

# Shivaji University, Kolhapur

# M.Sc. Part-II Inorganic, Organic, Physical, Analytical, Applied and Industrial Chemistry Syllabus as per National Education Policy 2020 (NEP 2.0)

To be implemented from June- 2024-25

**Applicable for University Department and Affiliated Colleges PG Centres** 

#### Name of Program: M.Sc. Organic Chemistry

M. Sc. Organic Chemistry, a post-graduate degree program of the Shivaji University, is one of the best in the country because it's curriculum involves most advanced topics like Organic reaction mechanism, Advance spectroscopic methods, Advance synthetic methods, Drug and Heterocycles, Theoretical Organic Chemistry, Stereochemistry, Chemistry of Natural Products, Applied organic chemistry, etc. and the practical training based on these advanced topics required to understand problems of the present time. Successful students of this course are capable of doing independent research work not only in relevant world class laboratories but also in R&D sectors and in quality teaching institutes.

#### 1. Program Outcomes (POs)

#### **Program Outcomes (POs)**

- PO1. Students will be able to acquire in depth knowledge about fundamental as well as applied organic chemistry concepts.
- PO2. Students will be able to solve various problems by identifying the essential parts of a problem, formulate strategy for solving the problem, applying appropriate techniques to arrive at a solution, test the precision an accuracy of the solution and interpret the results.
- PO3. Students will be able to acquire domain specific knowledge and technical skills needed for employment in industries, teaching fields and pursue research.
- PO4. Students will be able to apply the fundamental knowledge to address the cross-cutting issues such as sustainable development.
- PO5. Students will get perfect insight into organic chemistry research ethics for production of quality research.
- PO6. Students will be able to communicate effectively i. e. being able to comprehend and write effective reports, make effective presentations and documentation and capable of expressing the subject through technical writing as well as through oral presentation.

#### 2. Program Specific Outcomes (PSOs)

- PSO 1. Students will be able to qualify competitive examinations like NET, SET, GATE, etc.
- PSO 2. Students will have opportunities to serve in different Chemical, Pharmaceutical as well as food and agrochemical industries.
- PSO 3. Students will have global level research opportunities in Ph.D. programme.

- PSO 4. Collaborate effectively on team-oriented projects in the field of Chemistry or other related fields.
- PSO 5. Students can start their own chemical industry / business (entrepreneurship).
- PSO 6. Students will be able to interpret NMR, MS, IR for structural elucidation.

# 3. Framework of NEP 2.0 as per NEP-2020 for M. Sc. Degree in Organic Chemistry

M.Sc. Organic Chemistry

Year Level	Sen		Major	RM	OJT/FP	RP	Cumm.	Degree
		Mandatory	Elective [Chose any one elective]				Cr.	
I 6.0	I	OCH101 (4 Cr)	E-ICH103 (4 Cr) OR	RM-CH106			22	PG Diploma in
		ICH102 (4 Cr)	E-OCH103 (4 Cr) OR	(4 Cr)				Organic Chemistry
		PRCH104 (4 Cr-Major	E-PCH103 (4 Cr) OR					(After 3yr B.Sc.
		Experiments- 5 from	E-ACH103 (4 Cr) OR					Degree)
		each Section)						Note: Common
		PRCH105 (2 Cr-Minor						practicals for M.Sc-
		Experiments-3 from						I
		each Section)			0.00		22	
	-	DOTTO A CA OLA	E ICHOO (ICA OR		ОЛТ- ОСН206		22	M.ScII will be
	П	PCH201 (4 Cr)	E-ICH203 (4 Cr) OR					discipline specific
		ACH202 (4 Cr)	E-OCH203 (4 Cr) OR		(4 Cr) OR. FP-			i.e. Organic
		PRCH204 (4 Cr-Major	E-PCH203 (4 Cr) OR		OCH206 (4			Chemistry oriented
		Experiments- 5 from	E-ACH203 (4 Cr)		Cr)			
		each Section)			[Any One]			
		PRCH205 (2 Cr Minor Experiments-3 from each			[Any One]			
		Section))						
Cum. Cr. for	PG Diploma	28	8	4	4		44	
Cuin. Cr. 101	i o Dipionia		otion: PG Diploma (40-44 Credits):	after Three Year I	JG Degree		***	
II 6.5	III	OCH301 (4 Cr)	E-ICH304 (4 Cr) OR			RP-	22	PG Degree After 3-
		OCH302 (4 Cr)	E-OCH304 (4 Cr) OR.			OCH306 (4 Cr)		Yr UG
		OCH303 (4 Cr)	E-PCH304 (4 Cr) OR					Or
		PR-OCH305 (2 Cr)	E-ACH304 (4 Cr) OR					PG Degree after 4-
								Yr UG
	IV	OCH401 (4 Cr)	E-ICH404 (4 Cr) OR			RP-	22	Note: All the
		OCH402 (4 Cr)	E-OCH404 (4 Cr) OR.			OCH405		practicals/Project
		OCH403 (4 Cr)	E-PCH404 (4 Cr) OR.			(6 Cr)		will be discipline
			E-ACH404 (4 Cr) OR					specific i.e. Organic
								Chemistry oriented
Cum. Cr. For	1 Year PG	28	8	4	4	10	44	
Degree		20	5	7	•	10	-77	
Cum. Cr. For	2 Year PG	54	16	4	4	10	88	
Degree								

# 4. Course Structure: M.Sc. Part-II, Organic Chemistry

# **Semester III**

# **Major Mandatory**

Course Code	Course Title	Credits
OCH301	Organic Reaction Mechanism	4
OCH302	Advanced Spectroscopic methods	4
OCH303	Advanced Synthetic methods	4
PR-OCH305	Practical Course	2
RP-OCH306	Research Project	4

# **Major Elective (Choose any one)**

Course Code	Course Title	Credits
E-ICH304	Organometallic and Bioinorganic	4
	Chemistry	
E-OCH304	Drug and Heterocycles	4
E-PCH304	Solid State Chemistry	4
E-ACH304	Environmental Chemical Analysis	4
	and Control	

# **Semester IV**

# **Major Mandatory**

<b>Course Code</b>	Course Title	Credits
OCH401	Theoretical Organic Chemistry	4
OCH402	Stereochemistry	4
OCH403	Chemistry of Natural Products	4
RP-OCH405	Research Project	6

#### Major Elective (Choose any one)

<b>Course Code</b>	Course Title	Credits
E-ICH404	Energy and Environmental	4
	Chemistry	
E-OCH404	Applied Organic Chemistry	4
E-PCH404	Surface Chemistry	4
E-ACH404	Applied Analytical Chemistry	4

# 5. Detailed Syllabus

# M. Sc. II (Sem III) Organic Chemistry

# **OCH 301: Organic Reaction Mechanism**

#### UNIT-I: Methods of determining reaction mechanism

15 hrs.

- (A) Kinetic Methods: Order and Molecularity, Methods of following reaction rates, Types of reactions: 1<sup>st</sup>, 2<sup>nd</sup>, and 3<sup>rd</sup> order reactions, Reversible, Consecutive, and Parallel reactions. Energy of Activation, Entropy of Activation, Effect of Ionic strength, Solvent effect, and Kinetic isotopic effect
- (B) Non-Kinetic Methods: Identification of reaction products, Testing of the possible

intermediates, Trapping of the intermediates, Isotopic labeling, Reaction catalysis, Crossover experiments, Stereochemical studies, and Use of physical properties. Hammett and Taft equations.

#### **UNIT-II: Pericyclic reactions**

15 hrs.

Molecular orbital symmetry, Frontier orbital of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system, Classification of peri cyclic reaction, Wood-ward Hoffman correlation diagrams, FMO and PMO approach, Electrocyclic reactions, Conrotatory and disrotatary motions, 4n, 4n+2 and allyl systems, Cycloaddition, and supra and antara facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes, 1,3-dipolar cycloaddition and Chelotropic reactions, Sigmatropic rearrangement, supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

#### **UNIT-III: Study of the intermediate and name reactions**

15 hrs.

- (A) Ylids: Nitrogen, Sulfur and Phosphorous ylides: Synthesis and applications in organic synthesis.
- **(B) Name Reactions:** Alkyne metathesis reaction, Weinreb ketone synthesis, Petasis reaction, Henry reaction, Corey Kim oxidation. Reactions of carboxylic acids and esters.

#### **UNIT-IV: Free radical reactions**

15 hrs.

Types of free radical reactions, Detection by ESR, Mechanism of free radical substitution, Neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic halogenation (NBS), Oxidation of aldehydes to carboxylic acids, Auto-oxidation, Coupling of alkynes, Arylation of aromatic compounds by diazonium salt, Sandmeyers reaction, Hunsdiecker reaction.

#### **Reference Books:**

- 1. A guide book to mechanism in organic chemistry (orient- Longmans)- Peter Sykes
- 2. Organic Reaction Mechanism (Benjumin)- R. Breslow
- 3. Mechanism and structure in Organic Chemistry (Holt Reinhartwinston)- B. S. Gould
- 4. Organic chemistry (McGraw Hill)- Hendrikson, cram and Hammond
- 5. Basic principles of organic chemistry (Benjamin) J. D. Roberts and M. C. Caeserio.

- 6. Reactive intermediates in organic chemistry, (J. Wiley) N. S. Issacs.
- 7. Organic reaction mechanism (McGraw Hill ) R. K. Bansal
- 8. Fundamentals of photochemistry K. K. Rohtagi- Mukherji Wiley- Eastern
- 9. Essentials of molecular photochemistry, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
- 10. Molecular photochemistry, N.J. Urro, W. A. Benjamin
- 11. Introductory photochemistry. Cox and T. Camp McGraw -Hill
- 12. Photochemistry R.P. Kundall and A. Gilbert. Thomson Nelson.
- 13. Strategic applications of named reactions in organic synthesis by Laszlo Kurti and Barbara Czako.
- 14. Organic photochemistry J. Coxon and B. Hallon Cambridge University press.

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- Adopt the knowledge about the pathway and determine reaction rates using kinetic and non-kinetic methods. This involves steps such as reaction rate determination, order and molecularity, testing and trapping of intermediates, stereochemistry, and the Hammet-Taft equation.
- Familiarize with the concept of Pericyclic reactions, Woodward-Hoffmann correlation diagrams, and the Frontier Molecular Orbital (FMO) and Molecular Orbital (PMO) approaches. Understand conrotatory and disrotatory motion, and be able to identify reactions as 4n, 4n+2, and 2+2 addition of ketenes. Additionally, learn about sigmatropic shifts (3,3) and (5,5), Claisen and Cope rearrangements, and Aza-Cope rearrangement.
- CO3 Learn about the mechanisms, stereochemistry, migratory aptitude, and applications of different name reactions such as Dienone-phenol, Favorskii, Smiles, Brooke, Neber, Stevens, and Sommelet-Houser rearrangement reactions.
- CO4 Adapt the knowledge about photochemistry photochemical reactions, their types, and laws of photochemistry. Also, know quenching and chemiluminescence.

#### **OCH 302: Advanced Spectroscopic methods**

#### **UNIT-I: Study of Ultraviolet and IR Spectroscopy**

15 hrs.

#### (A) Ultraviolet Spectroscopy:

**(5)** 

Woodward-Fisher rules for conjugated dienes and carbonyl compounds, Calculation of  $\lambda$  max of conjugated dienes and carbonyl compounds. Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls.

#### (B) IR Spectroscopy:

(10)

Characteristic vibrational frequencies of (i) alkanes, (ii) alkenes, (iii) alkynes, (iv) aromatic compounds, (v) alcohols, (vi) ethers, (vii) phenols, (viii) amines. Detailed study of vibrational frequencies of carbonyl compounds; (i) ketones, (ii) aldehydes (iii) esters (iv) amides (v) acids (vi) anhydrides (vii) lactones (viii) lactams, and (ix) conjugated carbonyl compounds. Effect of hydrogen bonding and solvent effect on vibrational frequencies, Overtones, combination bands, and Fermi resonance, FT-IR of gaseous; solids and polymeric materials.

#### **UNIT-II: NMR Spectroscopy**

15 hrs.

General introduction and definition; chemical shift, spin-spin interaction, shielding mechanism of measurement, Chemical shift values, and correlation for protons bonded to (a) carbons: aliphatic, olefinic, aldehydic, and aromatic and (b) other nuclei: alcohols, phenols, enols, acids, amines, amides and mercaptons, Chemical exchange; effect of deuteration, Complex spin-spin interaction (first order spectra) between (i) two (ii) three (iv) four and (v) five nuclei, Virtual coupling, Stereochemistry; hindered rotation, Karplus curve variation of coupling constant with dihedral angle, Simplification: Simplification of complex spectra, nuclear magnetic double resonance, shift reagent, solvent effect. Fourier transform technique, Nuclear overhauser effect [NOE], NMR of F, and P nuclei.

#### **UNIT-III: Mass Spectrometry**

15 hrs.

Introduction of MS, Ionization methods; (i) EI, (ii) CI, (iii) FD (iv) FAB, and (v) MALDI-TOF, Factors affecting on fragmentation, Ion analysis, Ion abundance. Molecular ion peak, Metastable peak, McLafferty rearrangement, Nitrogen rule. Mass spectral fragmentation of organic compounds; (i) hydrocarbons (aliphatic and aromatic), (ii), carbonyls (aldehydes, ketones, acids, acid chlorides, esters, amides), (iii) halogen compounds (iv) amines, (iv) nitro compounds, High-resolution mass spectrometry (HRMS).

#### UNIT-IV: Study of <sup>13</sup>C NMR and Combined problems

15 hrs.

#### (A) Carbon-13 NMR Spectroscopy:

**(7)** 

General considerations; chemical shift; aliphatic, olefinic, alkyne, aromatic, heteroaromatic, and carbonyl compounds, problems associated with <sup>13</sup>C, FT- NMR, proton decoupled off-resonance.

#### (B) Structural Problems:

**(8)** 

Structural problems based on combined spectroscopic techniques (including reaction sequences)

#### **Reference Books:**

- 1. V.M. Parikh, Application spectroscopy of organic molecules. (Mehta)
- 2. D.W. Williams and Flemming, Spectroscopic methods of organic compound.
- 3. Silverstein and Basslar, Spectroscopic identification of organic compounds V.M. Parikh ORPTION SPECTROSCOPY OF ORGANIC MOLECULES ( J. Wiley )
- 4. P.S. Kalsi Spectroscope of organic compounds ( New age publisher )
- 5. J.R. Dyer. Application of absorption spectroscopy of organic compounds.
- 6. Jackman and Sterneil, Application of NMR spectroscopy
- 7. Nuclear magnetic resonance. J.D. Roberts (J. Wiley)
- 8. Theory and application of U.V. Jafee and Orchin.
- 9. Mass spectroscopy K. Benjamin.
- 10. The mass spectra of organic molecules. Beynon J H.
- 11. Interpretation of carbon 13 NMR Wehli F.W, Marchand A. P. (J. Wiley)
- 12. Organic Spectroscopy W. Kemp, ELBS
- 13. Instrumental methods of analysis CBS. Willard Merritt and Dean.
- 14. Mass Spectroscopy. Das and Jame
- Organic structural spectroscopy: J. B. Lambert, S. Gronert, H. F. Shurvell, D. Lightneli,
   R. G. Cooks (Prentice Hall 2<sup>nd</sup> edition).

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- CO1 Learn about the principles and theory behind UV and IR spectroscopy, including molecular vibrations due to IR radiation absorption and electronic excitations from UV radiation absorption. This will help students identify unknown organic compound structures and recognize functional groups such as alcohol, aldehyde, ketone, ester, and aromatic compounds. They will also study overtones, combination bands, and Fermi resonance in FT-IR spectroscopy.
- CO2 Recap proton NMR spectroscopy, factors affecting coupling constants, analyze first-order spectra, simplify complex spectra, understand second-order spectra, effect of deuteration, and spectra of Homotopic, Enantiotopic, and Diastereotopic systems. Also, learn about the Advanced NMR technique, Fourier transform technique, Nuclear Overhauser Effect (NOE), COSEY, NOSEY, and resonance of F19 and P31 nuclei.
- CO3 Learn about ion production methods (EI, CI, FD, and FAB) and factors affecting fragmentation analysis. Also understand mass spectral fragmentation of functional groups (e.g., aldehydes, ketones, esters, alcohols) to solve mass spectroscopy problems.
- Understand the concept of C13 NMR spectroscopy chemical shift values of alkanes, alkenes, alkynes, aromatic compounds, carbonyl and heterocyclic compounds. Also learn this advanced C13 technique NOE, DEPT, HETCOR and heteronuclear coupling. They will become confident to solve the problems on C13 NMR.

# **OCH 303: Advanced Synthetic methods**

#### **UNIT-I: Disconnection Approach**

15 hrs.

- (a) Terms involved in retrosynthesis; synthons, synthetic equivalents, disconnection approach, functional group interconversions.
- (b) Importance of the order of events in organic synthesis
- (c) Chemoselectivity, Regioselectivity, and Stereoselectivity, Protecting groups,
- (d) One group C-X and two group disconnections in (i) 1, 2, (ii) 1, 3 (iii) 1, 4, and (iv) 1, 5-difunctional compounds,
- (e) Retrosynthesis of (i) alkanes (ii) alkene, (iii) acetylenes, (iv) nitro (v) alcohols (vi) carbonyl compounds, (vii) amines, (viii) aromatic heterocycles (ix) 3, 4, 5 and 6 membered rings.
- (f) Reversal of polarity (Umpolung).
- (g) Use of Diels-Alder reaction, Michael addition, and Robinson annulation in retrosynthesis.

#### UNIT-II: Applications of the following in organic synthesis

15 hrs.

- (A) Reagents: Lithium diisopropylamide(LDA) Dicyclohexyl carbodiimide(DCC), lead tetra acetate, PPA, Diazomethane, ozone, phase transfer catalyst, Selenium dioxide, Dess-Martin periodinane, and iodoisobenzyldiacetate, periodic acid
- **(B) Reactions:** Woodward-Prevost hydroxylation, Barton and Shapiro reaction, Hoffmann–Loffler-Fretag, Peterson synthesis, Olefin metathesis using Grub's catalysts.

#### **UNIT-III:** Applications of metals and ligands in organic synthesis

15 hrs.

(A) Applications of metals in organic synthesis

**(7**)

- (i) Ti, (ii) Ce, (iii) Tl and (iv) Si
- **(B)** Applications of ligands in organic synthesis: Synthesis and Applications

**(8)** 

(i) Phosphines, (ii) N-heterocyclic carbenes (NHC), and (iii) Oxazoline

#### **UNIT-IV:** Applications of the following methods in organic synthesis

15 hrs.

- (a) Synthesis and applications of Merrifield resin
- (b) Electro-organic synthesis
- (c) Enzyme catalyzed reaction
- (d) Solvent free synthesis
- (e) Multicomponent reactions

- (f) Microwave techniques and their applications
- (g) Ultrasound techniques and their applications
- (h) Mechanochemical synthesis

#### **Reference Books:**

- 1. Designing of organic synthesis. S. Warren
- 2. Organic synthesis J. Fuhrhop & G. Penzlin. (2nd ed.)
- 3. Some modern methods of organic synthesis. Carruthres:
- 4. Modern synthetic reaction. H. O. House
- 5. Reagent in organic synthesis. Fieser & Fieser
- 6. Principle of organic synthesis. R. O. C. Norman
- 7. Advanced organic Chemistry. Carey & Sundharg
- 8. Organic synthesis. P. E. Realand:
- 9. Comprehensive organic Chemistry. Bartan and Ollis:
- 10. Organic reactions. R. Admas:
- 11. Advances in organometallic Chemistry. Stone & West:
- 12. Transition metal intermediate in organic synthesis. C. W. Bird:
- 13. Organometallic in organic synthesis. Swan & black :
- 14. Synthesis of prostaglandins. A. Mitra:
- 15. Total synthesis of natural products. John Apsimon:
- 16. Phosphorus ligands in homogeneous catalysis: Design and synthesis by Paul C. J. Kamer.
- 17. Phosphorus ligands effect in homogeneous catalysis and rational catalyst design by Jason A. Gillespie and Erik Zuidema. Polymers as aid in organic synthesis. M. K. Mathur, C. K. Narang & R. E. Williams:
- 18. Polymer supported reaction in organic synthesis. P. Hodge & D. C. Sherrington:
- 19. Enzyme catalysed reactions.C. J. Gray:
- 20. Electroorganic Chemistry. T. Shona:
- 21. Phase transfer catalyst in organic synthesis. Weber & Gokel

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- CO1 Understand the concept of the disconnection approach through the introduction of synthons, synthetic equivalents, and functional group interconversions. Also, understand retrosynthesis of difunctional compounds. Importance of the order of reaction in organic synthesis. They will learn Diel's Alder reaction, Michael addition, Robinson annulation, and what is meant by Umpolung reaction.
- CO2 Study the applications of different reagents in chemical reactions and also study of Woodward Prevost hydroxylation, Barton and Shapiro reaction as well as Grub's catalysis.
- CO3 Learn how the different metals and ligands in organic chemistry.
- CO4 Learn the new concept of supramolecular chemistry, advanced synthetic methods by using microwave ovens, ultrasound waves, using enzymes, electroorganic synthesis, use of multicomponent reactions as well as the use of Ionic liquids in chemical reactions.

# PR-OCH305 Organic Chemistry Practicals (2 Cr.) 60 hrs.

#### A) Qualitative Analysis

Separation, purification and identification of compounds (any two) of ternary mixtures using **semi-microanalysis**, TLC, column chromatography and chemical tests. IR spectra to be used for functional group identification.

#### **B)** Quantitative analysis

#### 1. Two step Preparations (Any Five)

- **a**) Preparation of m-Nitroaniline
- **b**) Preparation of Benzanilide from benzophenone
- **c**) Preparation of Phthalimide
- **d**) Preparation of N-Bromosuccinimide
- e) Preparation of 4-methyl -7-acetoxy coumarin
- f) Preparation of 1, 2, 3, 4- Tetrahydro carbazole
- **g**) Preparation of p-ethoxy acetanilide

#### **Reference books:**

- **1.** Textbook of Practical Organic Chemistry A. I. Vogel.
- **2.** Practical Organic Chemistry Mann & Saunders.
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
- **4.** Organic Synthesis Collective Volumes by Blat

**NOTE:** Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

# **RP-OCH306** Research Project (4 Cr)

See Annexture-I for details.

# M. Sc. II (Sem IV) Organic Chemistry

# **OCH 401: Theoretical Organic Chemistry**

#### **UNIT-I: Molecular Orbital Theory**

15 hrs.

Aromaticity in benzenoids, alternant and non-alternant hydrocarbon, Huckels rule, energy level of  $\pi$ - molecular orbital and concept of aromaticity, calculation of energies of orbitals cyclic and acyclic systems. Determination energies and stabilities of different systems calculation of charge densities PMO theory and reactivity index.

#### **UNIT-II: Non benzenoid aromatic Compounds**

15 hrs.

Aromaticity in non-benezenoid compounds Annulenes and heteroannulenes, fullerenes, azulene, fulvene, tropylium salts, ferrocene, five-membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes, and rotaxanes, bonding in fullerenes.

#### **UNIT-III: Green Chemistry**

15 hrs.

Introduction to the principles of green chemistry – prevention of waste, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, reducing derivatives, renewable feedstock, catalysis, design for degradation, real-time analysis for pollution prevention, and inherently safer chemistry for accident prevention. Green synthesis, clean routes using supercritical solvents, ionic liquids, and water.

UNIT-IV:

A) Kinetic and thermodynamic control of reactions

**(9)** 

Nitration and Sulphonation of naphthalene, Wittig, Enolization, Friedel-Crafts and Diels Alder reactions.

**B)** Non-classical carbocations: Formation, stability, and reactivity. (6)

#### **Reference Books:**

- 1. Lehar and Merchand: Orbital Symmetry.
- 2. R. B. Woodward and Hoffman: Conservation of orbital symmetry.
- 3. P. T. Anastas, J. C. Werner: Green Chemistry: Theory and Practice
- 4. V. K. Ahluwalia: Green chemistry, A textbook
- 5. V. K. Ahluwalia, R. S. Verma: Green Solvents: For Organic Synthesis
- 6. Ginsburg: Nonbenzenoid aromatic compound.
- 7. A. Streitwieser: Molecular orbital theory for organic chemistry.
- 8. E. Cler: The aromatic sextet.
- 9. Lloyd: Carbocyclic non- benzenoid aromatic compounds.
- 10. W. B. Smith: Molecular orbital methods in organic chemistry.
- 11. Grratt; Aromaticity

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- Understand the concept of aromaticity, Huckel's rule, the energy level of pimolecular orbital, calculation of energies of cyclic and acyclic systems, calculation of charge densities, PMO theory, and reactivity index.
- CO2 Learn synthesis and reactions of Linear and Non-linear polynuclear hydrocarbons.

  Understand the concept of aromaticity and anti-aromaticity as well as the concept of
  3- and 5- 5-membered carbocyclic compounds, crown ethers, cyclodextrins,
  catenanes, and rotaxanes.
- CO3 Understand the types of free radicals, detection by ESR, reaction mechanism, and reactivity. They also learn the effect of solvent on reactivity, Sandmeyer's reaction, Hunsdiecker reaction.
- CO4 Learn about the Kinetic and thermodynamic control of nitration and sulphonation, about Wittig reaction, Enolization, F. C. reaction, and Diel's Alder reaction. Understand Non-classical carbonation Formation, stability, reactivity, and synthetic applications.

#### **OCH 402: Stereochemistry**

#### UNIT-I: Conformational analysis and reactivity of acyclic and alicyclic compounds 15 hrs.

#### A) Conformational analysis of acyclic compounds

**(4)** 

The difference between configuration and conformation, torsion strain, Pitzer strain, the effect of (i) van der Waals interactions, (ii) hydrogen bonding, and (iii) dipole moment on the stability of conformation with examples, gauche effect.

#### B) Conformational analysis of cyclohexane compounds

**(4)** 

Concept of Baeyer ring strain, ring inversion, locking of conformations and groups. Conformations of (1, 4-di-t- butylcyclohexane, 1, 4-cyclohexanediol, menthol, cyclohexanone.

C) Effect of conformation on reactivity (mechanism) of acyclic and cyclic systems

(7)

Curtin-Hammett principle. Effect of conformation on the course and rate of reactions in cyclohexane; debromination of 2,3-dibromobutane, semipinacolic deamination of 1,2-diphenyl- 1-(pchlorophenyl)-2-amino ethanol, dehydrohalogination of stilbene dihalide and bromo-1,2- diphenyl propane,

# UNIT- II: Conformational analysis and reactivity of the fused and bridged ring system 15 hrs.

stereochemistry of molecular rearrangements; pyrolytic cis-elimination.

- **A) Fused rings:** Types of fused ring systems; (i) Fused bicycles: cis and trans-decalins, octalins, decalols, (ii) Fused poly-bicycles: perhydroanthracene and perhydrophenanthrene (iii) effect of angular methyl group on conformation of fused ring system.
- **B) Bridged rings:** Types of bridged ring systems, nomenclature, bridged bicycles: heptanes and octane, stereochemical restrictions, Bredt's rule.

#### **UNIT-III: Stereoselective Synthesis**

15 hrs.

#### A) Stereoselective addition of nucleophiles to carbonyl group

**(6)** 

Cram's rule, Felkin Ahn rule, Houk's model, Cram's chelate model. Asymmetric synthesis by use of chiral auxiliaries, use of chiral substrates, reagents, and catalysts

#### B) Asymmetric Synthesis

**(9)** 

Asymmetric epoxidation of allylic alcohols (Sharpless Epoxidation), Dihydroxylation of olefins: Sharpless asymmetric dihydroxylation, Upjohn process, Milas hydroxylation.

Asymmetric Diels-Alder Reactions using chiral Lewis acids: Chiral bissulfonamides (Corey's catalyst).

# UNIT- IV: Stereochemistry of compounds containing no chiral carbon atoms 15 hrs.

- A) Stereochemistry of allens, sprains and biphenyls, assignment of configuration (4)
- B) Configuration of diastereomers (4)

Geometrical isomerism based on physical and chemical methods.

C) O.R.D. and C.D. (7)

ORD and CD curves with Cotton effect. Empirical and semi-empirical rules; The octant rule, helicity rule, Lowe's rule, and axial haloketone rule.

#### **Reference Books:**

- 1. E.L. Eliel: Stereochemistry of carbon compounds.
- 2. D. Nasipuri : Stereochemistry of organic compounds
- 3. P.S. Kalsi: Stereochemistry, Conformation and Mechanism.
- 4. Eliel, Allinger, Angyal and Morrison: Conformational analysis.
- 5. Hallas: Organic stereochemistry
- 6. Mislow and Benjamin: Introduction to Stereochemistry.
- 7. H. Kagan: Organic stereochemistry.
- 8. Carl Djerassi; Optical Rotatory Dispersion.
- 9. P. Crabbe: Optical Rotatory Dispersion and C.D.

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- Approve the knowledge of about stereoselective, stereospecific synthesis, chemoselective and regioselective reactions. Undestand the enantioselective synthesis, reactions with hydride donar, catalytic hydrogenation via chiral hydrazones and oxazolines etc.
- Understand in depth stability and reactivity of diastereoisomers, Curtin-Hammett principle, some aspects of stereochemistry of ring compounds. The shapes of the 5, 6 and 7 membered rings. Also, they will learn the conformational effects in medium sized rings and the concept of I-strain.
- CO3 Knowledge about conformation and configuration of fused bicyclic rings and

bridged rings, stereochemical restrictions, and Bredt's rule.

Understand O. R. D. and C. D. curves, circular dichroism, the Octane rule and axial haloketone rule.

CO4 Explain the stereochemistry of Allenes, Spiranes, and Biphenyls and how to assign the configuration and by using physical and chemical methods.

# **OCH 403: Chemistry of Natural Products**

UNIT-I: Terpenoids 15 hrs.

Introduction of natural products and Terpenoids: Introduction of natural products: Classification and isolation methods. Terpenoids: Structure and synthesis of camphor, carvone, abietic acid, zingiberene,  $\alpha$ -santonin,  $\beta$ -cuparenone. Biogenesis of abietic acid.

UNIT-II: Alkaloids 15 hrs.

Structure, stereochemistry, synthesis, and biosynthesis of the following: Morphine, Reserpine, Papaverine, and Lysergic acid. Biogenesis of Coniine.

UNIT-III: Steroids 15 hrs.

Occurrence, nomenclature, basic skeleton, Diels hydrocarbon. **Study of the following:** ormones (Structure and synthesis): Cholesterol, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and cortisone Bile acid (only synthesis) and biosynthesis of lanosterol.

#### UNIT-IV: Study of Prostaglandins, Lipids and Vitamins

15 hrs.

A) Prostaglandins: (5)

Occurrence, nomenclature, classification, biogenesis and physiological effects, Synthesis of PGE2 and PGF2.

B) Lipids: (4)

Classification, Role of Lipids, Fatty acids and glycerol derived from oils and fats.

C) Vitamins: (6)

Synthesis and structure of biotin, vitamin B1 and B2, Biological functions of Vitamin B<sub>6</sub>, D and E.

#### **Reference Books:**

- 1. Apsimon: The total synthesis of natural products.
- 2. Manskey and Holmes: Alkaloids

- 3. A.A. Newmen: Chemistry of Terpenes.
- 4. P. D B. Mayo: The chemistry of natural products.
- 5. Simonson: Terpenes.
- 6. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry.
- 7. R.T. Slicken staff A.C. Ghosh and G.C. Wole: Total synthesis of steroids.
- 8. The chemistry of natural products, vol. Nakanishi
- 9. Biochemistry of Lipids, Lipoproteins and membranes by Neele Ridgway and Roger McLeod
- 10. Membranes (New comprehensive biochemistry) by J E Vance and E Vance
- 11. Schaum's easy outline of biochemistry by Philip W Kuchel.

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- CO1 Learn the classification, isolation of terpenoids, structure, and synthesis of Camphor, Carvone, Abietic acid, zingiberene, alpha-santonin, and beta-caryophyllene.
- CO2 Know all about Alkaloids the occurrence, isolation, structures, functions, stereochemistry, and synthesis of Morphine, Reserpine, Atropine, and Conin alkaloids.
- CO3 Learn the occurrence, nomenclature, and basic skeleton of steroids as well as the synthesis of hormones like cholesterol, Androsterone, Testosterone, and Estrone. Also study the nomenclature, classification, biogenesis, physiological effects, and synthesis of prostaglandin PGE2 and PGF2.
- CO4 Study about the Vitamins as well as synthesis and biological functions of vitamins B1, B2, B5, B6, and Biotin i.e. vitamin H.

# RP-OCH405 Research Project (6 Cr)

See Annexture-I for details.

Note: Study tour is the part of your syllabus for M.Sc. Part- II. Students shall visit Chemical Industries in India.

# **Major Electives (Choose any One)**

#### M.Sc. II, SEM-III

Students of Inorganic/Organic/Physical/Analytical/Applied/Industrial Chemistry shall choose any one of the following elective papers.

#### E-ICH304: Organometallic and Bioinorganic Chemistry

#### **Unit I: Organotransition Metal Chemistry**

15 hrs.

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways of alkyls and aryls of transition metals. Organocopper in Organic synthesis, Compounds of Transition Metal –Carbon Multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes–synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role in organic synthesis.

#### **Unit-II: Transition Metal Pi-complexes**

15 hrs.

Carbon multiple bonds. Nature of bonding, structural characteristics & synthesis, properties of transition metal Pi-Complexes with unsaturated organic molecules, alkenes alkynes, allyl, diene, dienyl, arene and trienyl complexes. Application of transition metal, organometallic intermediates in oraganic synthesis relating to nucleophilic and electrophilic attack onligands, role in organic synthesis.

#### **Unit III: Metal Compounds in Medicine**

15 hrs.

Medicinal use of metal complexes as antibacterial, anticncer, use of cis-platin as antitumor drug, antibiotics & related compounds. Metal deficiency and disease, iron deficiency, zinc deficiency and copper deficiency, Metal used for dignosis and chemotherapy with particular reference to anti-cancer drugs. Chelate therapy, chemotherapy with compounds of some non-essential elements; platinum complexes in cancer therapy. Antiviral activity of metal complexes. Gold containing drugs used in the therapy of Rheumatic-Arthritis, Gold complexes as anticancer drug. Lithium in psycho pharmacological drugs. Antimicrobial agents.

Heme proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanins & hemerythrin. Perutz mechanism for structural changes in porphyrin ring system, Oxygenation and deoxygenation. Oxygen adsorption isotherm and cooperativity, physiological significance of haemoglobin, role of globin chain in gaemoglobin, Cyanide poisoning and treatment.

#### **Reference Books:**

- 1. Yamamoto, Organo Transition Metal Chemistry, Wiley (1986).
- 2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals (4th edn.), John Wiley (2005).
- 3. A. J. Pearson. Metallo-Organic Chemistry, John Wiley & Sons (1985).
- 4. M. Bochmann. Organometallics-I Complexes with Transition Metal-Carbon σ-Bonds, Oxford Chemistry Primers (1994).
- 5. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 6. Biochemistry, L. Stryer, W. H. Freeman
- 7. Biochemistry, J. David Rawn, Neil Patterson.
- 8. Biochemistry, Voet and Voet, John Wiley.
- 9. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.
- 10. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford Univ. Press, 1990.

#### **Course Outcomes (COs):**

**CO1:** After successful completion of the course the students should be able to explain the synthesis, structure, bonding, properties and reactivity of Alkyls and Aryls of Transition Metals.

**CO2:** After successful completion of the course the students should be able to explain the synthesis, structure, bonding, properties and reactivity of Compounds of Transition Metalcarbon with Multiple bonds.

**CO3:** Students should be able to describe the role of metals in medicines, deficiency disorders of metals and use of platinum, gold and lithium compounds in the treatment of cancer, arthritis and psycho drugs, respectively.

**CO4:** At the end of the course student should be able to explain the natural proteins that carry dioxygen in various animals, the role of myoglobin and hemoglobin in carrying dioxygen in mammals and other non-heme proteins for oxygen uptake.

#### E-OCH304: Drug and Heterocycles

#### Part- A: DRUGS

#### **UNIT-I: Drug Design and Antibiotics**

15 hrs.

A. Drug Design (10)

Procedures followed in drug design, **factors affecting development of new drugs**, concepts of prodrugs and soft drugs, **Isosterism, bioisosterism,** Theories of drug activity, Quantitative structure activity relationship, QSAR theory, Concepts of drug receptors.

#### **B. Study of Antibiotics**

**(5)** 

(i) Classification of antibiotics, (ii) Preparation of semi synthetic penicillin, (iii) Penicillin G, (iv) Penicillin V, (v) Conversion of penicillin into cephalosporin.

#### **UNIT-II: Study of the Following Drugs**

15 hrs.

- a) Antimalerials: Trimethoprim, Amodiaquine
- b) Analgesic & Antipyretics: Meperidine, Aminopyrine, Diflunisal
- c) Anti- inflammatory: Oxyphenylbutazone, Indomethacin
- d) Antitubercular & antileprotic: Dapsone, Pyrazinamide, Ethionamide
- e) Anaesthetics: Lidocaine, Thiopental
- f) Antihistamines: Cyproheptadine, Cetirizine
- g) Psychoactive: Ethiosuximide, Glutethimide
- h) Antiinfective: Grisefulvin, norfloxacin
- i) Cardiovascular: Warfarim, Clofibrate, Quinidine, Methyldopa, Atenolol
- j) Anti-neoplastic: Recent development in cancer chemotherapy. Hormones and natural products. Synthesis of (i) Mechloraethamine, (ii) Cyclophosphamide, (iii) Mephalan, (iv) Uracils, (v) Mustards.
- k) Anti-AIDS: General study

#### **Part-B: HETEROCYCLES**

#### **UNIT-III: Study of following heterocycles**

15 hrs.

#### A) Small ring heterocycles:

**(5)** 

3 and 4 membered heterocycles: Synthesis and reactions of (i) aziridines, (ii) oxiranes, (iii) thiranes, and (iv) azetidines.

#### B) Six membered heterocycles with one heteroatom:

**(5)** 

Synthesis and reactions of (i) pyrilium salts, (ii) pyrones, (iii) coumarins, (iv) chromones.

#### C) Six membered heterocycles with two and more heteroatoms:

**(5)** 

Synthesis and reactions of (i) diazines (ii) triazines

#### **UNIT-IV: Study of following heterocycles**

15 hrs.

# A) Benzofused five membered heterocycles:

**(7)** 

Synthesis and reactions of (i) benzopyrroles, (ii) benzofurans and (iii) benzothiophene

#### B) Benzofused heterocycles with two heteroatoms:

(8)

Synthesis and reactions of

(i) benzimidazole, (ii) benzthiazole and (iii) benzoxazole

#### **Reference Books:**

- 1. Medicinal Chemistry. Burger
- 2. Medicinal Chemistry A. Kar. (Wiley East)
- 3. Principals of medicinal chemistry.W. O. Foye:
- 4. Text book of organic medical and pharmaceutical chemistry. Wilson, Gisvold & Dorque:
- 5. Pharmaceutical manufacturing encyclopedia.
- 6. D. Sriram, P. Yogeeswari: Medicinal Chemistry
- 7. An introduction to chemistry of heterocyclic compounds. R. M. Acheson :( Interscience).
- 8. Heterocyclic chemistry. Joule &Smith: (Van Nostrand).

- 9. Heterocyclic chemistry. R. K. Bansal: (Wiley E).
- 10. Principals of modern heterocyclic chemistry.L. A. Paquitte:
- 11. The structure and reactions of heterocyclic compounds.M. H. Palamer:
- 12. Advances in Heterocyclic chemistry. A. R. Katritzky: (A.P.).
- 13. Organic chemistry (Vol. 1& 2) Finar.
- 14. Outline of Biochemistry. Cohn & Stumpt
- 15. Introduction to the chemistry of enzyme action. Williams:
- 16. The Organic Chemistry of Drug design and Drug action. R. B. Silverman Academic press.
- 17. Strategies for Organic Drug synthesis and Design. D. Lednicer, J. Willey.
- 18. Heterocyclic Chemistry. Vol-1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Veriag.
- 19. The Chemistry of Heterocycles. T. Eicher and S. Hauptmann, Thieme
- 20. Heterocyclic Chemistry. J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
- 21. Heterocyclic Chemistry. T. L. Gilchrist, Longman Scientific Technical
- 22. Contemporary Heterocyclic Chemistry. G. R. Nikome and W. W. Poudler, Willey
- 23. An Introduction to Heterocyclic Compounds, R. M. Acheson, J. Willey
- 24. Comprehensive Heterocyclic Chemistry. A. R. Katritzky and C. W. Rees

#### **Course Outcomes (COs):**

#### CO No. On completion of the course, students will be able to:

- CO1 To know about the drug design, history, and development of quantitative structure-activity relationship (QSAR). Also, learn the concept of drug receptors and the relationship between structure and chemical reactivity. Learn about different types of antibiotics.
- CO2 Study the various types of drugs like antimalarials, Anti-inflammatory, anesthetics, Antitubercular, Tranquilizers cardiovascular, and Antineoplastic drugs.
- CO3 Understand synthesis and reactions of five, six-membered heterocycles.
- CO4 Learn the synthesis and reactions of diazines and triazines. Synthesis of the reactions of azepines, oxepines & thiepines.

# **E-PCH304: Solid State Chemistry**

#### UNIT-I: The Solid State 15 hrs.

Introduction, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Miller indices, Bragg's Method, Debye-Sherrer method of X-ray for structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem, procedure for an X-ray structure determination, Rietveld analysis, Problems.

#### **UNIT -II: Solid State Reactions**

15 hrs.

General principle, types of reactions: Additive, structure sensitive, decomposition and phase transition reactions, tarnish reactions, kinetics of solid-state reactions, Mechanochemical methods for preparations of semiconductors. Co-precipitations reactions, factors affecting the reactivity of solid-state reactions.

#### **UNIT –III: Electronic Properties and Band Theory**

15 hrs.

Metals, insulators and semiconductors, free electron theory and its applications, electronic structure of solids, band theory, band structure of metals, insulator, and semiconductors, doping in semiconductors, p- n junction, superconductors, organic semiconductors, charge carrier injection and transport, Optical properties of organic semiconductors, applications and devices involving optical properties, luminescence photoluminescence, effect of impurity levels on photoluminescence, light emitting diodes, luminous efficiency, photo-conduction and photoelectric effects, laser, principle of laser action, solid state laser and their applications, Problems.

#### **UNIT-IV: Preparation of Materials**

15 hrs.

Purification and crystal growth, kinetics of nucleation, critical radius, principle of nucleation, crystal growth during casting, zone refining, growth from solution, growth from melt and preparation of organic semiconductors for device applications.

Crystal defect and Non-Stoichiometry: Classification of defects subatomic, atomic and lattice defect in solids. Thermodynamics of vacancy in metals, Thermodynamics of Schottky

defects in ionic solids, Thermodynamics of Frenkel defects in silver halides. Calculation of number of defects and average energy required for defect.

#### **Reference Books:**

- 1. A guide to laser in chemistry by Gerald R., Van Hecke, Keny K. Karokitis
- 2. Principles of Solid-State Chemistry, H. V. Keer, Wiley Eastern,
- 3. Solid State Chemistry, N. B. Hannay
- 4. Solid State Chemistry, D. K. Chakrabarty, New Age International
- 5. An Introduction to Crystallography: F. G. Philips
- 6. Crystal Structure Analysis: M. J. Buerger 49
- 7. The Structure and properties of materials: Vol. III Electronic properties by John Walss
- 8. Electronic processes in materials : L. U. Azroff and J. J. Brophy
- 9. Chemistry of imperfect crystal: F. A. Krogen
- 10. Elements of X-ray Diffraction by B. D. Cullity, Addison-Weily.
- 11. Solid State Chemistry by A.R. West (Plenum)
- 12. Electronics made simple by Jacobwitz.
- 13. Principles of Physical Metallurgy, by Abhijeet Mallick,

#### **Course Outcomes (COs):**

The Solid-State Chemistry Course Outcomes. On completing the module students will be able to:

- CO1: Demonstrate an ability to describe, with confidence, the features of the most common crystalline structures.
- CO2: Demonstrate the ability to identify different bonding contributions in the solid state.
- CO3: Demonstrate the ability to relate the crystalline structure with the bonding to predict materials properties.
- CO4: Demonstrate assured ability to describe different defect structures in the solid state and how they affect the materials' properties.
- CO5: Demonstrate thorough analytical skills associated with the need to pay attention to detail and develop an ability to manipulate precise and intricate ideas, to construct desired materials for various applications in the industry.
- CO6: Demonstrate the ability to work independently for the preparation of solid materials and characterization.

# E-ACH 304: Environmental Chemical Analysis and Control

#### **UNIT-I: Sampling in analysis**

15 hrs.

Definition, theory and techniques of sampling, sampling of gas, liquids and solids, Criteria of Good sampling, Minimization of Variables, transmission and storage of samples, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, Filtering and gravity separation. Analysis of particulate matter like asbestos, mica, dust and aerosols etc

#### **UNIT-II: Electrochemical and spectral methods Environmental analysis** 15 hrs.

Introduction to instrumental techniques, principle instrumentation and applications with respect to environmental analysis of Conductometry, Potentiometry, Ion selective electrodes, Cyclic voltammetry, Amperometry, Coulometry, Atomic absorption spectrometry, Atomic fluorescence spectrometry, Inductively coupled plasma spectrometry, Turbidimetry, Non Dispersive Infrared Analysis (NDIR).

#### **UNIT-III: Air and Water Pollutant Analysis**

15 hrs.

Chemistry of Air pollutants, characterization. source, methods of analysis of air pollutants; CO, CO2, NOX, NH3, H2S, SO2 etc. Monitoring Instruments, Potable and Industrial water, major and minor components, dissolved oxygen (DO) Chemical oxygen demand(COD) Biochemical oxygen demand (BOD) and their measurements. Analysis of Pd, Cd, Hg, Cr, As and their physiological manifestations. Quality of industrial waste water analysis for organic and inorganic constituents. Chemistry of odour and its measurements.

#### **UNIT-IV: Organic Pollutants and Their Analysis**

15 hrs.

Sources, disposal, treatment and analysis of phenolic residues, methods of recovery of phenols from liquid effluents, Organomercurials and its analysis, Analysis of organochlorine pesticides, volatile organic pollutants and their analysis

#### **Reference books:**

- 1. A.K. De: Standard Methods of Waste and Waste water analysis.
- 2. P. M. S. Monk Fundamentals of Electroanalytical chemistry-John Wiley & Sons
- a. (2001) 3. Instrumental methods of chemical analysis H. Kaur

- 3. S.M. Khopkar, Environmental Chemistry; Environmental pollution analysis
- 4. M.S. Creos and Morr, Environmental Chemical Analysis, American publication
- a. (1988)
- 5. A.K. De, Environmental Chemistry, New Age International publishers. Moghe and
- a. Ramteke, Water and waste water analysis: (NEERI)
- 6. A.C. Stern, Air pollution: Engineering control Vol. IV(AP)
- 7. P.N. Cheremisinoff and R.A. Young, Air Pollution controland Design. Hand Book
- a. Vol. I & II (Dekker)
- 8. R.B. Pohasek, Toxic and Hazardous waste disposal, Vol. I & II (AAS)
- 9. M. Sitting, Resources Recovery and Recycling, Handbook of industrial Waste.
- 10. B.K. Sharma, Industrial Chemistry.
- 11. S.P. Mahajan, Pollution Control in Process Industries.
- 12. R.A. Horne, Chemistry of our Environment.

#### **Course Outcomes (COs):**

- CO1: Students will acquire knowledge about sampling, criteria of good sampling, handling, preservation and storage of the samples, pretreatment and post treatment of samples.
- CO2: Students will acquire knowledge of conditions and strategies required during sampling and electrochemical and spectral methods for analysis of environmental samples.
- CO3: Students will learn about the air and water pollution, sources of pollution, typical parameters and properties (physical, chemical and biological) to be measured in air and water pollution with relevance to specific case studies.
- CO4: Students will be acquainted with organic pollutants and their analysis with special reference to pesticide analysis.

# **Major Electives (Choose any One)**

#### M.Sc. II, SEM-IV

Students of Inorganic/Organic/Physical/Analytical/Applied/Industrial Chemistry shall choose any one of the following elective papers.

#### E-ICH 404: Energy and Environmental Chemistry

#### **Unit I: Energy Conversion Devices**

15 hrs.

Fuel Cells: Working of Fuel Cells, Types of fuel cells, Current capabilities/uses, Fuel cell stacks and systems, Hydrogen as a fuel, Production of hydrogen: Electrolysis, Thermochemical Processes, Steam Reformer Processes, Water Gas Processes, Bosch Process, Biosynthesis and Photochemical Processes, Coal Gasification, Steam Iron Process, Partial Oxidation Processes. Storage, Transport, and Handling of Hydrogen.

#### **UNIT II: Energy Storage Devices: Batteries**

15 hrs.

Li-ion batteries: Principle of operation, Battery components and design, Electrode materials (LiCoO<sub>2</sub>, LiNiO<sub>2</sub>, LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub>, LiMn<sub>2</sub>O<sub>4</sub>, LiFePO<sub>4</sub>, graphitic carbon) their synthesis and characterization, Theoretical capacity, Energy density, power density, cycle life, Electrode and battery fabrication, Battery modules and packs, Li-polymer batteries and applications, Electrolytes for Li-ion batteries, All solid-state batteries. Future developments and beyond lithium batteries: Li-S battery, Li-Air battery, Advanced lead-acid batteries, Sodium-battery, Magnesium battery, Aluminium battery, Silicon battery, Battery Recycling Technologies.

#### **UNIT III:**

#### A) Waste Treatment

8 hrs.

Electronic waste recycling programs, E-waste – non-recycling impacts, Materials Used in Manufacturing Electrical and Electronic Products, Solid Waste Management: Gas to Energy projects, Incandescent vs. compact florescent light bulbs, Value-added Material Recovery, Cost effective treatment of refractory organics,

#### B) Air and Water Pollution control

7 hrs.

Control of NOx, SOx and particulate pollution, Sewage and industrial waste water treatment, water softening, municipal water purification.

#### **UNIT-IV:**

#### A) Monitoring, sampling and Analysis of Air and water pollutants

8 hrs.

Methods of monitoring and sampling of gaseous, liquid and solid pollutants, analysis of CO, CO<sub>2</sub>, NO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>S, analysis of toxic heavy metals, Cd, Cr, Hg, As, Pb, analysis of anions SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>, NO<sub>3</sub><sup>-</sup>, estimation of COD and BOD

# B) Techniques in Environmental Analysis

7 hrs.

ND-IR Spectroscopy, FTIR, AAS, ICP-AES, GC, GC-MS, HPLC, Anodic stripping voltammetry with case studies

#### **Reference Books:**

- 1. Lithium ion Batteries: Basics and Applications, R. Korthauer, Springer
- Lithium ion Batteries: Fundamentals and applications, Yuping Wu, CRC Press, Taylor
   &

Francis group

- 3. Lithium ion batteries: Materials, Technology and new applications, K. Ozawa, Wiley 30 Years of Lithium-Ion Batteries, Advanced Materials, M. Li et al., Vol 30, issue 33, 2018,1800561
- 4. Fuel Cell Fundamentals, R. O'Hayre, et al., John Wiley & Sons, 2016
- 5. George Techobanoglous et al,"Integrated Solid Waste Management" McGraw Hill, 1993.
- 6. Environmental Chemistry, H. Kaur, PragatiPrakashan, 10th edition 2016.
- 7. Environmental Pollution, A. K. De
- 8. Environmental Pollution Analysis, S. M. Khopkar
- Compendium of R&D Projects, Waste Management Technologies (WMT) Programme,
   Technology Development and Transfer Division, Department of Science and
   Technology, New-Delhi 2018-2019.
- 10. Environmental Waste Management, Ed. Ram Chandra, CRC Press 2015, 1st Edition
- 11. Electronic Waste Management, RSC Publishers, Editors: R E Hester, R M Harrison, 2009

# **Course Outcome (COs):**

**CO1:** At the end, students will be able to: Learn basic concepts of solid waste management, beginning from source generation to waste disposal.

CO2: Students should be able to-Characterize the solid waste in terms of hazardous waste components; impact of waste management on health and environment; understand steps towards solid waste management-waste reduction at source, materials and resource recovery/recycling, treatment and disposal techniques.

**CO3:** After completion of the course student will be able to explain the advanced energy conversion devices such as Fuel cells, and the various techniques involves in the production of Hydrogen (future fuel).

**CO4:** Students will be able to demonstrate the reactions involved in the advanced energy storage devices, can predict the theoretical energy storage capacities of such devices, and understand the chemistry of various batteries.

# E-OCH404: Applied Organic Chemistry

#### **UNIT-I: Study of Agrochemicals and Perfumes**

15 hrs.

#### A) Agrochemicals (7)

(i) Organochlorine pesticides: Introduction, synthesis, and mode of action of endrin, aldrin, dieldrin. (ii) Herbicides: Synthesis and mode of action of Triazines, triazoles, pyridazinones, and bipyridylium compounds: diquat, paraquat. (iii) Juvenile hormone: introduction & structures JHA importance synthesis, IPM

#### B) Synthesis and applications of perfumery

**(8)** 

2-Phenylethanol, vanillin, and other food flavors, synthetic musk, and ionones.

#### **UNIT-II: Unit processes**

15 hrs.

Introduction to unit operation and unit processes. Nitration: Introduction, Nitrating agents, kinetics and mechanism, oxynitration, typical industrial nitration process.

Amination: Introduction, Bechamp reduction. Halogenation: Introduction, Kinetics and mechanism, catalytic chlorination, manufacturing process for chlorobenzene and monochloroacetic acid. Sulfonation- Introduction, sulphonating agents, kinetics and mechanism, manufacturing process for benzene sulphonic acid.

#### **UNIT-III: Dyes and Intermediates**

15 hrs.

Classification and synthesis of important dye intermediates by using nitration, sulphonation, diazotization reactions. Synthesis of Nitro dyes, xanthenes, reactive dyes, fluorescent brightening

agents, thermal sensitive dyes, dispersed dyes and reactive dyes.

UNIT-IV: Polymers 15 hrs.

Mechanism of polymerization. Industrial process for synthesis of polyethylene, acrylonitrile, acrylate and methacrylate polymer, biomedical polymer, polymer processing, Plasticizers and anti-oxidants for polymers,

#### **Reference Books:**

- 1. Allan: Colour Chemistry
- 2. K. Venkataraman: Chemistry of Synthetic Dyes Vol- 1 to 7
- 3. G. R. Chatwal: Synthetic dyes
- 4. Abrahart: Dyes & their intermediates
- 5. N. N. Melikov: The Chemistry of Pesticides and formulations
- 6. K. H. Buchel: Chemistry of Pesticides.
- 7. R. Clemlyn: Pesticides
- 8. K. H. Buchel: Chemistry of Pesticides
- 9. H. R. Alcock and F. W. Lambe: Contemporary Polymer Chemistry
- 10. J. M. G. Cowie, Blackie: Physics & Chemistry of Polymers
- 11. I. M. Campbell: Introduction to Synthetic Polymers
- 12. A. L. Gupta: Polymer Chemistry
- 13. M. S. Bhatnagar: A textbook of Polymers
- 14. F. W. Billmeyer: Textbook of Polymer Science

# **Course Outcomes (COs):**

#### CO On completion of the course, students will be able to:

No.

- CO1 Learn about the synthesis and uses of different types of Agrochemicals such as Carbamates, organophosphorous insecticides, and Natural and Synthetic Pyrethroids. They will learn the synthesis of some plant growth regulators as well as applications of Juvenile hormones and Pheromones.
- CO2 Learn about the perfumery compounds, commercial process, preparation and importance of essential oils. Also learn the synthesis of 2 phenyl ethanol, yara-yara, vanillin, synthetic musk, jasmine, ionone etc. from citral, phenyl acetate ester, benzyl acetate ester.

- CO3 Understand the classification, and synthesis of azo dyes, reactive dyes, optical brighteners, dispersed dyes.
- Understand the mechanism of polymerization. Also, study about the manufacturing processes of synthetic rubber plasticizers, and anti-oxidents required for natural polymers like starch and cellulose. They will get the knowledge about the Oxo and Wacker process necessary for Soap and Synthetic detergents.

# **E-PCH404: Surface Chemistry**

#### **UNIT-I: Surface Chemistry of Interfaces**

15 hrs.

Types of interfaces, liquid-vapour interface, surface tension and interfacial tension, surface tension across curved surfaces, capillary action, methods of determination of surface tension, vapor pressure of droplet (Kelvin equation), surface activity and adsorption phenomenon, Trube's rule, liquid-liquid interfaces, work of cohesion and adhesion, surface spreading, spreading of one liquid on the surface of other liquid, spreading coefficient and derivation for its relation with surface tension, surface films on liquids, criteria for spreading of one liquid on another. Experimental techniques for the study of monomolecular films, states of monomolecular films reaction on monomolecular films, heterogenous catalysis.

#### **UNIT -II: Solid-Liquid and Solid - Solid interfaces**

15 hrs.

Solid-liquid interfaces, Introduction, wetting phenomenon, contact angle and wetting, heat of wetting, methods of determination of contact angle, contact angle hysteresis, wetting agents, selective wetting, applications in detergency, and pesticide affectivity, solid-solid interfaces, introduction, surface energy of solids, adhesion, and adsorption, sintering and sintering mechanism, Tammann temperature, importance of impurities, surface structure and surface composition. Friction and lubrication, mechanism of lubrication, solid state lubricants.

#### **Unit-III: Solid-gas interfaces**

15 hrs.

Adsorption, mechanism of adsorption, adsorption of gases by solids, surface area measurement, factors affecting on adsorption, experimental methods of determining gases adsorption, adsorption of solutes from solution, heat of adsorption, measurement of heat of adsorption,

Chemisorption: kinetics of chemisorption, heat of chemisorption, surface film, Catalysis of gases reaction by solid surface, One reactant gases slightly/ strongly/ moderately adsorbed, Retarded reaction, ion exchange adsorption, Applications.

#### **UNIT- IV: Colloids and emulsion**

15 hrs.

Colloidal solution, classification of colloids, Theories of origin of charge on sol particles, determination of charge on a colloidal particle, stability of sols, properties of colloids, spontaneous ageing of colloids, factors affecting on the spontaneous ageing, theories of spontaneous ageing, coagulation, kinetics of coagulation.

Emulsion: Types of emulsion, preparation, properties, characteristics, identification test between two types of emulsions, emulsifiers, demulsification.

Gels: classification, methods for the preparation of gels, properties of gels, applications of colloids.

#### **Reference Books:**

- 1. Physical chemistry of surfaces: A. W. Adamson.
- 2. Introduction to colloid and surface chemistry by D. J. Shaw. 58
- 3. Surface chemistry by J. J. Bikermann
- 4.The Surface Chemistry of Solids, by S.J.Gregg, Second Edition, Chapman & Hall Ltd. London.
- 5. Advanced Physical Chemistry, by Gurdeep Raj, Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)
- 6. Physical Chemistry by Pahari S. New Central Book Agency (P) Ltd. Kolkata.
- 7. Advanced Physical Chemistry J.N. Gurtu, A. Gurtu. 11th Edition Pragati Prakashan.
- 8. Advanced Physical Chemistry D N Bajpai S Chand Publications
- 8. Essentials of Physical Chemistry by Arun Bahl, B S Bahl, G D Tuli . S Chand Publications 9. Principles of Physical Chemistry by S H Maron and C F Prutton
- 10. Physical Chemistry, P. W Atkin.

# **Course Outcomes (COs):**

After completion of course student will able to understand

CO1: Understand concepts of solid-liquid, solid-gas, liquid-gas interfaces.

CO2: Apply fundamental principles of chemistry to chemical processes occurring at interfaces.

CO3: Apply spectroscopic methods to study interfaces and interfacial phenomena.

CO4: Learning and understanding the importance, applications, and basic aspects of surface chemistry.

CO5: The course focuses on the fundamentals of surface chemistry, with the main emphasis on solid surfaces in contact with gas phase.

CO6: Adsorption, desorption and colloidal applications of surface chemistry are able to apply this knowledge in understanding and designing surface chemistry processes.

# E-ACH404: Applied Analytical Chemistry

#### **UNIT-I: Spectrochemical Methods of Analysis**

15 hrs.

Introduction to spectrochemical methods. Electronic spectra and molecular structure, NIR spectrometry for non-destructive testing. Solvents for spectrometry, FTIR spectrometer, fluorometry, optical sensors. Analysis of ores –bauxites, dolomites, monazites. Analysis of Portland cement.

#### **UNIT-II: Analysis of metals and alloys**

15 hrs.

Foundry materials, ferroalloys, and special steels, slags, fluxes. Analysis of alloys, bronze, brass, Alnico and Nichrom.

#### **UNIT-III:** Analysis of soil and fertilizers

15 hrs.

Method of soil analysis, soil fertility and its determination, determination of inorganic constituents of plant materials, Chemical analysis as measure of soil fertility, analysis of fertilizers, applications.

#### **UNIT-IV:** Analysis of Commercial materials

15 hrs.

Analysis of explosive materials, TNT, RDX, lead azide, EDNA (ethylene dinitramine). Analysis of conducting polymer, resins and rubber. Analysis of luminescent paints, Analysis of lubricants and adhesive.

#### **Reference Books:**

1. Hillebrand Lhundel, Bright and Hoffiman, Applied Inorganic Analysis, John Wiley.

- 2. Snell and Biffen, Commercial Methods of Analysis.
- 3. P. G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
- 4. Buchel, Chemistry of Pesticides. J Wiley.
- 5. Rieche, Outlines of Industrial Organic Chemistry, Butter Worth.
- 6. F. A. Henglein, Chemical Technology, Pergamon.
- 7. Kent, Riegl's Industrial Chemistry, Rainhold.
- 8. Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
- 9. Aubert and Pintes, Trace Elements in Soils.
- 10. Bear, Chemistry of Soil.
- 11. Hauson, Plant Growth Regulators, Noyes.
- 12. P. G. Jeffery and D.J. Hatchinson, Chemical Methods of Rock Analysis.
- 13. F. J. Weleher, Standard Methods of Chemical Analysis, A Series of Volumes Robert and Krigeger Publishing Company.
- 14. I. M. Kolthoff and PJ Ewing, Treatise o Analytical Chemistry, A series of Volumes.
- 15. R. D. Reeves and R.R. Brooks, Trace element Analysis of Geological Materials, John Wiley & Sons New Dehli.
- 16. W. M. Johnson and J.A. Maxwell, Rock and Mineral Analysis, John Wiley and Sons, New York.
- 17. W. F. Hildebrand, GHC Landell and HA Brighot, Applied Inorganic Analysis, John Wiley 2<sup>nd</sup> Ed.
- 18. K. J. Das, Pesticide Analysis (MD).

#### **Course Outcomes (COs):**

- CO1: The students will acquire knowledge of analysis of metals, alloys, minerals and ores commonly used in the industry.
- CO2: The students will be acquainted with the analysis of real samples like cement, plaster of Paris, different commercial ores, soil composition, soil fertility, fertilizers etc using conventional and instrumental methods of analysis.
- CO3: Students will also gain the knowledge of analysis of commercial materials, explosives, polymers, resins, rubber, luminescent paints, lubricants and adhesives.
- CO4: These would offer opportunity to the students to get employment in industries for quality assurance and quality control (QA-QC) of the product.

# **Annexture-I**

# **Research Project Paper Guidelines for all specializations**

(Inorganic, Organic, Physical, Analytical, Applied and Industrial Chemistry)

#### **Semester III**

# RP-ICH306, RP-OCH306, RP-PCH306, RP-ACH306, RP-APCH306, RP-INDCH306 Credits= 04, 120 Hours, 100 Marks

- The students should write synopsis of proposed research work.
- The students should perform detail literature survey related to research problem.
- The students should write review article related to research problem.
- It is expected to publish the review article either in Shivaji University Journal or peer reviewed journals.
- The students should design the problem and start experimental work. The students should complete at least 25% of their experimental work during the semester III and the same work to be continued in semester IV.
- The student should submit the spiral bound copy of research work carried out during semester III including the synopsis, research proposal, review article and certified progress report.
- The Research Project will be examined jointly by internal and external examiners during the practical examination at the end of the semester.
- The students should present their work during the evaluation in the form of power point presentation (PPT).

#### • Marking Scheme:

Sr. No.	Description	Marks
1	Synopsis	10
2	Research Proposal	20
3	Review article on proposed work	20
4	Daily Lab notebook record	10
5	Progress of Experimental work	20
6	Quality and effectiveness of presentation	20
	Total	100

#### **Broad guidelines for preparation of synopsis**

- A. The proposed synopsis for research should be self contained and should cover the rationale for carrying out research.
- B. There should not be repetition of the work or topic or theme.
- C. The synopsis of the proposed research shall contain the following points :
- 1. Title of the Research Proposal
- 2. Motivation with reasoning and significance of the proposed research
- 3. Statement of the problem
- 4. Review of the relevant literature
- 5. Objectives of the study
- 6. The methodology comprising
- a. Methods of research
- b. Sampling design and assumptions
- c. Conceptual framework if any
- d. Research design (explanation of how research is being conducted and the tools used for the same)
- e. Methods of data collection
- f. Methods of data analysis (use of parametric and non-parametric tools and techniques as the case may be)
- 7. Expected outcome
- 8. Bibliography.

#### **Template for Research Proposal**

- Title
- Introduction
- Origin of the research problem
- Interdisciplinary relevance
- Review of Research and Development in the Subject
- Significance of the study
- Objectives
- Plan of research work

#### M. Sc. II Semester IV

# RP-ICH405, RP-OCH405, RP-PCH405, RP-ACH405, RP-APCH405, RP-INDCH405 Credits= 06, 180 Hours, 150 Marks

- The student should submit the final bound dissertation/thesis copy of research work carried out during semester III and IV.
- It should include title page, certificate, declaration, acknowledgement, abbreviations, index, abstract, introduction, experimental section, results and discussion, conclusions, references, participation in conferences/seminars and publications if any.
- The students should present their work during the evaluation in the form of power point presentation (PPT) .

#### • Marking Scheme:

Sr. No.	Description	Marks
1	Dissertation/thesis bound copy	30
2	Quality of work ( Innovative concepts, social relevance, extent of work etc.)	50
3	Publications	20
4	Participation in conferences	10 maximum
	a) Oral/Poster Presentation (10 marks)	
	b) Only attended (7 marks)	
5	Final Dissertation/thesis defence	40
	Total	150

**Note:** The Project will be examined jointly by internal (Project Supervisor) and external examiners (preferably Associate professor and above with Ph. D.) at the end of the semester. The project can be given individually or a maximum group of three students is allowed. (Not more than three students allowed).