# MADRAS CHRISTIAN COLLEGE (AUTONOMOUS) (UGC – College with Potential for Excellence) (Reaccredited with 'A' Grade by NAAC, 2019)

# DEPARTMENT OF CHEMISTRY (Self Financed Stream)

Revised Curriculum and syllabi *for* **M. Sc. Chemistry** (Effective from the academic year 2022 – 2023)



**JUNE 2022** 

# MADRAS CHRISTIAN COLLEGE (Autonomous)

UGC – College with Potential for Excellence Chennai -600059

# DEPARTMENT OF CHEMISTRY (SFS)

Minutes of the Board of Studies Meeting held on Wednesday, 6th July, 2022 at 2:00 pm in the Staff Room, Department of Chemistry (Aided), Madras Christian College, Chennai-600 059

**Members Present:** 

Convenor:

Dr.S.Sahila

Assistant Professor i/c

J. Inth

Department of Chemistry (SFS), MCC.

**External Members:** 

**University Nominee:** 

Dr. M Saroja Devi

Professor, Department of Chemistry CEG Campus, Chennai.

Subject Experts:

Dr. S. J. Askar Ali Associate Professor. Department of Chemistry

New College, Chennai.

Dr. S. Muniraj

Assistant Professor, Department of Chemistry Vivekananda College, Chennai.

**Industrial Expert:** 

Mr. R. Shanmuga Sundaram (FL-1, Shift In-charge) Orchid Pharma, SIDCO Industrial Estate Alathur, Kanchipuram District.

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#### Alumna:

Mrs. y. Sudha,

Assistant Dean, Sri Chaitanya Techno School, Pallavaram.

# **Student Representative:**

Ms. J. K. Austina Thesnavis, I. M.Sc Chemistry, MCC.

#### **Internal Members:**

Dr. S. Sahila, Assistant Professor i/c.

Dr. S. Daniel Abraham, Assistant Professor.

Dr. K. Vijayalakshmi, Assistant Professor.

Dr. S. Saranya, Assistant Professor.

#### Agenda:

M.Sc Syllabi for the Academic Year 2022-2023 onwards.

- The Board of Studies meeting began with the college prayer by Dr. S. Daniel Abraham, Assistant Professor, Department of Chemistry (SFS), MCC.
- Dr. S. Sahila, Assistant Professor i/c, Department of Chemistry (SFS), MCC delivered the welcome address and introduced the Board of Studies panel members.
- She informed that the revision of all the papers comprising the four semesters of the syllabi of the M.Sc. program for the upcoming academic year (2022 2023) would be taken up for scrutiny and for ratification in the meeting and presented the papers before the Board.

The syllabus was presented for discussion and the following points were resolved.

# Course Title: Advanced foundations in organic chemistry (SEM I)

1. It was suggested that specific examples should be mentioned under heterocyclic compounds (Unit 1.1).

# Course Title: Solid state and organometallic chemistry (SEM I)

1. It was recommended to remove Isopolyacid and heteropolyacid of Chromium. (Unit 3.4).

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- 2. It was advised to include the organometallics as introduction followed by different reactions (Unit 5.1).
- 3. It was suggested to mention the specific catalyst used in olefin isomerization and to include the conversion process in Fischer-Tropsch method (Unit 5.2).

# Course title: Organic Reaction Mechanism (SEM II)

- 1. It was suggested to rearrange the topics as Woodward -Hoffmann rule, use of FMO and correlation diagrams electrocyclic (butadiene-cyclobutene system), cycloaddition (4+2) & (2+2) systems, sigmatropic and cheletropic reactions and asked to remove application of HMO theory to organic reaction mechanism (Unit 4.2).
- 2. It was recommended to expand LAH as LiAlH<sub>4</sub> (Unit 5.3).

# Course title: Analytical Techniques in Chemistry (SEM II)

1. Under Unit 3.1 instead of certain simple molecules it was suggested to specifically mention as ESR applications to radicals and ions.

#### Course title: Polymer Chemistry (SEM II)

1. Under Unit 1.1, it was advised to introduce the term functionality under basic concepts of polymer chemistry.

### Course title: Chemistry of Natural Products (SEM III)

- 1. Under Unit 1.1, it was recommended to remove furan, pyrrole, thiophene and pyridine.
- 2. Under Unit 1.3, It was suggested to remove stereochemistry, reaction and conformation of monosaccharide, disaccharide and polysaccharide and to include structural elucidation of sucrose followed by structural difference between starch and cellulose.
- 3. Unit 2.2 was modified as synthesis of Cholesterol, Structural elucidation and synthesis of estrone and progesterone.
- 4. In Unit 4.1, it was advised to remove Vitamin B2.

### Course title: Electrochemistry and Spectroscopy (SEM III)

1. In unit 5, It was suggested to remove solvents used in NMR, theory of spin-spin splitting, and factors influencing the coupling constants.

#### Course title: Coordination Chemistry (SEM IV)

- 1. Under 1.2, it was advised to remove site selections in spinels and anti-spinels.
- 2. Under Unit 3.3, it was suggested to remove the ESR of copper complex and ORD of  $[Co(en)_2(glu)^{3+}]$  complex.
- 3. Under Unit 4.2, it was advised to mention the theories of Trans effect (polarization and pi bonding theory).
- 4. Under Unit 4.3, it was recommended to specifically mention as formation and rearrangement of precursor complex and also to include the atom transfer reaction at the end of the unit.
- 5. In Unit 5.2, it was advised to mention specific example under photochemistry of Cr (III) and Co (III) complexes.
- 6. In Unit 5.3, it was recommended to remove the CO-TiO<sub>2</sub> and to include nano TiO<sub>2</sub> as photocatalyst.

# Course title: Bioinorganic Chemistry (SEM IV)

- 1. Unit 4.2, was rearranged as 'metal salts and complexes in therapeutics: Drugs used in treatment of metal deficiency- metal salts-gold-lithium-arsenic-antimony compounds- anticancer drugs (cis-platin and its alternatives).
- 2. Under Unit 5.1, it was suggested to change detoxification mechanism as Mechanism of detoxification.
- 3. Under Unit 5.3, it was suggested to shift <sup>67</sup>Ga and <sup>68</sup>Ga complex to the end.

After careful examination, the members of the board approved the revised syllabus of the M.Sc. program and, also recommended the same for presentation at the Academic Council of the college for further approval and ratification.

Thus, the meeting was concluded with vote of thanks proposed by Dr. K. Vijayalakshmi, Assistant Professor, Department of Chemistry, (SFS), MCC.

# Department of Chemistry (SFS) Master of Science in Chemistry-Curriculum Framework (Effective from the academic year 2022-2023)

SEMESTER-I						
COURSE NUMBER	NATURE OF COURSE	NAME OF COURSE	COURSE CODE	HOURS/ CYCLE	CREDIT	MARKS ICA + ESE (100)
C-1	CORE	ADVANCED FOUNDATIONS		4	4	50+50
	THEORY	IN ORGANIC CHEMISTRY				
C-2	CORE	SOLID STATE AND		4	4	50+50
	THEORY	ORGANOMETALLIC				
		CHEMISTRY				
C-3	CORE	THERMODYNAMICS AND		5	4	50+50
	THEORY	CHEMICAL KINETICS				
E-1	ELECTIVE	ENVIRONMENTAL		5	5	50+50
	THEORY-1	CHEMISTRY				
		ORGANIC CHEMISTRY		4	-	-
	CORE	PRACTICALS-I				
P-1	PRACTICALS-I	INORGANIC CHEMISTRY		4	-	
		PRACTICALS-I				
		PHYSICAL CHEMISTRY		4	-	
		PRACTICALS-I				
		CORE THEORY+ PRA	ACTICALS	25	12	300
			ELECTIVE	5	5	100
			TOTAL	30	17	400

	SEMESTER-II						
COURSE NUMBER	NATURE OF COURSE	NAME OF COURSE	COURSE CODE	HOURS/ CYCLE	CREDITS	MARKS ICA + ESE (100)	
C-4	CORE THEORY	ORGANIC REACTION MECHANISM		4	4	50+50	
C-5	CORE THEORY	ANALYTICAL TECHNIQUES IN CHEMISTRY		3	4	50+50	
C-6	CORE THEORY	GROUP THEORY AND QUANTUM MECHANICS		4	4	50+50	
E-2	ELECTIVE THEORY-2	POLYMER CHEMISTRY		5	5	50+50	
SS-1		SOFT SKILLS-I		2	4	50	
P-2	CORE PRACTICALS-I	ORGANIC CHEMISTRY PRACTICALS-I		4	4	100	
		INORGANIC CHEMISTRY PRACTICALS-I		4	4		
		PHYSICAL CHEMISTRY PRACTICALS-I	-	4	4		
CORE THEORY+ PRACTICALS				23	24	400	
			ELECTIVE	5	5	100	
		SO	FT SKILLS	2	4	50	
			TOTAL	30	33	550	

		SEMESTER	R-III			
COURSE NUMBER	NATURE OF COURSE	NAME OF COURSE	COURSE CODE	HOURS/ CYCLE	CREDIT	MARKS ICA + ESE (100)
C-7	CORE THEORY	CHEMISTRY OF NATURAL PRODUCTS		3	4	50+50
C-8	CORE THEORY	ELECTROCHEMISTRY AND SPECTROSCOPY		3	4	50+50
E-3	ELECTIVE THEORY-3	MEDICINAL CHEMISTRY		5	5	50+50
SS-II		SOFT SKILLS-II		2	4	50
P-3	CORE PRACTICALS-II	ORGANIC CHEMISTRY PRACTICALS-II		4	-	-
		INORGANIC CHEMISTRY PRACTICALS-II		4	-	
		PHYSICAL CHEMISTRY PRACTICALS-II		4	-	
PR-1		PROJECT		5	-	-
CORE THEORY+ PRACTICALS+ PROJECT				23	8	200
		SO	FT SKILLS	2	4	50
			ELECTIVE	5	5	100
			TOTAL	30	17	350

				SEMES	TER-IV	7			
	JRSE 1BER	NATURE		NAME OF COUP	RSE	COURSE CODE	HOURS/ CYCLE	CREDITS	MARKS ICA + ESE
C-9	)	CORE THE	ORY	COORDINATION			4	4	( <b>100</b> ) 50+50
0,				CHEMISTRY			·	·	50150
C-1	10	CORE THE		SCIENTIFIC RESEA	RCH		4	4	50+50
-	-			METHODOLOGY	-				
E-4	1	ELECTIVE		BIOINORGANIC			5	5	50+50
		THEORY-4		CHEMISTRY					
P-4	Ļ	CORE		ORGANIC CHEMIS	ſRY		4	4	100
		PRACTICAL	.S-II	PRACTICALS-II					
			_	INORGANIC CHEM	ISTRY		4	4	
				PRACTICALS-II					
			_	PHYSICAL CHEMIS	TRY		4	4	
				PRACTICALS-II					
				INTERNSHIP			-	2	_
PR	-1			PROJECT			5	6	20+80
			CO	RE THEORY+PRAC	FICALS	+ PROJECT	25	26	400
						ELECTIVE	5	5	100
					ľ	ITERNSHIP	-	2	-
					S	SUB TOTAL	30	33	500
					GRA	ND TOTAL	120	100	1800
	Seme	esters	Ι	II		III	IV	Г	otal
I		ctional	30	30		30	30		120
		urs dits	17	33		17	33		100
					NILL				
			RE OF P.		NU.	MBER OF PA	APERS	CREDIT	5
		CORE T	HEORY	PAPERS	10		40		
	CORE PRACTICAL PAPERS		6		24				
	PROJECT			1 6		6			
	ELECTIVE THEORY PAPERS			4		20			
	INTERNSHIP			IIP		-		2	
		SC	OFT SKIL	LS		-		8	
							100		

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<b>Course Code</b>		<b>Revised</b> /	New/Revised		% of
(will be filled by EO)	Existing syllabus	Renamed/ Replaced	Subjects	Paper	Change
	Basic Concepts in	Revised and	Advanced Foundations	Major-	10%
	Organic Chemistry	renamed	in Organic Chemistry	Core	
	Material Science	Revised and	Solid State and	Major-	60%
		renamed	Organometallic Chemistry	Core	
	Thermodynamics and Chemical Kinetics	Revised	Thermodynamics and Chemical Kinetics	Major- Core	15%
	Environmental Chemistry	Revised	Environmental Chemistry	Elective	60%
	Organic Chemistry Practicals-I	No Revision	Organic Chemistry Practicals-I	Practicals	-
	Inorganic Chemistry Practicals-I	No Revision	Inorganic Chemistry Practicals-I	Practicals	-
	Physical Chemistry Practicals-I	No Revision	Physical Chemistry Practicals-I	Practicals	-
SEMESTER-II					2004
	Organic Reaction Mechanism	Revised	Organic Reaction Mechanism	Major- Core	30%
	Analytical Techniques in Chemistry	Revised	Analytical Techniques in Chemistry	Major- Core	30%
	Group Theory and Quantum Mechanics	Revised	Group Theory and Quantum Mechanics	Major- Core	15%
	Polymer Chemistry	Revised	Polymer Chemistry	Elective	40%
	Organic Chemistry Practicals-I	No Revision	Organic Chemistry Practicals-II	Practicals	-
	Inorganic Chemistry Practicals-I	No Revision	Inorganic Chemistry Practicals-II	Practicals	-
	Physical Chemistry Practicals-I	No Revision	Physical Chemistry Practicals-II	Practicals	-

<b>Course Code</b>	Existing syllabus	<b>Revised</b> /	New/Revised	Paper	% of
(will be filled		<b>Renamed</b> /	Subjects	_	Change
by EO)		Replaced			C
	Chemistry of Natural Products	Revised	Chemistry of Natural Products	Major Core	30%
	Electrochemistry and Spectroscopy	Revised	Electrochemistry and Spectroscopy	Major Core	20%
	Medicinal Chemistry	Revised	Medicinal Chemistry	Elective	20%
	Organic Chemistry Practicals-II	No Revision	Organic Chemistry Practicals-II	Practicals	-
	Inorganic Chemistry Practicals-II	No Revision	Inorganic Chemistry Practicals-II	Practicals	-
	Physical Chemistry Practicals-II	No Revision	Physical Chemistry Practicals-II	Practicals	-
SEMESTER-I	V				
	Coordination Chemistry	Revised	Coordination Chemistry	Major Core	60%
	Scientific Research Methodology	Revised	Scientific Research Methodology	Major Core	30%
	Bioinorganic Chemistry	Revised	Bioinorganic Chemistry	Elective	15%
	Organic Chemistry Practicals-II	No Revision	Organic Chemistry Practicals-II	Practicals	-
	Inorganic Chemistry Practicals-II	No Revision	Inorganic Chemistry Practicals-II	Practicals	-
	Physical Chemistry Practicals-II	No Revision	Physical Chemistry Practicals-II	Practicals	-

# SCHEME OF EVALUATION FOR PRACTICAL COURSES

The assessment for practical papers done internally as per the following scheme:

Assessment type	Odd semester	Even semester	Average / Year
In-class assessment	50 marks	50 marks	50 marks
Internal continuous assessment	-	-	50 marks
		Total	100 marks

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In-class assessment	At the end of a semester, a student's performance for all
	the classes is evaluated as follows:
	Quantum of work: 20 marks
	(Attendance: 10 + Number of experiments: 10)
	Accuracy for selected experiments: 20 marks*
	Record (regularity and neatness): 10 marks
	Total: 50 marks
	*Accuracy for at least 60% of the experiments carried
	out to be considered for average
Internal continuous assessment*	Three department centralized ICA will be conducted (one
	in odd semester and two in even semester). Better of two
	out of three ICA will be considered for final ICA-
	Average. ICA test will be evaluated as follows:
	Experiment – Procedure, Observation and
	Calculation: 20 marks
	Accuracy: 20 marks
	Viva: 5 marks
	Record: 5 marks
	Total: 50 marks
Total marks	100

Note: No end of semester examination will be conducted for practical courses.

	EXPERIMENTAL WORK	REVIEW WORK
INTERNAL	By project supervisor:	By project supervisor:
	Literature survey-10 marks	Literature survey-15 marks
	Originality/planning-5 marks	Critical analysis/comparison- 20 marks
	Accuracy-10 marks	By project coordinator:
	Quantum of work-10 marks	Attendance-5 marks
	By project coordinator:	Presentation-10 marks
	Attendance-5 marks	Total : 50 marks
	Presentation-10 marks	
	Total : 50 marks	
EXTERNAL	Report-80 marks	Report-80 marks
	Viva-20 marks	Viva-20 marks
	Total : 100 marks	Total : 100 marks

# SCHEME OF EVALUATION FOR PROJECT

# PROGRAM SPECIFIC OUTCOMES

On successful completion of M.Sc Chemistry program, students will be able

PSO No.	PROGRAM SPECIFIC OUTCOMES				
	Integrate advanced knowledge in organic, inorganic, physical, analytical				
PSO-1	chemistry and relate the theoretical aspects of chemistry in different fields of				
	medicine, materials, technology, energy and environment.				
	Describe the basic concept of reaction pathways, stereochemistry, chemical				
PSO-2	reactivity, mechanisms of organic reactions including the structure and synthesis				
of natural compounds					
	Develop the mastery of chemistry to conduct formal scholarly research,				
PSO-3	investigating a research problem through dissertation /project work in different				
	arena of chemistry and to emerge as a perspective chemical entrepreneur				
	Discuss the structure, function, various disasters caused by natural/human				
PSO-4	activities and to carry out advanced analysis/experiments to provide solutions to				
	industrial and global environmental issues				
	Apply the basic concepts/ideas involved in the separation and preparation of the				
	organic and inorganic compounds, classical techniques to perform experiments				
PSO-5	developing skills to interpret and to pursue career in industry, research and				
	academics.				
	Correlate the various concepts and express the core/elective subject to develop				
	critical thinking ability by way of solving problems to succeed in competitive				
PSO-6	examinations, data interpretation, scientific report writing and to emerge as				
	successful entrepreneurs.				

#### SEMESTER-I

#### COURSE TITLE: ADVANCED FOUNDATIONS IN ORGANIC CHEMISTRY

Course Code: (will be filled by EO)

(60 hours)

Number of hours/cycle: 4

Nature of Course : Core Theory

Credits: 4

Le	Learning Objective				
(i)	To understand the concept and mechanisms of aromaticity of benzenoid, non-				
	benzenoid and heterocyclic compounds.				
(ii)	To learn the configuration and stereo chemical aspects of acyclic and cyclic molecules.				
(iii)	To study the conformational analysis of cyclic and acyclic molecules.				
(iv)	To learn the reaction mechanisms through non-kinetic and kinetic methods.				
( <b>v</b> )	To study the correlation between the structure and reactivity of molecules				

CO No	<b>Course Outcome</b> Upon completion of this course, students will be able to	PSO's addressed	CL
CO-1	Assign the aromaticity in benzenoid and non- benzenoid molecules	PSO-1, PSO-2, PSO-6	Ар
CO-2	Analyze and Assign the configuration for stereo isomers.	PSO-2, PSO-6	An
CO-3	Differentiate the conformation and configuration in stereo chemistry	PSO-2, PSO-6	An
CO-4	Apply the reaction mechanism through kinetic and non-kinetic methods	PSO-1, PSO-2	Ар
CO-5	Predict the structural effects and reactivity of molecules and the nature of intermediates.	PSO-2, PSO-5	Ар

# <u>Unit I</u>

(12 hours)

(12 hours)

- 1.1 Aromaticity: Benzenoid and non-benzenoid, heterocyclic compounds (furan, pyrrole, thiophene, imidazole and pyridine). Huckel and Craig rules. Frost Circle. Alternant and non-alternant hydrocarbons. Homo-and antiaromatic compounds.
- 1.2 Study of cyclopropenium cation, cyclopentadienyl anion, cycloheptatrienyl cation, aromatic, nonaromatic and antiaromatic compounds. Aromatic and antiaromatic ions. Annulenes [10],[14],[18],[22], tropolone and azulene.

# <u>Unit II</u>

2.1 Stereochemistry: Optical activity and chirality. Classification of chiral molecules as asymmetric and dissymmetry of allenes, biphenyls, spiro-compounds, cyclobutane and cyclononane and molecules with helical structures. Absolute configuration - R-S Notation of simple molecules. Stereochemistry of molecules with axial chirality – biphenyls, allenes, spiranes - concept of atropisomerism. Molecules with more than one asymmetric centre -

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#### erythro and threo compounds. Asymmetric synthesis, Cram's rule - optical purity.

2.2 Geometrical isomerism- E-Z nomenclature of olefins. Geometrical and optical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentanes. Helicity, chirality and topocity. Identification of enantiotopic, homotopic, and diastereotopic hydrogens and prochiral carbons in compounds containing upto ten carbon atoms only. Stereospecific and stereoselective synthesis.

#### <u>Unit III</u>

- 3.1 Conformation and conformational analysis: Conformation and reactivity in acyclic systems conformations of some simple 1,2- disubstituted ethane derivatives. Sawhorse and Newmann projections.
- 3.2 Conformation and reactivity in cyclic systems cyclobutane, cyclopentane, cyclohexane, cycloheptane and cyclooctane. Conformational analysis of disubstituted cyclohexanes and their stereochemical features Conformation and reactivity of cyclohexanols (oxidation and reduction) and cyclohexanones (reduction). Conformation and stereochemistry of cis-and trans- decalins.

### <u>Unit IV</u>

- 4.1 Study and description of organic reaction mechanisms: Non-kinetic methods- Energy profile diagrams, intermediate versus transition state, identification of products, cross-over experiments, stereochemical studies- uses of isotopes.
- 4.2 Kinetic methods-Kinetic isotopic effects, salt effects, solvent effects- solvent isotopic effects, kinetic and thermodynamic controlled products. Hammond postulates. Curtin-Hammett principle and Winstein-Holness equation.

#### <u>Unit V</u>

- 5.1 Structural effects: Correlation of structure with reactivity. Inductive, mesomeric, steric effects, linear free energy relationship Hammett equation, Taft equation, comparison of the acidity of carboxylic acids and phenols, comparison of basicity of aliphatic and aromatic bases.
- 5.2 Reactive intermediates: Generation, detection, stability and reactivity of carbocations (classical and non-classical), carbanions, carbenes, arynes, nitrenes, free radicals and enolates.

#### **TEXT BOOKS**

- 1. Advanced Organic Chemistry Part (A & B) Francis A Carey and Richard J Sundberg, V Edition, 2008, Springer, New York, USA.
- 2. March's Advanced Organic Chemistry, Michael B Smith, Jerry March, 2007, Wiley Students Edition, India.
- 3. Advanced Organic Chemistry, Jagdamba Singh and L.D.S Yadav Pragati, 2017, Prakashan Educational Publishers.
- 4. Stereochemistry: Conformation and Mechanism, P S Kalsi, X Edition, 2019, New Age

(12 hours)

(12 hours)

(12 hours)

International Publisher.

#### REFERENCES

- 1. Stereochemistry of Carbon Compounds, Ernest L Eliel, Tata McGraw Hill Edition, 2008, India.
- Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, II Edition, 2019, Oxford University Press, New Delhi – 110 001, India
- 3. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, IV Ed., New Age International Publishers.
- 4. A Guidebook to Mechanism in Organic Chemistry, Peter Sykes, VI Edition, 2020, Pearson India Education Services, India.
- 5. Organic Reaction Mechanism, V K Alhuwalia and Rakesh Kumar Parashar, IV Edition, 16<sup>th</sup> Reprint, 2019, Alpha Narosa Publishing House, New Delhi, India

### SUGGESTED READING

- 1. Stereochemistry of organic compounds, principles and applications, D. Nasipuri, II Edition New Age International Publishers
- 2. N.S. Isaacs, Physical Organic Chemistry, 1987, ELBS. Longman, UK.
- 3. T. H. Lowry K. S. Richardson, Harper and Row, Mechanism and theory in organic chemistry, 2nd edition, 1981, Pearson Publication, New York.

- 1. <u>https://onlinecourses.nptel.ac.in/noc22\_cy34/preview</u>
- 2. https://nptel.ac.in/courses/104103071
- 3. https://nptel.ac.in/courses/104105086
- 4. <u>https://onlinecourses.nptel.ac.in/noc22\_cy08/preview</u>
- 5. <u>https://onlinecourses.nptel.ac.in/noc22\_cy18/preview</u>

## COURSE TITLE: SOLID STATE AND ORGANOMETALLIC CHEMISTRY

Course Code: (will be filled by EO)

(60 hours)

Number of hours/cycle: 4

Nature of Course : Core Theory

Credits: 4

Lear	Learning Objective		
(i)	To understand the structure, bonding, cohesive forces in crystals, structural aspects of		
	different crystal systems, crystal geometry and space group in crystal lattices		
<b>(ii)</b>	To gain knowledge about the crystal growth methods, crystal defects, magnetic		
	behaviour and various analytical techniques to determine the structure of solids		
(iii)	To understand the synthesis, bonding and structural aspects of various ionic		
	conductors, metal carbonyl clusters, boranes, carboranes, isopolyacids and polysulphur		
	nitrogen compounds		
(iv)	To learn the bonding and structural aspects of metal carbonyls, nitrosyls,		
	organometallic compounds and macrocyclic ligands.		
<b>(v)</b>	To acquire knowledge on the utilization of various organometallic complexes as industrial		
	catalysts in numerous applications.		

CO No	Course Outcome	PSO's	CL
	Upon completion of this course, students will be able	addressed	
	to		
CO-1	Describe the crystal structure in terms of atom	PSO-1,	U
	positions, unit cells, crystal lattices, crystal symmetry and different types of crystal systems	PSO-6	
CO-2	Explain the crystal growth methods, properties of	PSO-1,	An
	crystals, crystal defects and demonstrate various	PSO-3	
	diffraction and microscopic techniques to determine		
	the structure of solids		
CO-3	Relate the properties of ionic conductors, metal	PSO-1,	Ар
	carbonyl clusters, boranes, carboranes, isopolyacids	PSO-3	
	and polysulphur nitrogen compounds.		
<b>CO-4</b>	Predict the concepts and properties of metal	PSO-4,	An
	carbonyls, nitrosyls, organometallic compounds and	PSO-6	
	macrocyclic ligands.		
CO-5	Develop novel applications of organometallic	PSO-1,	Ар
	complexes as industrial catalysts.	PSO-3,	
		PSO-4	

## <u>Unit I</u>

(12 hours)

- 1.1 Structure and bonding in solids Cohesive force in crystals, van der Waals interactions, ionic bonding, covalent bonding and hydrogen bonding in solids.
- 1.2 Structural aspects of rutile, fluorite, antifluorite, zinc blende, wurtzite, crystobalite, spinels, inverse spinels and silicates.
- 1.3 Crystal geometry- Symmetry elements (including glide planes and screw axis) and their symmetry

operations, Miller indices, point groups and space groups- definition and examples- classification of crystals- seven crystal systems and fourteen Bravais lattices.

Unit II

- 2.1. Crystal growth techniques- Single crystal growth solution growth technique–gel and sol-gel method. Melt growth - Bridgeman-Stockbarger and Czochralski method.
- 2.2. Techniques of structure determination in solid state X-ray diffraction- Debye Scherrer equation, electron and neutron diffraction-powder diffraction and electron microscopy principle, instrumentation and applications.
- 2.3. Defects in crystals Frenkel and Schottky defects, F-centres, effect of defects on the electrical, optical, magnetic, thermal and mechanical properties of crystals - magnetic behaviour of solids-diffusion in solids.
- 2.4. Theories of metallic state free electron theory, Brillouin and band models.

# **Unit III**

- 3.1. Liquid crystals: Thermotropic and lyotropic classification- nemetic, smectic and cholestric applications.
- 3.2. Optimised ionic conductors: Silver ion, alumina and related electrolytes. Superconductors principle and applications- optical materials (LED's and lasers)
- 3.3. Synthesis and structure of boranes closo, nido and arachno boranes  $(B_4H_{10}, B_5H_9, B_5H_{11})$ and  $B_{10}H_{14}$ ) - STYX number-Wades rule, carboranes ( $C_2B_{10}H_{12}$ ), phosphazenes (cyclic trimer  $(NPCl_2)_3$  and cyclic tetramer  $(N_4P_4Cl_8)$  and polysulphur nitrogen compounds  $((SN)_x)$ .
- 3.4. Isopolyacids and heteropolyacids of vanadium, molybdenum and tungsten- metal clustersstructure of  $[\text{Re}_2\text{Cl}_8]^{2-}$  and  $[\text{Re}_3\text{X}_{12}]^{3-}$ .

# **Unit-IV**

- 4.1. Complexes of alkali and alkaline earth metals with macrocyclic ligands like porphyrin, corrin, crown ethers and cryptands.
- 4.2. Organometallic compounds of transition elements: 16 and 18 electron rule. Synthesis, reactions, bonding and structure of metal-olefin, metal-acetylene, metal-allyl and metalcyclopentadienyl complexes of transition elements.
- 4.3. Stabilisation of the unusual oxidation states of metals metal carbonyls nitrosyls carbonyl halides - carbonyl hydrides - synthesis, bonding and structure - complexes with oxygen and fluorine ligands.

# <u>Unit V</u>

- 5.1 Organometallics: Oxidative addition. reductive elimination, insertion, alpha and beta elimination reactions- fluxional isomerism.
- 5.2 Industrial applications of organometallics as catalysts: Homogeneous and heterogeneous catalytic reactions - hydrogenation of olefins (Wilkinson's catalyst) - hydroformylation of olefins using cobalt and rhodium catalysts (Oxoprocess) - olefin isomerization using rhodium catalyst - oxidation of olefin (Wacker process) - cyclo-oligomerisation of acetylenes using Reppe's catalysts- Fischer-Tropsch process (olefins to higher alkanes).

(12 hours)

(12 hours)

(12 hours)

(12 hours)

#### **TEXT BOOKS**

- 1. Solid state Chemistry, D.K. Chakrabharthy Second edition, 2010, New Age International publishers, New Delhi, India
- 2. Structure and Properties Of Solid State Materials, Viswanathan B , 2009, Narosa Publishing House (Publisher), Chennai, Tamilnadu
- 3. Crystallography and crystal structure, G. D. Arora, First Edition, 2000, Published by Sarup& Sons, New Delhi, India
- 4. Fundamentals of crystal chemistry, T.R.N Kutty, J.A.N Tareen, 2000, Universities Press.
- 5. Introduction to Solid State Physics, Charles Kittel, Eighth edition, 2005, John Wiley & Sons, Inc, New York, United Sates.
- 6. Concise Coordination Chemistry, R.Gopalan and V.Ramalingam, 2001, Vikas PublishingHouse Pvt Ltd, New Delhi.
- 7. Introduction to Organometallic chemistry, A.W. Parkins and R.C.Poller,1986, Palgrave Macmillan Publishers Ltd,UK
- 8. Basic Organometallic Chemistry-Concepts, synthesis and applications, Anil Elias and B.D.Gupta, Second edition, 2013, University Press.

#### SUGGESTED READING

- 1. Advanced Inorganic Chemistry, Cotton & Wilkinson, 1972, Third edition, InterScience Publishers, John Wiley and Sons Inc, New York, United Sates.
- 2. Inorganic Chemistry, Principles of Structure and Reactivity, James E Huheey, Fourth Edition, 2006, Pearson Education India.

#### REFERENCES

- 1. Solid state Chemistry and its applications, Anthony R West, Second edition, 2007, John Wiley & Sons, New York, United Sates.
- 2. Inorganic Chemistry, Keith.F.Purcell and john C Kotz, 1980, Holt Saunders International Editions, W.B.Saunders Company, Philadhelpia, Toronto, London

- 1. https://nptel.ac.in/courses/113104014
- 2. https://nptel.ac.in/courses/104101094
- 3. https://nptel.ac.in/courses/104101079
- 4. <u>https://www.coursera.org/lecture/semiconductor-physics/defects-in-crystals-byFXL</u>
- 5. https://www.classcentral.com/course/swayam-organometallic-chemistry-10004

### COURSE TITLE: THERMODYNAMICS AND CHEMICAL KINETICS

Course Code: (will be filled by EO)

(75 hours)

Number of hours/cycle: 5

Nature of Course : Core Theory

Credits: 4

Lear	Learning Objective		
(i)	To understand the concept of partial molar properties, fugacity, activity and activity		
	coefficient in thermodynamics and to know the importance of irreversible processes.		
<b>(ii)</b>	To acquire knowledge about the concept of statistical thermodynamics and its		
	significance.		
(iii)	To know more about the kinetics and mechanisms of chemical transformation.		
(iv)	To apply the theories and concepts of kinetics for homogenous and heterogeneous		
	catalysed reactions.		
<b>(v)</b>	To learn the fundamental concepts in chemical kinetics, enzyme kinetics, surface		
	reactions and fast reactions.		

CO No	Course Outcome	PSO's addressed	CL
	Upon completion of this course, students will be able to	auuresseu	
CO-1	Describe the concept of partial molar properties, fugacity, activity and activity coefficient in chemical thermodynamics and the importance of irreversible processes.	PSO-1	U
CO-2	Explain the concept of statistical thermodynamics and its significance.	PSO-1, PSO-6	Ар
CO-3	Apply the theories of kinetics and mechanisms of chemical transformation	PSO-2	Ар
CO-4	Discuss the fundamental concepts of chemical kinetics, enzyme kinetics and surface reactions	PSO-1, PSO-2	Ар
CO-5	Explain the concepts and kinetics of photochemistry in addition to fast reactions	PSO-1, PSO-2, PSO-3	U

# <u>Unit I</u>

(15 hours)

- 1.1 Chemical thermodynamics: Partial molal properties- partial molar free energy (chemical potential)- partial molar volume- partial molar heat content- their significance- variation of chemical potential with temperature and pressure. Fugacity and its determination- variation of fugacity with temperature and pressure. Concept of activity and activity coefficient, determination of activity and activity coefficients for non-electrolytes.
- 1.2 Non-equilibrium thermodynamics: Postulates of non-equilibrium thermodynamics-entropy production-linear laws relative to fluxes and forces-Onsager's reciprocity relation-relaxation phenomena. Application of irreversible thermodynamics to biological and non- linear systems.

(15 hours)

- 2.1 Statistical thermodynamics: Permutation and combination-laws of probability-distribution laws-Gaussian distribution-ensembles. Microstates and macrostates for distinguishable and indistinguishable particles-thermodynamic probability-velocity space and phase space.
- 2.2 Partition functions: Translational, rotational, vibrational and electronic partition functionsrelationship between partition functions and thermodynamic properties-calculation of equilibrium constants from partition functions– Maxwell-Boltzmann distribution law.
- 2.3 Quantum statistics: Bose-Einstein (B.E.) and Fermi-Dirac (F.D.) distribution equationscomparison of B.E. and F.D. statistics with Boltzmann statistics. Liquid helium and BE condensation- negative absolute temperature.
- 2.4 Heat capacities of monoatomic crystals Einstein theory and Debye theory.

# <u>Unit III</u>

Unit II

- 3.1 Collision theory- effectiveness of collision- reaction cross section.
- 3.2 Reaction mechanisms CTST potential energy surfaces, reaction coordinate. Kinetic isotope effect-principle of microscopic reversibility-detailed balancing. Unimolecular and termolecular reactions.
- 3.3 Reactions in solution- comparison of gas phase reactions with reactions in solutions, factors influencing reaction rates in solution- effect of dielectric constants primary and secondary salt effects. Application of CTST to reactions in solution and diffusion-controlled reactions in solutions (cage effect).

# <u>Unit IV</u>

- 4.1 Homogeneous catalysis: Acid-base catalysis, acidity functions, Zucker-Hammett and Bunnet hypothesis. Enzyme catalysis-Michael Menton kinetics- effect of substrate concentration, temperature and pH on the rate of enzyme catalysed reaction.
- 4.2 Heterogeneous catalysis: Physical adsorption and chemisorption- Lennard-Jones plot. Adsorption isotherms- Langmuir and BET equation-surface area measurement. Role of surface in catalysis-catalysis by semiconductors. Langmuir-Hinshelwood and Eley-Rideal mechanisms.

# <u>Unit V</u>

- 5.1 Photochemistry-Laws of photochemistry-photophysical process (Jablonski diagram)-kinetics -Stern Volmer equation of fluorescence and phosphorescence.
- 5.2. Kinetics of photochemical reactions: Comparative study of thermal and photochemical mechanisms in hydrogen-bromine reaction-thermal decomposition of carbonyl compound (acetaldehyde) Rice Herzfeld mechanisms-explosion limits.
- 5.3 Fast reactions: Methods of studying fast reactions- flow methods continuous, stopped and quenched flow method, relaxation technique and flash photolysis.

(15 hours)

(15 hours)

(15 hours)

# **TEXT BOOKS**

- 1. A Textbook of Physical Chemistry Application of Thermodynamics, K.L.Kapoor, fifth edition, 2020, McGraw Hill India.
- Thermodynamics for students of chemistry, J. Rajaram and J.C. Kuriacose, 1986, Lal Nagin Chand, New Delhi.
  Statistical Thermodynamics by M. C. Gupta,2007, New Age International, Chennai, Tamilnadu.
- 3. Chemical Kinetics, K.J. Laidler, 3<sup>rd</sup> edition, 1987, Pearson.
- 4. Kinetics and Mechanisms of Chemical Transformations, Rajaram & Kuriacose, 1993, Macmillan India Ltd, Delhi.

#### SUGGESTED READING

- 1. Elements of Statistical Thermodynamics, Leonard K. Nash,2<sup>nd</sup> edition, Dover Publications Inc, New York.
- 2. Physical Chemistry, G.M. Barrow, 1988, McGraw Hill, India.
- 3. Chemical Kinetics, Principles and selected topics, I. Amdur and G.G. Hammes, 1986, McGraw Hill, New York.
- Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, C. Kalidas, 2005, New Age International, Chennai, Tamilnadu

#### REFERENCES

- Donald A.McQuarrie and John D.Simon, "Physical Chemistry-A Molecular Approach" 1st Edition, 1998, Viva Books Private Limited, New Delhi.
- 2. Statistical Thermodynamics, B. J. McClelland, 1973, Chapman and Hall.
- 3. Kinetics and Mechanism, 3rd Edition John W. Moore, Ralph G, 1981, Pearson, .
- 4. Kinetics and Mechanism: A Study of Homogeneous Chemical Reactions Arthur Atwater Frost, 1961, Ralph G. Pearson, Wiley,UK

- 1. https://nptel.ac.in/courses/104103112
- 2. <u>https://dituniversity.digimat.in/nptel/courses/video/112105266/L35.html</u>
- 3. https://nptel.ac.in/courses/104106089
- 4. https://nptel.ac.in/courses/104101128
- 5. https://nptel.ac.in/courses/104105041

#### COURSE TITLE: ENVIRONMENTAL CHEMISTRY

Course Code: (will be filled by EO) (75 hours) N

Number of hours/cycle: 5

Credits: 5

#### Nature of Course : Elective Theory

Lear	ming Objective
(i)	To acquire knowledge about the various energy resources, environmental health
	hazards and certain social issues
(ii)	To understand how the various pollutants have contributed to the degradation of the
	environment and the ways by which these effects can be reduced.
(iii)	To determine and calculate simple physicochemical characteristics of water and
	wastewater samples and to discuss the various methods of treating waste water and effluents.
(iv)	To learn about the solid waste management methods, biomedical waste, plastic waste,
	e waste and the waste minimization technologies
<b>(v)</b>	To gain knowledge about the energy recovery from wastes and the various green
	methods as alternatives to control the pollution

CO No	<b>Course Outcome</b> Upon completion of this course, students will be able to	PSO's addressed	CL
CO-1	Classify different types of energy resources, and to analyze various social issues, natural and manmade hazards associated with the environment	PSO-1, PSO-4	U
CO-2	Demonstrate familiarity with common groups of environmental air, soil, water pollutants and its abatement	PSO-3,PSO-4	U
CO-3	Appraise the various strategies and parameters involved in wastewater treatment, industrial pollution abatement in addition to radioactive pollution and its effects	PSO-1, PSO-4	An
<b>CO-4</b>	Adapt sustainable development, different modes of waste management and its control measures	PSO-1, PSO-4, PSO-6	Ар
CO-5	Prioritize the principles involved in green chemistry and the use of green alternative methods in day to day life	PSO-1, PSO-3, PSO-6	E

#### <u>Unit I</u>

(15 hours)

- 1.1 Environmental studies- Definition, scope, importance and need for public awareness.
- 1.2. Energy resources-Renewable and non-renewable energy- principles of generation of electricity from hydroelectric power, tidal power, wind power, geothermal power, solar power, ocean thermal power, fossil fuels and nuclear power.
- 1.3. Natural hazards-Earthquakes, tsunami's, volcanic eruptions, landslides, cyclones and floods. Man-made hazards- improper irrigation and deforestation. Industrial hazards- fire explosion, toxic release and dispersion.
- 1.4. Social issues and the environment: Water conservation and rain water harvesting.

#### (15 hours)

(15 hours)

- 2.1. Structure of earth's atmosphere : Layers of earth's atmosphere-air pollution- sources- oxides of nitrogen, sulphur and carbon, hydrogen sulphide, photochemical smog and dioxins from burning of plastics-ozone layer depletion and consequences- acid rain, greenhouse effect, global warming- analysis of air quality standards and air pollution abatement.
- 2.2. Noise pollution-sources- decibel scale-physiological, psychological, acute and chronic effects- control of noise pollution.
- 2.3. Soil pollution causes, consequences and its effects on human and environment- modern agriculture and its impact on the environment.
- 2.4. Marine pollution- the chemical constituents of sea water organic matter and suspended material - ocean dumping - oil pollution- need for protecting and conservation of marine environment.

#### **Unit III**

- 3.1. Water pollution Sources, analysis of water quality standards-sewage water treatment: different stages of treatment- primary, secondary (trickling filter, activated sludge and oxidation pond) and tertiary or advanced treatment (effluent polishing, removal of plant nutrients (eutrophication/denitrification)- sludge treatment (aerobic and anaerobic digestion process)- sludge disposal.
- 3.2. Pollution control in the following industries: Fertiliser, pulp and paper, tanning and electroplating.
- 3.3. Analysis of pollutants-SO<sub>2</sub>, NO<sub>x</sub>, H<sub>2</sub>S, O<sub>3</sub> and CO- Sum, specific and group parameters-pH, BOD, COD, DOC, TSS, TDS - Analysis of toxic heavy metals- As, Cr, Hg, Pb and Cd.
- 3.4. Radioactive pollution-ionizing and non-ionizing radiation- sources of radioactive pollutionnatural and anthropogenic - biological effect of radiation on human body-radioactive waste management.

#### <u>Unit- IV</u>

- 4.1. Solid waste management: Sources, composition and collection of solid waste- treatmentincineration, composting, sanitary land filling-treatment of organic waste- vermicompostingaerobic and anaerobic composting- steps to sustainability-7R's of waste management.
- 4.2. Biomedical waste: Sources, types of biomedical waste impacts of biomedical waste onenvironment - control measures of biomedical waste.
- 4.3 Plastic waste sources, facts & figures of plastic waste scenarios in national and international effect of plastic waste on environment and humans-control measures of plastic waste.
- 4.4. e-waste: Sources, types of e-waste-impacts of e-waste on environment control measures of e-waste.

5.1. Green chemistry-need for green chemistry- principles of green chemistry- control of environmental pollution by green alternatives- simple emphasis on biosolvents-limonene, methyl soyate-solvents in organic synthesis-ionic liquids, supercritical carbon dioxide. Green

#### Unit-V

(15 hours)

(15 hours)

### <u>Unit-II</u>

quantitative analysis using flower petals as indicator.

5.2. Green chemistry in day-to-day life- green dry cleaning of clothes- green bleaching agentseco-friendly paint - green solution to turn turbid water clear - bioplastics - starch based bioplastics- biofuels-power alcohol, benzol.

#### **TEXT BOOKS**

- 1. Natural Hazards Risk Assessment and Public Policy Anticipating Unexpected, Petak WJ and Allissoon AA , 1982, Springer-Verlag, New York
- 2. Environmental Risk and Hazards, Cuttler SI ,1994, Prentice Hall of India, New Delhi
- 3. Environmental Chemistry , A.K.De, 8th Edition, 2016, New Age Publishers International Pvt Ltd, New Delhi.
- 4. Solid Waste Management, Subash Anand , 2010, Mittal Publication, New Delhi.
- 5. Green Chemistry , V.K. Alluwaliah, 2012, Narosa Publishing House Pvt Ltd, Chennai, Tamilnadu
- 6. E-waste implications, regulations & Management in India and Current, Rakesh Johri, 2008, TERI Press, New Delhi.

#### SUGGESTED READING

- 1. Environmental chemical analysis, Iain L, Marr and Malcom S.Cresser,1982, Blackie Academic & Professional (an Imprint of Chapman & Hall).
- 2. Pollution control in processes industries, S.P.Mahajan, 2003, McGraw Hill Publication, Europe.

#### REFERENCES

- 1. Chemistry of our environment, K.A.Home, 1979, Wiley, NewYork.
- Handbook of Solid Waste Management and Waste Minimization Technologies, Nicholas P Cheremisinoff, 2002, Butterworth-Heineman for Elsevier Science, e-Book ISBN: 9780080507811.

- 1. https://nptel.ac.in/courses/104103020
- 2. https://www.ripublication.com/ijoo17/ijoov11n2\_07.pdf

#### SEMESTER-II

#### **COURSE TITLE: ORGANIC REACTION MECHANISM**

Course Code: (will be filled by EO)

(60 hours)

Number of hours/cycle: 4

Nature of Course : Core Theory

Credits: 4

Learning Objective		
To learn the concept and mechanism of nucleophilic substitution at aliphatic and aromatic		
carbons.		
To understand the concepts of electrophilic substitution reactions and rearrangement		
reactions.		
To study the elimination, electrophilic and nucleophilic addition reactions and their		
mechanism		
To learn the concepts of organic photochemistry, pericyclic reactions and mechanisms.		
To understand the mechanisms of oxidation and reduction reactions.		

CO No	<b>Course Outcome</b> Upon completion of this course, students will be able to	PSO's addressed	CL
CO-1	Apply the concept of nucleophilic substitution in aliphatic and aromatic carbons	PSO-1, PSO-2	Ар
CO-2	Apply and analyze the electrophilic substitution in aromatic and aliphatic carbons and rearrangement reactions	PSO-1, PSO-2	An
CO-3	Explain the electrophilic, nucleophilic addition and elimination reactions	PSO-1, PSO-2, PSO-5	Ар
CO-4	Recognize and apply the mechanism of photochemistry and pericyclic reactions	PSO-2, PSO-5	U
CO-5	Analyze different kind of reagents related to the functional group transformation, oxidation and reduction	PSO-1, PSO-2,	An

#### <u>Unit I</u>

(12 hours)

- 1.1. Nucleophilic substitution at carbon: S<sub>N</sub>1, S<sub>N</sub>2, S<sub>N</sub>i, nucleophilic substitution at vinylic and allylic carbons. (S<sub>N</sub>1', S<sub>N</sub>2'), tetrahedral mechanism, solvolytic reactions, neighbouring group participation, ambident nucleophiles, mechanisms of ester hydrolysis and trans esterification.
- 1.2. Aromatic nucleophilic substitution in aryl halides by Meisenheimer complex mechanism and benzyne mechanism-various methods of benzyne generation and reactions of benzynes. Reactions of aryldiazonium salts, Zeigler alkylation, vicarious nucleophic substitution (VNS)-Chichibabin, Balz-Schiemann and Von Ritchter reaction.

#### (12 hours)

- 2.1. Electrophilic substitution in aliphatic carbon:  $S_E1$ ,  $S_E2$  and  $S_Ei$  mechanisms, electrophilic substitution via enolization, Stork-enamine reaction. Electrophilic displacements at an aromatic carbon: General mechanism, kinetics of  $S_E2$  -Ar reactions. Ortho- para selectivity ratio, Vilsmeyer formylation, Gatterman-Koch reaction and Jacobson reaction.
- 2.2. Molecular rearrangements: Carbon to carbon migration Wagner-Meerwein and Pinacol-Pinacolone. Carbon to nitrogen migration - Beckmann and Hofmann. Carbon to oxygen migration - Baeyer-Villiger and Dakin. Rearrangements proceeding through carbanions-Demjanov, dienone-phenol, Neber and Favorskii.

#### <u>Unit III</u>

- 3.1. Elimination reactions:  $E_1$ ,  $E_2$  and  $E_1cB$  mechanisms Saytzeff and Hoffman elimination stereochemistry of  $E_2$ , intramolecular pyrolytic elimination ( $E_i$ ) Chugaev and Cope elimination. Competition between elimination and substitution reactions.
- 3.2. Addition reactions: Electrophilic addition to alkenes, kinetics, effect of structure, isotope effects, orientation and stereochemistry, the nature of the intermediates, ozonolysis, hydroboration, additions to dienes, alkynes (halogenation and hydrogenation) and allenes. Diels-Alder and 1,3-dipolar addition reactions.
- 3.3 Nucleophilic addition to multiple bonds: Mannich, aldol condensation, Stobbe, Cannizzaro and Wittig reaction.

### <u>Unit IV</u>

- 4.1. Organic photochemistry: General principles- photochemistry of carbonyl compounds-Norrish Type I and Type II reactions. Photoreduction of ketones- Paterno-Buchi reaction, di-pi-methane and Barton rearrangement. Cis-trans isomerization, photo sensitization and Hofmann Loffler Freytag reaction.
- 4.2. Pericyclic reactions: Woodward-Hofmann rule, use of FMO and correlation diagram to electrocyclic (butadiene-cyclobutene system), cyclo-addition ((4+2) and (2+2)) systems), sigmatropic and cheletropic reactions.

# <u>Unit V</u>

- 5.1. Reagents in organic synthesis and functional group transformation-complex metal hydrides, lithium dimethylcuprates, lithium di-isopropylamide (LDA), 1,3 dithiane (umpolung synthesis) and trimethylsilyliodide.
- 5.2.Carbon-carbon bond formation through coupling reactions Heck, Suzuki, Stille, Sonogoshira and Negishi.
- 5.3. Oxidation and reduction reactions: Oxidation of alcohols using chromic acid- DMSO-DCC- hydroxylation of olefins (both cis and trans), oxidation of alkenes using organoboranes, manganese dioxide, permanganate, mercuric acetate, lead tetraacetate and SeO<sub>2</sub>. Cleavage of 1,2-glycols using periodate, catalytic hydrogenation, metal hydride reduction-NaBH<sub>4</sub>, NaBH<sub>3</sub>CN, LiAlH<sub>4</sub> and Birch reduction.

# (12 hours)

(12 hours)

(12 hours)

<u>Unit II</u>

#### **TEXT BOOKS**

- 1. Organic Reaction Mechanism, V K Alhuwalia and Rakesh Kumar Parashar, IV Edition, 16<sup>th</sup> Reprint, 2019, Alpha Narosa Publishing House, New Delhi, India
- 2. Photochemistry and Pericyclic reactions, Jagdamba Singh and Jaya singh, III Revised Edition, 2012, New Age International Publishers.
- 3. Organic Photochemistry, J.M.Coxon, B.Halton, 2011, Cambridge University Press.
- 4. A Guidebook to Mechanism in Organic Chemistry, Peter Sykes, VI Edition, 2020, Pearson India Education Services, India.
- 5. Reaction Mechanism in organic chemistry, S.M.Mukerji , S.P.Singh. 2014, Laxmi Publications.

#### REFERENCES

- 1. Writing Reaction Mechanisms in Organic Chemistry by Audrey Miller, Philippa H. Solomon, II Edition, 1999, Elsevier Science & Technology Books
- 2. Name reactions and reagents in organic synthesis, Bradford P. Mundy, Michael G. Ellerd and Frank G. Favaloro, Jr, Second Edition, 2005, Wiley Inter-science
- 3. Modern Methods of Organic Synthesis, William Carruthers and Iain Coldham, IV Edition, 2020.
- 4. Advanced Organic Chemistry Part (A & B) Francis A Carey and Richard J Sundberg, Fifth edition, 2007, Springer, New York, USA.
- 5. Organic Synthesis, Michael B Smith, III Ed, 2010, Elsevier, USA.

# SUGGESTED READING

- 1. March's Advanced Organic Chemistry, Michael B Smith, Jerry March, 2016, Wiley Students Edition, India.
- 2. Organic Chemistry Structure and Function, Peter Volhardt, Neil Schore, 8<sup>th</sup> Edition, 2018. W.H.Freeman, Macmillan Learning, NewYork.
- 3. Advanced Organic Chemistry Structure and Mechanisms, Ashutosh Kar, 1<sup>st</sup> Edition, 2017, MedTech.

- 1. https://nptel.ac.in/courses/104101115
- 2. <u>https://nptel.ac.in/courses/104101005</u>
- 3. <u>https://onlinecourses.nptel.ac.in/noc22\_cy25/preview</u>
- 4. <u>https://nptel.ac.in/courses/104103023</u>

## COURSE TITLE: ANALYTICAL TECHNIQUES IN CHEMISTRY

Course Code:(will be filled by EO)

(45 hours)

Number of hours/cycle: 3

Nature of Course : Core Theory

Credits: 4

Lear	rning Objective
(i)	To acquire knowledge about the use of UV-Visible spectrophotometric method for the estimation of various transition metals using specific reagents.
(ii)	To predict, interpret and identify the spectral patterns of different molecules using multiprobe NMR techniques
(iii)	To understand the concepts of various spectral techniques like UV, IR, NMR, mass and Mossbauer and to apply these techniques for the quantitative and structural analysis in organic and inorganic compounds
(iv)	To understand the basic principles and applications of separation, thermo and spectroanalytical techniques
( <b>v</b> )	Gain knowledge about the synthesis of organic and inorganic compounds by irradiation radiometric analysis and radiography

CO	Course Outcome	PSO's	CL
No	Upon completion of this course, students will be able to	addressed	
CO-1	Describe the principle, working and instrumentation of UV-	PSO-1,	Ар
	visible, IR and Raman spectroscopic techniques	PSO-5,	
		PSO-6,	
<b>CO-2</b>	Understand the principle, instrumentation, structural	PSO-1,	Ар
	applications and spectral interpretation of various molecules	PSO-5,	
	using multiprobe NMR and NQR spectroscopic techniques.	PSO-6,	
CO-3	Identify, formulate and recognize various spectroscopic	PSO-1,	An
	techniques like UV-Visible, IR, NMR, ESR, Mass and	PSO-5,	
	Mossbauer in the structural elucidation of molecules	PSO-6,	
	through simple problems.		
<b>CO-4</b>	Predict the configuration of simple coordination complexes	PSO-4,	An
	and understand the different kinds of separation and	PSO-5	
	thermoanalytical methods.		
CO-5	Explain the significance of electroanalytical techniques,	PSO-4,	An
	neutron activation analysis and the synthesis of molecules	PSO-5	
	using irradiation radiometric analysis including radiography		

#### <u>Unit I</u>

(9 hours)

- 1.1. Optical methods of analysis: Colorimetric analysis-importance and applications of Beer-Lambert's law. UV-visible spectrophotometric analysis - principle - single and double beam instruments - instrumentation- solvent effects on electronic transitions.
- 1.2. Spectrophotometric determination of iron in various oxidation states using ammonium thiocyanate and 1,10 phenanthroline as ligands manganese using formaldoxime and picolinaldehyde nicotinoyl hydrazone (PANH) as ligands titanium using hydrogen

peroxide in presence of xylenol orange and cobalt as cobalt (II)-benzoin oxime complex. Analysis of organic compounds - olefins, ketones and aromatics by UV- visible spectroscopy (Woodward - Fieser rules).

- 1.3. Infrared spectrophotometric analysis principle instrumentation vibrational frequencies and factors affecting them fingerprint region group frequencies molecular structure determination.
- 1.4. Raman spectra-principle, instrumentation mutual exclusion principle-diagnostic structural analysis.

#### <u>Unit II</u>

(9 hours)

(9 hours)

- 2.1. Nuclear magnetic resonance spectroscopy- <sup>1</sup>H NMR- principle, instrumentation-double resonance nuclear overhauser effect (NOE) structure determination of simple organic molecules like ethanol, aldehydes, amines, acids and esters-NMR shift reagents
- 2.2. <sup>13</sup>C NMR principle of OFF resonance decoupling comparison with <sup>1</sup>H NMR chemical shifts (aliphatic, olefinic, alkynic, aromatic and carbonyl compounds)
- 2.3. <sup>31</sup>P, <sup>19</sup>F applications in structural problems based on number of signals in molecules namely oxyacids of phosphorous, HPF<sub>2</sub>, P<sub>4</sub>S<sub>3</sub>, TiF<sub>4</sub>, SF<sub>4</sub>, fac-Rh (PPh<sub>3</sub>)<sub>3</sub>Cl<sub>3</sub>, P<sub>4</sub>N<sub>4</sub>Cl<sub>6</sub>(NHC<sub>6</sub>H<sub>5</sub>)<sub>2</sub>, PF<sub>5</sub> and H<sub>2</sub>PF<sub>3</sub>.

### <u>Unit III</u>

- 3.1. Electron spin resonance principle, instrumentation- hyperfine splitting- zero field splitting-Kramers degeneracy-applications of ESR in study of coordination complexes like bis(salicylaldimine) copper(II) complex and [Cu(bpy)<sub>3</sub>]<sup>2+</sup>. ESR applications to radicals and ions - methyl, benzene and biphenyl radicals- naphthalene, pyrazine and p-benzosemiquinone ions.
- 3.2. Mass spectrometry principle, instrumentation fragmentation patterns organic molecular structural determination applications in the study of inorganic compounds (metal carbonyls).
- 3.3. Mössbauer spectroscopy principle, instrumentation and applications (Fe and Sn).
- 3.4. Structure determination of organic molecules like 2-butanone, isopropyl cyanide, o-nitrophenol, 2-butanoic acid, mesitylene, phenyl acetaldehyde using combined UV-visible, IR, NMR and mass spectral data with examples.

# <u>Unit IV</u>

- 4.1. ORD and circular dichroism cotton effect axial-haloketone rule octant rule -applications.
- 4.2. Flame photometry, atomic absorption analysis (AAS) and atomic fluorescence- principle and applications.
- 4.3.Thermal methods: Thermogravimetric (TGA), differential thermal analysis (DTA), thermometric titrations and differential scanning calorimetry (DSC) instrumentation and applications.
- 4.4 Chromatographic methods: TLC, column, gas, ion exchange, HPLC and gel permeation chromatography principles and applications.

(9 hours)

#### (9 hours)

### <u>Unit V</u>

- 5.1 Electroanalytical methods: Polarography principle, instrumentation and applications.
- 5.2 Derivative polarography: Cyclic voltametry(CV), amperometric titration principle and applications.
- 5.3 Radiochemical methods: Hot atom chemistry Szilard-Chalmers process, chemistry of recoil atoms, chemical effects of radioactive decay and solvated electron.
- 5.4 Uses of radiations in the study of matter, neutron activation analysis, dilution analysis, dosimetry, synthesis of organic and inorganic compounds by irradiation radiometric analysis and radiography.

# **TEXT BOOKS**

- 1. Physical Methods in chemistry, Russell's Drago, Second edition, 1977, Thomson Learning, London, UK.
- 2. Physical Methods in Inorganic chemistry, Russell's Drago, 2012, East West Press Pvt. Ltd.-New Delhi.
- 3. Fundamentals of Molecular spectroscopy, C.N. Banwell,Forth Edition, 1991, McGraw HillPublication, United states.
- 4. Organic spectroscopy, William Kemp, Third Edition, 1991, Palgrave Macmillan, USA.
- 5. Elementary Organic Spectroscopy, Y.R.Sharma, Fifth Edition, 2013, S Chand Company andPvt Ltd, Chennai.
- 6. Analytical chemistry, J.G.Dick, 1973, McGraw Hill Publication, United Sates.
- 7. Instrumental Methods of Chemical Analysis, Gurdeep R. Chatwal and Sham K Anand, 2011, Himalaya Publishing House, Chennai, Tamilnadu

# REFERENCES

- 1. Spectrometric identification of organic compounds, Robert Silverstein, 2014, Wiley Publishers, Hoboken, New Jersy
- 2. Fundamentals of Analytical chemistry, Skoog Douglas A, West M Donald, Holler F James, Crouch Stanley R, 9<sup>th</sup> Edition, 2014, Belmont, CA: Brooks/Cole Cengage Learning.

# SUGGESTED READING

- 1. Physical Methods for Chemists, Russell S Drago, Second edition, 1977, Saunders College Publishing, Harcourt Brace Jovanovich College Publishers, California
- 2. Instrumental methods of analysis, Willard Merritt and Dean and Settle, 7<sup>th</sup> Edition, 2001, Wadsworth Publishing Co Inc, Belmont CA.
- 3. Instrumental methods of analysis, B.K.Sharma, 2011, Krishna Prakashan Media P Ltd, Meerut, Uttar Pradesh.

- 1. <u>https://archive.nptel.ac.in/courses/104/108/104108078/</u>
- 2. <u>https://onlinecourses.swayam2.ac.in/ugc19\_bt16/preview</u>
- 3. <u>https://onlinecourses.nptel.ac.in/noc20\_cy08/preview</u>
- 4. <u>https://onlinecourses.nptel.ac.in/noc22\_cy45/preview</u>

#### **COURSE TITLE: GROUP THEORY AND QUANTUM MECHANICS**

Course Code: (will be filled by EO)

(60 hours)

Number of hours/cycle: 4

Nature of Course : Core Theory

Credits: 4

Lear	Learning Objective			
(i)	To learn the concepts of group theory and its applications to simple molecules.			
( <b>ii</b> )	To construct the character table and their use in prediction IR and Raman active			
	fundamental vibrational modes, hybridization and electronic spectrum.			
(iii)	To understand the fundamental of quantum mechanics and develop the skills to apply			
	required mathematics for solving quantum mechanical problems.			
(iv)	To know the Schrödinger wave equation and their importance for a simple systems.			
( <b>v</b> )	To learn and appreciate the quantum mechanical approach to the atomic and molecular			
	electronic structure.			
CO	No Course Outcome PSO's CL			

CO No	Course Outcome	PSO's	CL
	Upon completion of this course, students will be able to	addressed	
CO-1	Discuss about the fundamentals of group theory and its	PSO-1,	Ар
	applications to simple molecules.	PSO-6	-
CO-2	Construct the character table and utilize their use in	PSO-6	An
	prediction IR and Raman active fundamental vibrational		
	modes, hybridization and electronic spectrum.		
CO-3	Explain the fundamentals of quantum mechanics and its	PSO-1,	U
	application to simple systems.	PSO-3	
<b>CO-4</b>	Describe the applications of basic mathematics in quantum	PSO-1,	Ар
	chemistry.	PSO-6	-
CO-5	Predict the electronic structure of atoms and molecules in	PSO-1	An
	terms of quantum mechanics.		

# <u>Unit I</u>

(12 hours)

(12 hours)

- 1.1 Principles of group theory -symmetry elements- symmetry operations in molecules.
- 1.2 Properties of group abelian, non abelian and cyclic groups multiplication tables classes subgroups identification of point groups of molecules and Schoenflies symbols optical activity and dipole moment on the bases of point groups.
- 1.3 Matrices for symmetry operations reducible and irreducible representations-direct product representation great orthogonality theorem (GOT) and its consequences– construction of character table for  $C_{2v}$ ,  $C_{3v}$ ,  $C_{2h}$  and  $D_2$  point groups.

# <u>Unit II</u>

- 2.1 Applications of group theory standard reduction formula relating reducible and irreducible representations use of character tables in predicting hybridisation of molecules like tetrahedral, triangular planar and square planar systems.
- 2.2 Symmetry selection rules in fundamental vibrational modes of H<sub>2</sub>O, NH<sub>3</sub>, trans-N<sub>2</sub>F<sub>2</sub> and BF<sub>3</sub>-

integration method-mutual exclusion principle.

2.3 Symmetry selection rules for electronic transition to ethylene and carbonyl chromophore (formaldehyde) - construction of projection operators and molecular orbitals by symmetry adapted linear combinations (SALC) to benzene and naphthalene.

# <u>Unit III</u>

- 3.1 Introduction to quantum mechanics-general principles of classical mechanics and its failurepostulates of quantum mechanics.
- 3.2 Functions and operators eigen functions and eigen values. Hamiltonian, linear, angular momentum and commutation operators.
- 3.3 Application of quantum mechanics particle in a 1-D and 3-D boxes, simple harmonic oscillator rigid rotor, hydrogen atom atomic units.

# <u>Unit IV</u>

(12 hours)

(12 hours)

(12 hours)

- 4.1 Degeneracy and degenerate wave functions, quantum mechanical tunnelling, s hapes and nodal properties of orbitals space quantisation.
- 4.2 Approximation methods-variation and perturbation method (time-independent)-simple examples.
- 4.3 Many electron atoms- helium atom, general principle of setting up wave function for other many electron atoms Pauli's exclusion principle.
- 4.4 Slater type orbitals-Hartree and Hartree-Fock SCF methods-Born-Oppenheimer approximation.

# <u>Unit V</u>

- 5.1 HMO theory calculations-evaluation of coefficients and eigen values for ethylene, allyl system and 1,3-butadiene. Delocalization energy, electron density,  $\pi$ -bond order and free valence index.
- 5.2 Extended HMO theory-application to simple ring molecules containing hetero atoms.
- 5.3 Bonding- VB and MO treatment of  $H_2$  and  $H_2^+$ . MO models of  $C_2$ ,  $N_2$ ,  $O_2$  and CO.

# **TEXT BOOKS**

- 1. Symmetry and spectroscopy of molecules by K.Veera Reddy, 1988, New Age International.
- 2. A Simple approach to group theory in Chemistry by S.Swarnakakshmi, 2008, University press.
- 3. Quantum Chemistry, Levine, 4<sup>th</sup> edition, 1983, Allyn & Bacon Inc.
- 4. Quantum Chemistry, R.K. Prasad, 1992, New Age, India, 1992.
- 5. Quantum Chemistry, D.A. McQuarrie, University Science Books, Mil Valley.

#### SUGGESTED READING

- 1. Chemical Application of Group Theory, 2<sup>nd</sup> edition, 1971, F.A. Cotton, John Wiley & Sons.
- 2. Group Theory in Chemistry by V. Ramakrishnan and M.S. Gopinathan, 1988, Vishal

Publications.

- 3. Quantum Chemistry through problems and Solutions by R.K. Prasad, 1997, New Age International Publishers, New Delhi.
- 4. Physical Chemistry, P.W. Atkins and Julio de Paula, 7<sup>th</sup> edition, 2002, Oxford University Press.
- 5. Physical chemistry A Molecular Approach, Donald A. McQuaric & John D. Simon, 1998, Viva Books Pvt. Ltd.. New Delhi.

### REFERENCES

- 1. Group Theory and its applications to Chemistry, K. V. Raman, 1990, McGraw Hill.
- 2. Molecular Symmetry and Group Theory. A Programmed Introduction to Chemical Applications, Alan Vincent, 1977, John and Willy & Sons Ltd.
- 3. Fundamentals of quantum chemistry, Anantharaman, 2001, Macmillan India Limited.
- 4. An Introduction to Quantum Mechanics of Chemical Systems, R.P. Rastogi and V.K. Srivastava, 1986, Oxford &: IBH Publishing Co., New Delhi.

- 1. http://www.digimat.in/nptel/courses/video/104101094/L60.html
- 2. https://www.digimat.in/nptel/courses/video/104101094/L01.html
- 3. https://www.digimat.in/nptel/courses/video/104108057/L11.html
- 4. <u>https://onlinecourses.nptel.ac.in/noc22\_cy33/preview</u>
- 5. https://nptel.ac.in/courses/104101124

#### **COURSE TITLE: POLYMER CHEMISTRY**

Course Code: (will be filled by EO)

(75 hours)

Number of hours/cycle: 5

Nature of Course : Elective Theory

Credits:	5
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Lear	Learning Objectives		
(i)	To impart fundamental knowledge on chemistry of polymers.		
( <b>ii</b> )	To learn the synthesis of various polymer synthesis techniques and understand the		
	importance of additives in polymers.		
(iii)	To learn the concepts of Glass transition temperature and crystallinity of polymers		
(iv)	To gain fundamental knowledge of biopolymers and their applications in various fields.		
<b>(v)</b>	To understand the different types of polymer degradation methods		

CO No	Course Outcomes	PSO's	CL
	Upon completion of this course, students will be able to	addressed	
CO-1	Explain the basic concepts, classification and mechanism of	PSO-1,	U
	different types of polymerization	PSO-6	
CO-2	Enumerate the numerous methods of molecular weight	PSO-3	U
	determination and various polymer synthesis techniques and	PSO-5	
	understand the importance of additives in polymers		
CO-3	Apply the concepts of glass transition temperature and	PSO-1,	Ар
	crystallinity of polymers with respect to the polymer material	PSO-3	-
	applications in various fields.		
<b>CO-4</b>	Acquire knowledge on various biopolymers, surface coatings	PSO-1,	E
	and surface modification of biomaterials for improved	PSO-4	
	functionality		
CO-5	Understand the different types of polymer degradation	PSO-4	U
0.00	enderstand die anterent types of porjiner degradation	1001	

#### <u>Unit I</u>

(15 hours)

- 1.1 Basic concepts of polymer chemistry: Repeat unit, functionality, degree of polymerisation, classification, stereochemistry of polymers and nomenclature of stereoregular polymers.
- 1.2 Types of polymerization : Chain polymerisation, free radical polymerisation, ionic polymerisation and its kinetics. Coordination polymerisation Zeigler- Natta catalyst, step polymerisation and ring opening polymerisation.
- 1.3 Copolymerisation: Block and graft copolymers preparation and polymer blends.

# <u>Unit II</u>

(15 hours)

- 2.1 Molecular weight and size: Number average and weight average molecular weights, polydispersity and molecular weight distribution in polymers, the practical significance of polymer molecular weights and size of polymers.
- 2.2 Molecular weight determination gel permeation chromatography light scattering viscometry

- molecular weight distribution curve.

2.3 Polymerisation techniques: Bulk, solution, suspension and emulsion polymerisation - melt, solution and interfacial polycondensation - solid and gas phase polymerisation.

## <u>Unit III</u>

(15 hours)

- 3.1 The glassy state and glass transition temperature influencing factors (main chain structure, side groups, H-bonding, molecular weight, plasticisation) importance of glass transition temperature.
- 3.2 Crystallinity in polymers: Polymer crystallisation-structural and other factors affecting crystallisability-effect of crystallinity on the properties of polymers.
- 3.3 Additives for polymers: Fillers, plasticisers, thermal stabilizers, photo stabilizers, antioxidants and colourants.
- 3.4 Effect of chemical structure on mechanical, e lectrical and optical properties of polymers.

## <u>Unit IV</u>

(15 hours)

(15 hours)

- 4.1. Biodegradable polymer materials: Definition, structures and methods of preparation biodegradable polymers from renewable resources-poly lactic acid (PLA)-poly hydroxy alkanoates (PHA)-thermoplastic starch (TPS)-other compostable polymers from renewable resources- cellulose-chitosan-proteins. Biodegradable polymers from petrochemical sources-aliphatic polyesters and copolyesters-aromatic polyesters and copolyesters-poly capro lactone-PCL.
- 4.2 Biopolymer films and composite coatings- mechanism of film formation- film-application stages and methods for testing films- selecting biopolymers for specific applications- edible protective films- packaging materials fit for human consumption- inclusion of food additives within edible coatings.
- 4.3 Polymeric biomaterials: Polymeric biomaterials in ophthalmology- polymeric contact lens and polymeric artificial cornea. Polymeric biomaterials in orthopedics-polyethylene, polyacrylates and natural polymers.

## <u>Unit V</u>

- 5.1 Polymer degradation: Types of degradation- thermal, mechanical, photo, hydrolytic and oxidative degradation.
- 5.2 Polymer biodegradation: modes of biological degradation enzymatic degradation of biopolymers (poly saccharides, proteins, nucleic acids) and synthetic polymers microbial degradation of synthetic polymers.

## **TEXT BOOKS**

- 1. Introduction to Polymers, Robert J. Young and Peter A. Lovell, Third Edition, 2011, CRC Press.
- 2. Text book of Polymer Science, Fred W. Billmeyer, Third Edition, 2007, Wiley India.
- 3. Polymer Science, V R Gowariker, N V Viswanathan and Jayadev Sreedhar, 2019, New Age

International Publishers.

- 4. Handbook of Biopolymers and Biodegradable Plastics Properties, Processing and Applications, Sina Ebnesajjad, 2013, Elsevier Publication.
- 5. A first course in Polymer Chemistry, Alexander A Stepikheyev, Varvara A Derevitskaya and Grigory L Slonimsky, 1971, University press of the Pacific publisher.

## SUGGESTED READING

- 1. Polymer Chemistry A Practical Approach, Fred J. Davis, First Edition, 2004, Oxford University Press.
- 2. Introduction to Polymer Chemistry, Charles E. Carraher, Jr, Fourth Edition, 2017, CRC Press.
- 3. Polymer Chemistry, Paul C. Hiemenz, Timothy R Lodge, Second Edition, 2007, CRC Press.
- 4. Polymer Chemistry, Sebastian Koltzenburg, Michael Maskos, Oskar Nuyken, Springer-Verlag Berlin Heidelberg.

## REFERENCES

- 1. Principles of polymer science, P.Bahadur N.V Sastry, 2002, Narosa Publishing House.
- 2. Polymer Science and Technology, Joel R. Fried, Third Edition, 2014, Prentice Hall Publisher.
- 3. Chemical and Physical properties of polymers,2005, Gennady E.Zaikov and Ryszard Kozlowski, Nova Publishers,.
- 4. Natural fibres, Biopolymers and biocomposites, Amar.K.Mohanty, Manjusri Misra and Lawrence T.Drzal, First Edition, 2005, CRC Press.

## **ONLINE SOURCES**

- 1. https://nptel.ac.in/courses/105106205
- 2. https://nptel.ac.in/courses/104105124
- 3. https://nptel.ac.in/courses/104105039
- 4. https://nptel.ac.in/courses/113105077
- 5. https://nptel.ac.in/courses/113105028

#### SEMESTER-III

## COURSE TITLE: CHEMISTRY OF NATURAL PRODUCTS

Course Code: (will be filled by EO)

(45 hours)

Number of hours/cycle: 3

and

Nature of Course : Core Theory

#### Credits: 4

Lear	rning Objective		
(i)	To understand the chemistry of heterocyclic compounds, natural pigments		
	carbohydrates.		
<b>(ii)</b>	To learn the structural aspects of terpenes and steroids.		
(iii)	To study the chemistry of alkaloids and antibiotics.		
(iv)	To learn the synthetic and structural aspects of vitamins and proteins.		
( <b>v</b> )	To understand the synthetic methodology and biosynthesis of natural products		

CO No	Course Outcome	PSO's	CL
	Upon completion of this course, students will be able to	addressed	
CO-1	Describe the synthesis and reactions of heterocyclic compounds, pigments and carbohydrates	PSO-1, PSO-2	U
CO-2	Explain the chemistry of terpenes and steroids	PSO-1, PSO-2	An
CO-3	Deduce the importance of chemistry of alkaloids and antibiotics	PSO-1, PSO-2, PSO-6	Ар
CO-4	Discuss the structure and synthesis of various vitamins and amino acids	PSO-1, PSO-2, PSO-6	U
CO-5	Apply the concepts of the chemistry of protection and deprotection for the functional groups in biosynthetic routes of terpenes, alkaloids and proteins.	PSO-1, PSO-2, PSO-6	Ар

#### <u>Unit I</u>

(9 hours)

- 1.1 Heterocyclic compounds: Structure, preparation, properties and reactions of indole, quinoline and isoquinoline.
- 1.2 Natural pigments: Anthocyanins general methods of determining structure and synthesis cyanin and hirsutine chlorides. Flavones and flavanols general method of determining structure and synthesis Quercetin Isoflavones.

1.3 Carbohydrates: Structural elucidation of sucrose - structural difference between starch and cellulose.

#### <u>Unit II</u>

(9 hours)

- 2.1 Terpenes: Classification, structural elucidation by chemical degradation and synthesis of  $\alpha$ -pinene, zingiberene,  $\beta$ -carotene.
- 2.2 Steroids: Synthesis of cholesterol structural elucidation and synthesis of estrone and progesterone.

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# 3.1 Alkaloids: Classification, structural elucidation by chemical degradation and synthesis of papaverine, morphine and reserpine.

3.2 Antibiotics: Structure and synthesis of chloramphenicol, penicillin, streptomycin and terramycin.

## <u>Unit IV</u>

**Unit III** 

- 4.1 Vitamins: Structure and synthesis of vitamin A,  $B_1$ , C, D, E and K.
- 4.2 Amino acids Synthesis of α -amino acids (Strecker and Gabriel synthesis)- peptides synthesis of dipeptides and polypeptides (Merrifield resin synthesis)-end group analysis structure of proteins primary, secondary, tertiary and quaternary. Nucleic acids purine and pyrimidine bases nucleosides and nucleotides– structure of DNA and RNA.

## <u>Unit V</u>

- 5.1 Synthetic methodology: Illustration of protection and deprotection of groups in synthesis (hydroxyl, amino, carboxyl, and carbonyl- groups) synthesis of target molecules based on disconnection and synthon (acceptor and donor), chiron approach. -retrosynthetic analysis (FGI, FGA, FGR)-umpolung reactions.
- 5.2 Biosynthesis: Biosynthetic routes for terpenes, alkaloids and proteins.

## TEXT BOOKS

- 1. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry of Natural Products, I.L Finar, 5<sup>th</sup> edition, 2002, Pearson Education India.
- 2. Organic Chemistry on Natural Products, G. K. Chatwal, Vol. 1, 2009, Himalaya Publishing House, Mumbai
- 3. Organic Chemistry on Natural Products, G. K. Chatwal, Vol. 2, 2009, Himalaya Publishing House, Mumbai
- 4. Chemistry of Organic Natural Products, O. P. Agarwal, Vol. 1, 1997, Goel Publishing House, Meerut.
- 5. Chemistry of Organic Natural Products, O. P. Agarwal, Vol. 2, 1997, Goel Publishing House, Meerut.

## SUGGESTED READING

- 1. Natural Products Chemistry Sources, Separations, and Structures, Raymond Cooper George Nicola. 2015, CRC Press.
- 2. Chemistry of Plant Natural Products, Stereochemistry, Conformation, Synthesis, Biology, and Medicine, Sunil Kumar Talapatra, Bani Talapatra, 2015, Springer.

(9 hours)

(9 hours)

(9 hours)

#### REFERENCES

- 1. Chemistry of Terpenes and Terpenoids, A.A. Newman, 1972, Academic Press Inc
- 2. Natural Products Chemistry, Koji Nakanishi, Toshio Goto, Shô Itô, Volume 1, 1st Edition,1974, Elesevier.
- 3. Chemistry of the alkaloids, S. W Pelletier, 1970, Van Nostrand Reinhold Inc, United States.
- 4. Chemistry of the Steroids, Charles W. Shoppee, 1st edition, 1995, Springer.
- 5. Introduction to carbohydrate chemistry, Guthrie and Honeyman's, 4th edition, 1974, Clarendon Press, New York
- 6. Heterocyclic Chemistry , John A. Joule , Keith Mills, 5th Edition Wiley Publications, New York .
- 7. The chemistry of flavonoid compounds, T. A Geissman, First American Edition, 1962, Macmillan, United Kingdom

#### **ONLINE RESOURCES**

- 1. <u>https://www.coursera.org/lecture/bioinformatics-methods-2/lecture-5ZHrb</u>
- 2. <u>https://onlinecourses.swayam2.ac.in/cec20\_bt12/preview</u>
- 3. <u>https://onlinecourses.nptel.ac.in/noc22\_cy30/preview</u>

### COURSE TITLE: ELECTROCHEMISTRY AND SPECTROSCOPY

Course Code: (will be filled by EO)

(45 hours)

Number of hours/cycle: 3

Nature of Course : Core Theory

#### Credits: 4

Lear	Learning Objective		
(i)	To understand the behaviour of electrolytes in solution		
(ii)	To know the structure of the electrode surface and the applications of electrode process		
(iii)	) To study the interaction of electromagnetic radiations with mater and its significance.		
(iv)	To know the importance and essential concepts involved in different branches of		
	spectroscopy.		
( <b>v</b> )	7) To understand and appreciate the concepts of molecular spectroscopy like electronic,		
	rotational, vibrational and NMR spectroscopy and its applications		

CO No	Course Outcome	PSO's	CL
	Upon completion of this course, students will be able to	addressed	
CO-1	Discuss the behaviour of electrolytes and their activity	PSO-1	U
	coefficients in solution.		
CO-2	Explain the structure of the electrode surface and the various	PSO-3,	Ap
	applications of electrode process.	PSO-4	
CO-3	Examine the quantization of energy and the interaction of	PSO-1	An
	electromagnetic radiation with matter.		
<b>CO-4</b>	Describe the fundamentals of molecular spectroscopy and	PSO-1,	U
	their mathematical foundations in different branches of	PSO-3,	
	spectroscopy.	PSO-5	
CO-5	Enumerate the recent advancements in NMR spectroscopy	PSO-1,	Ар
	and to apply the concepts in the study of molecular structure.	PSO-3,	
		PSO-6	

#### <u>Unit I</u>

(9 hours)

- 1.1 Ion-solvent interaction: Born's treatment of ion solvent interaction its validity and modification-a brief account of ion-dipole and ion-quadrupole models of ion-solvent interactions.
- 1.2 Ion-Ion interactions and activity coefficients: Debye Huckel ionic atmosphere model of the strong electrolytes derivation of Debye Huckel limiting law validity of the equation-extension of Debye Huckel equation significance of the activity coefficient of electrolytes.
- 1.3 Ion transport in solutions: Theory of strong electrolytes for electrolytic conduction- Debye Huckel ion atmosphere model - derivation of the Onsager equation - validity of the equation - modification of the Onsager equation.

1.4 Ion association: Bjerrum treatment of association - Bjerrum ion association constant - factors influencing ion association - effect of ion association on conductivity and activity coefficient of electrolytes in solution.

#### <u>Unit II</u>

(9 hours)

- 2.1 Dynamic electrochemistry: Electrified interface IHP, OHP, contact adsorption surface excess and its importance use of mercury in double layer studies.
- 2.2 Thermodynamics of electrified interfaces: Electrocapillarity measurements Lippmann potential polarisable and non-polarisable interfaces Billiter potential.
- 2.3 Structure of electrified interfaces: Discussion of various models Helmholtz- Perrin, Gouy-Chapman and Stern models - derivations of equations and their validity. Electrokinetic phenomenon - Electrokinetic effects - concepts and derivations of equations - zeta potential and its determination- Tsilius method of separation of proteins - stability of colloids.
- 2.4 Electrodics: Charge transfer across the electrified interface its chemical and electrical implications basic electrodic equation- Butler Volmer equation derivation and its significance- special cases of Butler-Volmer equation and Tafel equation. Concept of overpotential types of overpotential quantification of polarisable and non-polarisable interfaces.
- 2.5 Power generation: Fuel cells construction and principle of operations and applicationsphotovoltaic phenomenon in electrochemical cells - corrosion and passivation metals-Pourbaix diagram – Evans diagram- techniques for inhibiting corrosion.

## <u>Unit III</u>

- 3.1 Atomic spectra: Total angular momentum vector- spectral notations term symbols selection rules spectra of one and two electron systems- effect of magnetic and electric fields Zeeman and Stark effects.
- 3.2 Electronic spectroscopy: Electronic spectra of diatomic molecules Frank-Condon principledissociation and predissociation - simple chromophores - fluorescence and phosphorescence. Electronic spectrum of polyatomic molecules- conjugated system.
- 3.3 Photoelectron spectroscopy: Origin chemical shift MO's spectra involving core and valence electrons applications.

#### <u>Unit IV</u>

- 4.1 Pure rotational spectra: Quantum mechanical results on the rigid rotor-rotational constant and centrifugal distortion -classification of molecules according to their moment of inertia Stark effect inversion spectrum of ammonia.
- 4.2 Raman Spectra: Rotational raman spectra anisotropic polarizability-Stokes and antistokes lines-vibrational raman spectra of diatomic molecules.
- 4.3 Vibrational spectra: Harmonic oscillator diatomic molecules, force constants, fundamental

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(9 hours)

(9 hours)

vibration frequencies - anharmonicity of molecular vibrations and its effect on vibrational frequencies - second and higher harmonics- vibration - rotation spectra: P,Q and R branchesvibrational raman spectra of diatomic molecules - vibrations of polyatomic molecules-normal modes of vibrations - CO<sub>2</sub>, H<sub>2</sub>O and acetylene.

## <u>Unit V</u>

(9 hours)

- 5.1 Nuclear magnetic resonance spectra: Theory nuclear spin Larmor frequency, NMR isotopes, population of nuclear spin levels relaxation processes. Chemical shift shielding constant ring current aromaticity shifts for <sup>1</sup>H and <sup>13</sup>C. Solvents shift concentration and temperature effects-hydrogen bonding. Spin-spin splitting- magnitude of coupling constant J-first-order spectra of complex systems-chemical and magnetic equivalence in NMR- proton exchange reactions. FT-NMR-principle.
- 5.2. Nuclear magnetic double resonance inter nuclear double resonance (INDOR) and selective population inversion (SPI)-nuclear overhauser effect (NOE)-distortionless enhancement by polarization transfer (DEPT) <sup>13</sup>CNMR.
- 5.3 Basics of 2D NMR: Principle and types- <sup>1</sup>H-<sup>1</sup>H Correlation spectroscopy (COSY) for simple molecules (methyl ethyl ketone and nitropropane)-working of magnetic resonance imaging (MRI).

## TEXT BOOKS

- 1. Modern Electro Chemistry by J.O.M.Bockris and A.K.N.Reddy, Vol.1 & 2, 1970, Plenum Press, New York.
- 2. Electro chemistry, S.Glasstone, 1974, Affiliated East-West Press, Pvt., Ltd., New Delhi.
- 3. Fundamentals of Molecular Spectroscopy, Banwell and E. M. McCash, 4th ed., 2000, C. N. Tata McGraw Hill, New Delhi
- 4. Molecular structure and spectroscopy, G. Aruldas, 2002, Prentice Hall.
- 5. Introduction of spectroscopy, D. L. Pavia et al., 4th Ed., 2008, Brooks Cole.
- 6. Spectroscopic Identification of Organic Compounds, R. M. Silverstein, F. X. Webster, and D. Kiemle, 7th Ed., 2005, John Wiley & Sons, New York.

## SUGGESTED READING

- 1. Physical Chemistry, P. Atkins and J. de Paula, 7th ed., 2002, Oxford University Press, UK.
- 2. Theoretical Electro Chemistry by L. Antropov, 1977, Mir Publications, Moscow.
- Physical Chemistry-A Molecular Approach, D.A.McQurrie and J.D.Simon, 1999, Viva Books Pvt. Ltd., New Delhi
- 4. Molecular Spectroscopy, Barrow, 1962, McGraw Hill Book Co, New Delhi.

#### REFERENCES

- 1. Kinetics and Mechanism of Electrochemical Transformations, J.Rajaram and J.C. Kuriakose,1993, Macmillan India Ltd., New Delhi.
- 2. Physical Methods in Chemistry, R. S. Drago, 1977, Saunders: Philadelphia.
- 3. Nuclear Magnetic Resonance-Basic Principles by A. Rahman, 1986, Springer-Verlag, New York
- 4. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, 4th edition, 1988, Tata McGraw-Hill Publishing Company, New Delhi.
- 5. Molecular Spectroscopy, K. V. Raman, R. Gopalan and P. S. Raghavan, 2004, Thomson and Vijay Nicole, Singapore.

#### **ONLINE RESOURCES**

- 1. https://www.digimat.in/nptel/courses/video/104106105/L01.html
- 2. https://nptel.ac.in/courses/103108162
- 3. https://nptel.ac.in/courses/104106105
- 4. https://nptel.ac.in/courses/104101099
- 5. https://nptel.ac.in/courses/104106122

## COURSE TITLE: MEDICINAL CHEMISTRY

(75 hours)

Course Code: (will be filled by EO)

Number of hours/cycle: 5

Nature of Course : Elective Theory

Credits: 5

Lea	Learning Objective		
(i)	To learn the interdisciplinary nature of medicinal chemistry		
(ii)	To learn the structure of cell and their functions, QSAR studies, drug action at receptors and drug-receptor theories.		
(iii)	To learn the mechanism of drug action at enzymes and DNA		
(iv)	To learn about the nervous system, drug metabolism and metabolic processes		
(v)	To understand and learn the structure – activity relationship for the development of drugs		

CO No	<b>Course Outcome</b> Upon completion of this course, students will be able to	PSO's addressed	CL
CO-1	Enumerate the interdisciplinary nature of medicinal chemistry, the classification of drugs and different routes of administration of drugs.	PSO-1, PSO-6	U
CO-2	Understand the drug action based on physiochemical properties and to explore the various drug-receptor theories	PSO-2,PSO-3	Ар
CO-3	Explain the mechanism of drug action at enzymes and DNA	PSO-4 PSO-3	An
CO-4	Discuss about the nervous system, drug metabolism and metabolic processes	PSO-1, PSO-4	U
CO-5	Evaluate the structure – activity relationship of various functional groups for the development of drugs	PSO-2,PSO-4	Ар

## <u>Unit-I</u>

(15 hours)

- 1.1 Interdisciplinary nature of medicinal chemistry: Pharmacology, molecular pharmacology, microbiology, biochemistry, physiology, medicine and pharmacy.
- 1.2 Classification of drugs Central nervous system acting drugs (general and local anaesthetics, sedatives and hypnotics, anticonvulsants, narcotic and non-narcotic analgesics, antiparkinsonian agents, antidepressants, tranquilizers, psychomimetics) pharmacodynamic agents (antiarrythmics, antianginals, vasodialators, antihypertensives, diuretics, antihistamines)-chemotherapeutic agents (antibiotics, antivirals, antifungals)-drug for metabolic and endocrine disorders (antihyroid drugs, antidiabetic drugs,

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## biosynthetic insulin)- therapeutic index (definitions with examples).

1.3 Pharmaceutical phase – Routes of administration (gastrointestinal, lungs, parenteral)-dosage forms - ingredients, their role and manufacture (tablets, capsules, liquids, injectables, suppositories, creams and pastes) - slow release drug formulations.

## <u>Unit-II</u>

- 2.1 Pharmacokinetic phase- Structure of eucaryotic cell cell components and their functions, cell membrane models, passive and active transport of materials across cell membranes pinocytosis.
- 2.2 Drug action and physiochemical properties hydrophobicity, electronic effect and steric effect.
- 2.3 Quantitative structure activity relationships (QSAR Studies) Hansch equation, Craig Plot, Topliss decision tree approach Bioisosterism.
- 2.4 Pharmacodynamic phase- drug action at receptors (the concept of receptors-structurally specific and structurally non-specific drugs-radiochemical studies of receptor sites-agonists and antagonists-binding force between drug and receptor).
- 2.5 Drug receptor theories: Occupancy theory, rate theory, induced fit theory and activationaggregation theory.

## <u>Unit-III</u>

- 3.1 Mechanism of drug action at enzymes competitive (reversible) inhibitors, non-competitive (irreversible) inhibitors and non-competitive reversible (allosteric) inhibitors.
- 3.2 Mechanism of transamination reaction and its inhibition.
- 3.3 Mechanism of action of pencillins and cephalosporins.
- 3.4 Mechanism of drugs acting on DNA intercalating agent (proflavin), alkylating agents (uracil mustard and cis-platin) and chain cutting agents (bleomycin).

## <u>Unit-IV</u>

- 4.1 The nervous system- Structure of nerve cells blood-brain barrier synapse neuro-transmitters (acetyl choline, adrenaline) and central nervous system neurotransmitters.
- 4.2 Drug metabolism routes of elimination (kidney and bilary excretion) factors affecting drug metabolism.
- 4.3 Metabolic processes phase I reactions (oxidation, reduction, hydrolysis), phase-II reactions glucuronide conjugation, acylation, methylation, mercapturic acid formation and sulphate conjugation.

## <u>Unit-V</u>

- 5.1 Drug development-optimizing drug interactions structure–activity relationships- binding role of alcohols and phenols- aromatic rings- alkenes- ketones and aldehydes-amines-amides-quaternary ammonium salts- carboxylic acids-esters alkyl and aryl halides- alkyl groups and the carbon skeleton- heterocycles.
- 5.2 Strategies in drug design -variation of substituents extension of the structure chain extension/contraction ring expansion/contraction ring variations ring fusions isosteres

(15 hours)

(15 hours)

(15 hours)

(15 hours)

and bioisosteres - simplification of the structure - rigidification of the structure-conformational blockers.

### **TEXT BOOKS**

- 1. An introduction to medicinal chemistry, G.L. Patrick, 4<sup>th</sup> Edition, 2013 Oxford University Press,UK
- 2. Medicinal Chemistry An Introduction, Gareth Thomas, 2nd Edition, 2007 Wiley, UK
- 3. Medicinal Chemistry, Ashutosh Kar, VII Edition 2018 New Age Publishers, India
- 4. An Introduction to Medicinal Chemistry, Bijoy Kundu, 2020 Wiley India.
- 5. Foye's Principles of Medicinal Chemistry, Victoria F. Roche and Thomas Lemke, 6<sup>th</sup> Edition, 2019, Lippincott Williams and Wilkins, Philadelphia, Pennsylvania, United States.
- 6. Introductory Medicinal Chemistry, J.B.Taylor, D.P.Kennewell, 1984, John Wiley and Sons.

## SUGGESTED READING

- 1. Principles of Organic Medicinal Chemistry, Rama Rao Nadendla, 2005 New Age International (P) Ltd Publishers, India.
- 2. Burger's Medicinal Chemistry, Donald J.Abraham, 8<sup>th</sup> Edition,2021, Wiley-Interscience, A John-Wiley and Sons Inc., Publication.
- 3. Essentials of Medical Pharmacology, K.D.Tripathy, 8<sup>th</sup> Edition 2018, Jaypee brothers Medical Publishers.

### REFERENCES

- Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry, John M. Beale, Jr, John H. Block, 12<sup>th</sup> edition 2011, Lippincott Williams & Wilkins, A Wolters Kluwer business, Philadelphia, Pennsylvania, United States.
- 2. Medicinal Chemistry, A Molecular and Biochemical Approach, Thomas Nogrady Donald F. Weaver, 3<sup>rd</sup> Edition 2005, Oxford University Press.
- 3. Textbook of medicinal chemistry Volume I, V. Alagarsamy, 2010, Reed Elsevier India Private Limited, Haryana.
- 4. Fundamentals of Medicinal Chemistry, Gareth Thomas, 2003 John Wiley & Sons Ltd, New York.

## **ONLINE RESOURCES**

- 1. <u>https://onlinecourses.nptel.ac.in/noc21\_cy05/preview</u>
- 2. https://archive.nptel.ac.in/courses/102/106/102106070/
- 3. https://nptel.ac.in/courses/102106070

## **SEMESTER-IV**

## COURSE TITLE: COORDINATION CHEMISTRY

Course Code: (will be filled by EO) (60 hours)

Number of hours/cycle: 4

Nature of Course : Core Theory

Credits: 4

Lear	Learning Objective		
(i)	To understand the basic concepts of coordination chemistry like bonding and theories of coordination complexes		
( <b>ii</b> )	To gain knowledge on the stability of coordination compounds and its determination		
(iii)	To acquire knowledge on the electronic transitions, magnetic properties and various spectroscopic applications of coordination complexes		
(iv)	To learn and understand the kinetics/mechanisms of substitution and electron transfer phenomenon of different coordination complexes		
( <b>v</b> )	To understand the mechanisms and applications of various coordination complexes in photochemical and photoelectrochemical processes		

CO No	Course Outcome	PSO's	CL
	Upon completion of this course, students will be able to	addressed	
CO-1	Describe the basic concepts of coordination chemistry like IUPAC nomenclature, bonding and theories of coordination complexes	PSO-1	Ар
CO-2	Explain the sigma bonding, pi bonding and the stability of various coordination complexes	PSO-1	U
CO-3	Predict the d-d transitions, electronic spectra, magnetic behaviour and the applications of various spectroscopic techniques in study of coordination compounds	PSO-1, PSO-5 PSO-6	An
CO-4	Describe the kinetics/mechanisms of substitution, electron transfer of different coordination complexes	PSO-2	Ар
CO-5	Identify and understand the photochemical reactions of different coordination complexes	PSO-4, PSO-6	Ар

#### Unit I

(12 hours)

- 1.1 Review of the fundamentals of coordination chemistry: Distinction between double salts and coordination compounds-IUPAC nomenclature-stable, unstable, inert and labile complexesmethods of preparation of complexes - detection of complex formation - applications of complexes in analysis and metallurgy. Isomerism- types, stereoisomerism in 4 and 6 coordinate complexes, chiral and achiral isomers and 18 electron rule.
- 1.2 Theories of bonding in complexes: Limitations of Werner theory and valence bond theorycrystal field theory - splitting of d orbitals in octahedral, tetrahedral and square planar symmetries- crystal field stabilisation energy-measurement of 10Dq - factors affecting 10Dq - octahedral site stabilisation energy - evidences for crystal field splitting energylimitations of CFT.

## Unit II

- 2.1 Evidences for metal-ligand orbital overlap- ligand field theory and molecular orbital theoryenergy level diagrams-concept of weak and strong field ligands- group theoretical treatment of the sigma and pi bonding in octahedral complexes.
- 2.2 Stability of complexes: Thermodynamic stability and kinetic stability stable, unstable, inert and labile complexes, stepwise and overall stability constants - their relationships - factors affecting the stability of complexes - chelate effect - importance of chelates-HSAB approach.
- 2.3 Determination of stability constant of complexes by spectrophotometric, ion exchange, pH, solubility and polarographic method.

#### Unit III

- 3.1 Spectral and magnetic characteristics of complexes: Term states for d ions characteristics of d-d transitions - Jahn Teller distortions and its consequences-charge transfer spectra selection rules for electronic spectra - Orgel correlation diagrams - Sugano-Tanabe energy level diagrams - spectrochemical series - nephelauxetic series.
- 3.2 Spin-orbit coupling effect of spin-orbit coupling on magnetic moments magnetic properties of transition metal complexes- quenching of orbital magnetic moments.
- 3.3 Applications of IR for identification of carbonyl complexes and geometrical isomers- ESR of iridium, manganese and vandium complexes- <sup>1</sup>H and <sup>13</sup>C NMR as applied to hydrido, carbonyl complexes and fluxional isomers- Mossbauer spectrum of carbonyl and cyano complexes of iron and application of ORD in the study of coordination compounds namely cobalt complexes like  $[Co(en)3]^{3+}$  and  $[Co(ala)_3]^{3+}$ .

#### **Unit-IV**

- 4.1. Kinetics and mechanisms of reactions of complexes: Substitution reactions of octahedral complexes - mechanism of water replacement - acid hydrolysis of octahedral complexes base hydrolysis - S<sub>N</sub>1cB mechanism.
- 4.2. General mechanism of square planar substitution reactions two parallel pathways factors affecting the reactivity of square planar complexes of d<sup>8</sup> metal ions - trans effect - theories of trans effect (polarisation and pi bonding theory).
- 4.3. Mechanism of electron transfer reactions outer sphere electron transfer reactions -

(12 hours)

(12 hours)

(12 hours)

Marcus Hush theory - inner sphere electron transfer reactions- formation and rearrangement of precursor complex-nature of bridging ligand-two electron transfer reactions- complementary, non-complementary and atom transfer reactions.

#### <u>Unit-V</u>

(12 hours)

- 5.1. Lanthanides and actinides: Periodic properties, spectral and magnetic properties of lanthanide and actinide complexes.
- 5.2.Photochemistry of transition metal complexes- photosubstitution photoisomerisation photoredox photochemistry of Cr (III) and Co (III) complexes ([Cr(NH<sub>3</sub>)<sub>6</sub>]<sup>3+</sup>, [Cr(H<sub>2</sub>O)<sub>6</sub>]<sup>3+</sup>, [Cr(en)<sub>3</sub>]<sup>3+</sup> and [Co(NH<sub>3</sub>)<sub>6</sub>]<sup>3+</sup>, [Co(CN)<sub>6</sub>]<sup>3-</sup>, [Co(NH<sub>3</sub>)<sub>5</sub>X]<sup>2+</sup>), photophysical and photochemical properties of [Ru(bpy)<sub>3</sub>]<sup>2+</sup> and solar energy conversion.
- 5.3.Inorganic photochemistry at semi-conductor electrodes catalyzed photoreduction of  $CO_2$  and nano TiO<sub>2</sub> as photocatalyst in removing air and water pollutants.

## **TEXT BOOKS**

- 1. Concise Inorganic Chemistry, J D Lee, 5<sup>th</sup> Edition, 2008, Oxford University Press, Wiley, New York.
- 2. Coordination Chemistry, D.Banerjea, 3<sup>rd</sup> edition, 2009, Asian Books, Hyderabad.
- 3. Modern aspects of inorganic chemistry, H.J Emeleus, J.S.Anderson and Alan G Sharpe, Revised ed A.G.Sharp ed edition, 1973, Routledge & Kegan Paul PLC.
- 4. Concise Coordination Chemistry, R.Gopalan and V.Ramalingam, 2001, Vikas Publishing House Pvt Ltd, New Delhi.
- 5. Inorganic Chemistry, Principles of Structure and Reactivity, James E Huheey, Fourth Edition, 2006, Pearson Education India.
- 6. Selected topics in Inorganic chemistry, Wahid U Malik, G.D.Tuli, R.D.Madan 2010, S Chand and Company Limited, New Delhi.
- 7. Fundamentals of inorganic photochemistry, Rhohatghi Mukherjee, 4<sup>th</sup> edition, 2021, New Age International Publishers, Chennai.

#### SUGGESTED READING

- 1. Advanced Inorganic Chemistry, Cotton & Wilkinson, 1972, Third edition, Inter-Science Publishers, John Wiley and Sons Inc, New York, United Sates.
- 2. Concepts and models of inorganic chemistry by Douglas, Darl H McDaniel and John J Alexander,1994 John Wiley and Sons, New York
- 3. Inorganic chemistry by Gary Wulfsberg, 2018, Viva Books, Chennai, TamilNadu .
- 4. Essential Trends in Inorganic Chemistry, D.M.P.Mingos (1998) Oxford University Press.
- 5. Principles of Inorganic Chemistry, B.R.Puri, L.R.Sharma, K.C.Kalia.(2020), Vishal Publishing company.

#### REFERENCES

- 1. Inorganic Chemistry, Keith.F.Purcell and john C Kotz, 1980, Holt Saunders InternationalEditions, W.B.Saunders Company, Philadhelpia, Toronto, London.
- 2. Shriver and Atkin's Inorganic Chemistry, 5<sup>th</sup> edition, 2009.
- 3. Inorganic Chemistry, Gary L. Miessler, Donald A.Taar, 3<sup>rd</sup> edition, 2008 Pearson India.
- 4. Theoretical Inorganic Chemistry, M.C.Day and J.Selbin, 1969, Van Nostrand Reinhold Inc.,U.S.
- 5. Coordination Chemistry: The Chemistry of metal Complexes, Fred Basolo, 1964, Benjamin-Cummings Pub Co.

#### **ONLINE RESOURCES**

- 1. https://nptel.ac.in/courses/104105033
- 2. <u>https://onlinecourses.nptel.ac.in/noc22\_cy20/preview</u>
- 3. <u>https://onlinecourses.nptel.ac.in/noc21\_cy10/preview</u>
- 4. https://nptel.ac.in/courses/115103123

#### COURSE TITLE: SCIENTIFIC RESEARCH METHODOLOGY

Course Code: (will be filled by EO)

(60 hours)

Number of hours/cycle: 4

Credits: 4

Nature of Course : Core Theory

Lear	ning Objective	
(i)	To introduce the aim, purpose and importance of research for development and sustenance.	
(ii)	To identify the scope and utility of various indexing and abstracting services in science and	
	technology as a source of information.	
(iii)	To appreciate about the safety and safe handling of chemicals in laboratories.	
(iv)	To understand the function of the entrepreneur in the successful, commercial application of	
	innovations.	
<b>(v)</b>	To comprehend the various ways of literature survey, collect data in an organized and	
	controlled manner and to statistically analyse the data appropriate to the problem.	

CO No	Course Outcome	PSO's	CL
	Upon completion of this course, students will be able to	addressed	
CO-1	Discover the different ways to identify and collect	PSO-3	U
	information on a particular topic of interest.		
CO-2	Articulate appropriate style for an academic or scientific	PSO-6	Ap
	report writing		
CO-3	Recognize business opportunities, self-esteem, knowledge	PSO-1	U
	and skills to act on them in addition to commercializing a		
	concept, managing resources and initiating business		
	speculation		
CO-4	Equip students with necessary skills and knowledge to	PSO-6	Ap
	assess, handle and dispose the chemicals safely in the work		
	place.		
CO-5	Communicate concepts in probability and statistics using	PSO-5	An
	both technical and non-technical language.		

#### <u>Unit-I</u>

(12 hours)

- 1.1 Chemistry literature survey-types of chemistry literature- primary, secondary and tertiary examples.
- 1.2 Journals published by the ACS and RSC- CA and its importance indian journals reviews, monographs, data books and indexes.
- 1.3 Literature survey: Methods of searching literature, methods of compilation and preservation and retrieval of collected literature.

## <u>Unit II</u>

(12 hours)

- 2.1. Research experiments: Planning and conducting experiments, methodology of collecting scientific data (with three types of project titles as examples).
- 2.2. Project report writing: The general format, chapter format and page format.

2.3 Procedure for presenting tables, graphs and figures, foot-notes, bibliography and appendices.

- 2.4 Abbreviations, symbols, SI units and nomenclature.
- 2.5 Scientific exactness and proper language, editing, plagiarism, copy right and patent laws.

## <u>Unit III</u>

(12 hours)

- 3.1 Entrepreneurship: Concept of entrepreneurship, types, characteristics and importance of entrepreneurship-steps in establishing a chemical factory.
- 3.2 Methodology of market survey for chemicals and chemical-based products.
- 3.3 Principles of designing bench scale production and scaling up for a chemical production.
- 3.4 Computer hardware and software, software *vs* hardware, data representation, computerised instrumentation systems and computer-controlled laboratory automation systems.

## <u>Unit IV</u>

(12 hours)

(12 hours)

- 4.1 Chemical safety and ethical handling of chemicals-safe working procedure- first aid and emergency procedure- general guidelines for safe handling of chemicals in laboratory- toxic, corrosive and carcinogenic chemicals-flammable or explosive hazards safe storage use and working protocol for hazardous chemicals- transportation of hazardous chemicals.
- 4.2 Storage and disposal of chemical waste and laboratory waste segregation of laboratory waste-minimization-disposal of chemicals in the sanitary sewage system-incineration.

## <u>Unit V</u>

- 5.1 Statistical calculation: Presentation of data- measures of central tendency-mean, median, mode and standard deviation- measures of variability- precision and accuracy, significant figures and errors in chemical analysis-simple sampling techniques.
- 5.2. Statistical treatment of finite samples-the student's t-test and F-test criteria for rejection of an observation Q-test linear regression and correlation- method of least squares.

## TEXT BOOKS

- 1. The Literature Review- A Step-by-Step Guide for Students , Diana Ridley, Second Edition, Sage publication.
- 2. EntrepreneurshipWilliam Bygrave and Andrew Zacharakis Second Edition, 2011, Wiley, New York.
- 3. Statistical Methods Book, SP Gupta, 2011, Sultan Chand & Sons
- 4. Chemical process safety fundametals with applications, Daniel A. Crowl and Joseph F. Lowar second Edition, Prentice Hall PTR.
- 5. Prudent Practices in the Laboratory Handling and Disposal of Chemicals, 1995, National Academy Press Washington, D.C.
- 6. Computer software applications in Chemistry, Peter C.Jurs, 1196, Wiley-Interscience.

#### SUGGESTED READING

- 1. Chemical publications: Their nature and use, M.G.Mellon , 5<sup>th</sup> edition , McGraw Hill,NewYork , United States.
- 2. CRC Handbook of Chemistry and Physics, W. M. Haynes, David R. Lide, Thomas J. Bruno, 97th Edition, 2017 CRC Press.
- 3. Introduction to Chemical Principles A Laboratory Approach, Susan A, Weiner, Blaine Harrison, Seventh Edition ,2010, Brooks Cole Cengage Learning, United States.
- 4. Statistical methods in analytical chemistry, Peter C. Meier, Richard E. Zund, <sup>2nd</sup> Edition, 2000, Wiley-Interscience publication, John Wiley & Sons, inc.
- 5. Toxic Chemicals Risk Prevention through Use Reduction, Thomas E. Higgins, 2011, CRC Press.
- 6. Computer-Assisted Organic Synthesis, ACS Symposium Series (1977) Robert F. Gould, American Chemical Society.
- 7. Computers for Chemist, Pandir Bansal, 2020, Pragati Prakashan.

#### REFERENCES

- 1. Literature Reviews-A Guide for Students of the Social and Behavioral Sciences, Jose L. Galvan and Melisa C. Galvan 7<sup>th</sup> Edition Tailor and Francis 2017.
- 2. How to write Dissertations & Project Reports , Kathleen McMillan and Jonathan Weyers, Pearson Education Limited, 2010.
- 3. Entrepreneurship and Innovation, James C Barrood, Rothman Institute of Entrepreneurship,2010.
- 4. Modern Elementary Statistics. by John Freund and Benjamin Perles, 12th edition, Prentice-Hall

#### **ONLINE SOURCES**

1. https://nptel.ac.in/courses/109108158

#### COURSE TITLE: BIOINORGANIC CHEMISTRY

Course Code: (will be filled by EO)

(75 hours)

Number of hours/cycle: 5

Nature of Course : Elective Theory

Credits: 5

Lear	Learning Objective		
(i)	To understand the interaction between biomolecules and nucleic acids		
(ii)	To comprehend the role of metal ions in biological systems and to study the interactions of metal ions and complexes with nucleic acids.		
(iii)	To realize the role of metalloenzymes in carrying out reactions that cannot easily be performed by the limited set of functional groups found in amino acids.		
(iv)	To recognize the role of calcium in extracellular and intracellular biological process.		
<b>(v)</b>	To appreciate the role of metals in medicine and diagnosis.		

CO No	<b>Course Outcome</b> Upon completion of this course, students will be able to	PSO's addressed	CL
CO-1	Explain the role of metals, non-metals and essential trace elements in biological system	PSO-1	U
CO-2	Interpret the important aspects of calcium in biochemistry	PSO-1, PSO-2	Ар
CO-3	Identify and describe the structure and different functions of metalloenzymes	PSO-1, PSO-6	U
CO-4	Sketch the different binding sites of nucleic acids with metal complexes and to appreciate its role in therapy and diagnosis	PSO-1, PSO-2	An
CO-5	Adapt knowledge on toxicity of metal ions and its chelation therapy	PSO-1	U

#### <u>Unit 1</u>

(15 hours)

- 1.1 Biomolecules and their metal coordination behavior: Metal ion binding with nucleosides, nucleotides and nucleic acids- metal and non-metals in biological system- importance of essential trace elements.
- 1.2 Metal storage and transport: Ferritin, transferrin and siderophores ion transport in membranes (active and passive) membrane potential ionophores biomineralization process.

- 2.1. Calcium in biology: Calcium in mineralized tissues (apatite family) essentials of Ca<sup>2+</sup> in chemistry coordination of Ca<sup>2+</sup> ion with oxygen. Transport and regulation of Ca<sup>2+</sup> ions in higher organisms Ca<sup>2+</sup> uptake and secretion, intracellular Ca<sup>2+</sup> transport Ca<sup>2+</sup>-ATP ases, Na<sup>+</sup>/Ca<sup>2+</sup> exchanger of the plasma membrane- other voltage-gated or receptor-activated Ca<sup>2+</sup> channels Ca<sup>2+</sup> intracellular messenger system (inositol trisphosphate).
- 2.2 Role of intracellular calcium binding proteins troponin, calmodulin, calbindin, calpin, protein kinase C role of extracellular calcium binding proteins like phospholipase, prothrombin and serine protease.

## <u>Unit III</u>

(15 hours)

(15 hours)

- 3.1 Metalloporphyrin: Structure and functions of haemoglobin, myoglobin, chlorophyll, vitamin  $B_{12}$  and iron sulphur proteins
- 3.2 Metalloenzymes: Zinc enzymes carboxy peptidase and carbonic anhydrase, iron enzymescatalase and peroxidase, copper enzymes - superoxide dismutase and hemocyanin (oxygen transport) and molybdenum oxatransferrase enzyme- xanthine oxidase.

## <u>Unit IV</u>

- 4.1 Metal nucleic acid interactions: Structure of DNA and RNA- structural characteristics of Watson-Crick model of DNA-different conformations of DNA double helix strand- general features of DNA-metal complex interaction modes of association (coordination, intercalation and hydrogen bonding) and chemical reaction between coordination complex and polynucleotides (redox and hydrolytic reactions).
- 4.2 Metal salts and complexes in therapeutics: Drugs used in the treatment of metal deficiencymetal salts - gold, lithium, arsenic and antimony compounds - anti-cancer drugs (cis-platin and its alternatives).

## <u>Unit V</u>

(15 hours)

- 5.1 Effect of deficiency and excess of essential metal ions, toxicity due to non-essential metals like mercury, lead, cadmium, arsenic, aluminium, tin and beryllium. Mechanism of detoxification of metals.
- 5.2. Chelating drugs used in metal ion detoxification: Drugs with SH group (BAL, Unithiol, disodium meso-2,3-dimercaptosuccinate, D-penicillamine and N-acetyl D-penicillamine), polyaminocarboxylic acid (EDTA).
- 5.3 Metals used for diagnosis: Radio diagnostic agents- radioisotopes used in radio therapy and radio diagnosis (<sup>60</sup>Co, <sup>57</sup>Co,<sup>123</sup> I, <sup>131</sup> I, <sup>32</sup> P, <sup>24</sup> Na, <sup>10</sup>B, m<sup>99</sup>Tc, <sup>67</sup>Ga and <sup>68</sup> Ga complex).

#### <u>Unit II</u>

#### **TEXT BOOKS**

- 1. Metal Ions in Biochemistry Hardcover by P. K. Bhattacharya published by Alpha Science International Ltd; 1st edition (2005)
- 2. Principles of Bioinorganic Chemistry by Stephen J. Lippard, Jeremy M. Berg published by University Science Books (21 September 1994)
- 3. Biochemistry by U. Satyanarayana ,U.Chakrapani, 5th Edition, Revised And Updated Edition published by Elsevier.
- 4. Bioinorganic chemistry, Asim K Das, 2007, Books & Allied Ltd, Kolkatta, West Bengal.

#### SUGGESTED READING

1. Principles of bioinorganic chemistry, S.J. Lippard and J.M. Berg, 1994, University science books, Sausalito, CA, United States

#### REFERENCES

- 1. Bioorganic Chemistry: A Chemical Approach to Enzyme Action by Hermann Dugas Springer; 3rd ed. 1996. 2nd printing 1999 edition (1 September 1999).
- 2. Bioorganic Chemistry: Nucleic Acids, Edited by Sidney M. Hecht, Oxford University Press. Publication Date - April 1996

#### **ONLINE RESOURCES**

1. https://archive.nptel.ac.in/courses/104/101/104101116/

#### ORGANIC CHEMISTRY PRACTICAL – I (Semester I and II) (120 hours)

Course Code: (For EO use only) Nature of Course: Core Practical Number of hours/cycle: 4 Credits: 4

Learning Objective	1. To achieve the separation of organic mixtures with two and three components and identify each component through systematic qualitative
Ŭ	analysis.
	2. To develop bench and psychomotor skills in organic preparations involving two and three stages.

CO No	<b>Course Outcomes</b> Upon completion of this course, the students will be able to	PSO's addressed	CL
CO-1	Demonstrate the analytical skill in the separation and identification of organic compound from a binary mixture.	PSO-5	Ар
CO-2	Demonstrate the analytical skills in the separation and identification of organic compound from a ternary mixture.	PSO-5	Ap
CO-3	Demonstrate the preparation and recrystallization of an organic compound in a two-step process	PSO-1, PSO-5	An
CO-4	Demonstrate the preparation and recrystallization of an organic compound in a three-step process	PSO-1, PSO-5	Ар

#### I. Separation and analysis of two component organic mixture by chemical methods

#### II. Separation and analysis of three component organic mixture by chemical methods

(Benzoic acid, cinnamic acid, phthalic acid,  $\alpha$  and  $\beta$ -naphthol, aniline, N, N-dimethylaniline, glucose, sucrose, fructose, benzaldehyde, acetophenone, benzophenone, nitrobenzene, benzamide, acetanilide and urea).

#### III. Two stage organic synthesis (any five)

Synthesis of organic compounds based on the following types of reactions: Acetylation, bromination, oxidation, reduction, dehydration, cyclization, benzoylation, hydrolysis, condensation and esterification.

- 1. p-bromoacetanilide from aniline (acetylation, bromination)
- 2. p-aminobenzoic acid from p-nitrotoluene (oxidation, reduction)
- 3. Benzil from benzaldehyde (condensation, oxidation)
- 4. 1,2,3,4-tetrahydrocarbazole from cyclohexanone (condensation, cyclization)
- 5. Phthalimide from phthalic acid (sehydration, Substitution)
- 6. 4-methyl-7-acetoxy coumarin from resorcinol (cyclization, acetylation)
- 7. Acetyl salicyclic acid from methyl salicylate (hydrolysis, esterification)
- 8. Stilbene from benzaldehyde (condensation, reduction)

#### **IV.** Three stage organic synthesis: (any three)

- 1. p-bromoaniline from aniline (acetylation, bromination, hydrolysis)
- 2. Ethyl p-aminobenzoate from p-nitrotoluene (oxidation, reduction, esterification
- 3. Benzilic acid from benzaldehyde (condensation, oxidation, rearrangement)
- 4. Anthranilic acid from phthalic acid (dehydration, substitution, hydrolysis)
- 5. Stilbene dibromide from phthalic acid benzaldehyde (condensation, reduction, addition)

## TEXTBOOKS

- 1. N. S. Gnanapragasam and G. Ramamurthy, Organic Chemistry Lab manual, S. Viswanathan Co. Pvt. Ltd, 1998.
- 2. J. N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987
- 3. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, Department of Science & Technology, GoI, 2009.

## REFERENCES

- 1. Vogel's Text Book of Practical Organic Chemistry, 5<sup>th</sup> Ed, ELBS/Longman, England, 1984.
- 2. V K Ahluwalia, Sunitha Dhingra, Adarsh Gulati, College Practical Chemistry, University Press, India, 2008.
- 3. Jag Mohan, Organic Analytical Chemistry, Narosa Publishing House, India, 2003

#### INORGANIC CHEMISTRY PRACTICALS I (for Semester I and II) (120 hours)

Course Code: By EO Nature of Course: Core Practical Number of Hours /cycle: 4 Credits: 4

Learning Objective	To apply physical and inorganic chemistry concepts in identifying
	the metal ions through semi-micro analysis

CO No	Course Outcomes	PSO's	CL
	Upon completion of this course, the students would be	addressed	
	able to		
CO-1	Understand and apply solubility product principles and	PSO-1,	Ар
	common ion effect and apply them in identification and	PSO-3	
	analysis of familiar and less familiar cations in the given		
	inorganic mixture		
CO-2	Understand the principles of and develop skills in	PSO-1,	Ар
	photocolorimetric estimation of selective metal ions	PSO-3	-
CO-3	Understand and apply different preparative routes for the	PSO-1,	Ар
	complexes	PSO-3,	_
		PSO-5	
CO-4	Prepare required solutions by meticulous planning and	PSO-1,	Ар
	execution of experiments	PSO-3,	-
		PSO-5	

**I. Semimicro qualitative analysis** of mixtures containing two common cations and two cations of the following less familiar elements.

Tl, W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be and U and Li

#### II. Photo-colorimetric estimation of metal ions:

- 1. Colorimetric estimation of iron by Fe-NH<sub>4</sub>SCN complex.
- 2. Colorimetric estimation of copper by Cu-NH<sub>3</sub> complex.
- 3. Colorimetric estimation of nickel by Ni-DMG complex.
- 4. Colorimetric estimation of manganese

#### **III.** Complex preparations (any five):

- 1. Preparation of tetramminecopper(II) sulphate.
- 2. Preparation of tris(thiourea)copper(I) sulphate.

- 3. Preparation of potassium tris(oxalato)chromate (III).
- 4. Preparation of sodium hexanitrocobaltate(III).
- 5. Preparation of potassium bis(oxalato)cuprate(II) dihydrate.
- 6. Preparation of sulphatotris(thiourea)zinc(II).
- 7. Preparation of hexamminenickel(II)chloride.
- 8. Preparation of cis-potassium dioxalatodiaqua chromate(III).
- 9. Preparation of sodium trioxalato ferrate(III)
- **IV. Green synthesis:** Preparation of manganese dioxide nano-particles and preparation of iron oxide nanoparticles.

#### TEXTBOOKS

- 1. Semimicro qualitative analysis of inorganic ions by V. V. Ramanujam
- Vogel's textbook of Macro and Semimicro qualitative analysis, 5<sup>th</sup> Edition, Revised by G. Svehla, Longman GroupLimited, London, 1979

## REFERENCES

1. Experimental Inorganic Chemistry, W.G. Palmer, Cambridge University Press, Cambridge, 1965

#### **ONLINE RESOURCES**

- 1. https://www.frontiersin.org/articles/10.3389/fnano.2021.655062/full
- 2. https://jnanobiotechnology.biomedcentral.com/articles/10.1186/s12951-018-0408-4

#### PHYSICAL CHEMISTRY PRACTICALS I (Semester I and II) (120 hours)

Course code: (For EO use only) Nature of course: Core Practical Number of hours/cycle: 4 Credits: 4

LearningTo apply the theoretical concepts of physical chemistry in determining and<br/>understanding various physical parameters

CO No.	Course Outcomes	PSO's Addressed	CL
INU.	Upon completion of this course learners will be able to	Auuresseu	
CO-1	Prepare required solutions by meticulous planning and execution of experiments.	PSO-1, PSO-5	Ар
CO-2	Acquire the skills to determine and evaluate various physical parameters through Conductometry and Refractometry	PSO-1, PSO-5	Ap
CO-3	Realize the importance of phase rule and its implications in chemical research	PSO-1, PSO-5	Ap
CO-4	Estimate pH, pKa, solubility product and standard electrode potentials through emf experiments.	PSO-1, PSO-5	Ap
CO-5	Acquire 21 <sup>st</sup> century skills such as critical thinking, creativity, collaboration, and communication as well as bench skills.	PSO-6	Ap
CO-6	Attain skills in generating and interpreting data through designing experiments.	PSO-5, PSO-6	Ap

#### **I. Experiments**

- 1. Determination of integral and differential heat of solution by calorimetry.
- 2. Determination of heat of neutralization of a strong acid by a strong base using calorimetry.
- 3. Determination of phase diagram for two component solid systems.
- 4. Determination of phase diagram for three component liquid systems.
- 5. Determination of bond refractions by refractometry.
- 6. Understanding the interaction between the components of a binary mixture using refractometry.
- 7. Determination of equivalent conductance of a strong electrolyte at infinite dilution using conductometry.
- 8. Determination of equivalent conductance of a weak electrolyte at infinite dilution using conductometry.

- 9. Determination of dissociation constant of a weak acid by conductometry.
- 10. Determination of solubility of sparingly soluble salt by conductometry.
- 11. Verification of Beer-Lambert's law.
- Beer-Lambert's law Simultaneous estimation of Mn and Cr in a solution containing KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>.
- 13. Conductometric titration strong acid vs strong base.
- 14. Conductometric titration mixture of strong acid and weak acid vs strong base.
- 15. Conductometric titration mixture of halides vs silver nitrate.
- 16. Conductometric titration CuSO<sub>4</sub> vs NaOH or MgSO<sub>4</sub> vs BaCl<sub>2</sub>
- 17. Determination of standard electrode potential.
- 18. Determination of solubility of AgCl from emf measurements.
- 19. Determination of pKa of a weak acid from emf measurements.
- 20. Determination of pH of buffer solutions from emf measurements.

#### **II. Project based learning**

- 1. Spectrophotometric analysis of coloured samples (dyes, natural pigments, metal ions etc.)
- 2. Study of interaction between samples by refractometry.
- 3. Use of conductance measurements to study interactions, determine physical quantities, etc.

#### TEXTBOOKS

- 1. A. Findlay, J.A. Kitchener, Findlay's Practical Chemistry, 8<sup>th</sup> Edition, Prentice Hall Press, 1954.
- 2. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books, 2012.

#### REFERENCES

1. R.C. Das and B. Behera, Experimental Physical Chemistry, McGraw-Hill Education, 1984.

#### SUGGESTED READING

1. Farrington Daniels, Experimental Physical Chemistry, 7th Edition, McGraw-Hill Inc., US, 1970.

#### ORGANIC CHEMISTRY PRACTICAL II (Semester III and IV) (120 hours)

Course Code: (For EO use only) Nature of Course: Core Practical Number of hours/cycle: 4 Credits: 4

Learning Objective	1. To estimate quantitatively the organic compounds with various functional	
Objective	groups	
	2. To understate and utilize various chromatographic techniques to monitor	
	the reaction progress	
	3. To understand the nuances and apply it in the isolation of natural products.	
	4. To elucidate the structure of simple organic compounds from spectra data	

CO No	Course Outcome Upon completion of this course, the students will be able to	PSO's addressed	CL
CO-1	Estimate quantitatively an organic compound with certain functional groups	PSO-1, PSO-2	Е
CO-2	Apply thin layer chromatographic technique to identify the components present in a given organic mixture	PSO-5	Ap
CO-3	Develop column chromatography technique for the separation of mixture of organic compounds	PSO-5	An
CO-4	Estimate or characterize certain organic compounds	PSO-2	An
CO-5	Isolation and purification of organic compounds from natural sources	PSO-5	Ap
CO-6	Identify the structure of an organic compound using UV- visible, FT-IR, NMR and mass spectral data	PSO-1, PSO-5	An
CO-7	Acquire 21 <sup>st</sup> century skills such as critical thinking, creativity, collaboration and communication as well as bench skills	PSO-6	Ар
CO-8	Attain skills in generating and interpreting data through designing experiments	PSO-6	Ap

I.

#### **Estimations:**

- 1. Phenol (bromination)
- 2. Aniline (bromination)
- 3. Methyl ketone (iodometry)
- 4. Glucose (redox)
- 5. Acetyl group (hydrolysis)
- 6. Methoxy group
- 7. Degree of unsaturation
- 8. Aromatic nitro groups (reduction)
- 9. Glycine (acidimetry)
- 10. Iodine value of an oil
- 11. Saponification number of an oil
- 12. Ascorbic acid (iodometry)

## **II.** Identification and Separation of components of an organic mixture (any 4):

- 1. Thin layer chromatography (monitoring the reaction progress).
- 2. Preparative thin layer chromatography.
- 3. Column chromatography (purification of organic mixtures).
- 4. Gas chromatography (monitoring the reaction progress).

## **III. Project based learning:**

#### Extraction/separation of:

- 1. Casein from milk
- 2. Caffeine from tea leaves
- 3. Vitamin C from fruits
- 4. Lycopene from tomatoes
- 5. Piperine from Pepper
- 6. Curcumin from Turmeric
- 7. Pigment from Red Chili

## IV. Structural Elucidation using spectral data: (any 10):

Phenol, anisole, benzoic acid, aniline, acetanilide, benzaldehyde, cinnamic acid, 1,3,5-

trimethylbenzene, n-propylamine, p-methoxy benzyl alcohol, benzyl bromide, phenylacetone, pyridine, 4-picoline and cinnamaldehyde.

#### **TEXT BOOKS**

- 1. Advanced Experimental Chemistry, J. N. Gurtu and R. Kapoor, S. Chand and Co., 1987
- 2. Organic Spectroscopy, William Kemp, III Edition, Palgrave USA

#### REFERENCES

- 1. Vogel's Text Book of Practical Organic Chemistry, 5th Ed, ELBS/Longman, England, 1984.
- 2. College Practical Chemistry, V K Alhuwalia, Sunitha Dhingra, Adarsh Gulati, University Press,2008, Hyderabad
- 3. Organic Analytical Chemistry, Jag Mohan, Narosa Publishing House, New Delhi, 2003

#### INORGANIC CHEMISTRY PRACTICAL II (Semester III and IV) (120 hours)

Course Code: For EO use only Nature of Course: Core Practical

Number of Hours /cycle:4 Credits: 4

	1.	To apply physical and inorganic chemistry concepts in quantitative estimation	
Learning		of metal ions by fundamental analytical techniques	
Objective	2.	To acquire 21 <sup>st</sup> century skills such as critical, creative thinking, collaboration	
		and communication as well as bench skills	

CO No	Course Outcomes	PSO's	CL
	Upon completion of this course, the students would be able to	addressed	
CO-1	Understand and apply the basic principles involved in redox and	PSO-1,	Ар
	complexometric titrations	PSO-3,	
		PSO-5	
CO-2	Understand the significance of back and blank titrations and	PSO-1,	Ap
	apply them in inorganic quantitative analysis	PSO-3,	_
		PSO-5	
CO-3	Analyse quantitatively the materials given with high precision	PSO-1,	An
		PSO-3,	
		PSO-5	
CO-4	Analyse, separate and quantitatively evaluate the individual	PSO-1,	An
	metal components present in the mixture by using more than one	PSO-3,	
	method	PSO-5	
CO-5	Draft a mini project proposal including hypothesis and design of	PSO-1,	C
	experiments	PSO-3,	
		PSO-5	
CO-6	Acquire 21 <sup>st</sup> century skills such as critical thinking, creativity,	PSO-6	Ар
	collaboration and communication as well as bench skills		
CO-7	Attain skills in generating and interpreting data through	PSO-6	Ap
	designing experiments		

#### I. Double Burette method:

- a. Estimation of iron by cerimetry
- b. Estimation of zinc by complexometric method

## **II. Single Burette method:**

- a. Estimation of nitrite
- b. Estimation of calcium
- **c.** Estimation of hardness of water

- **III. Quantitative separation and analysis** (one by volumetric and one by gravimetric method) of **any two** the following artificial mixtures:
  - a. Cu and Ni b. Cu and Fe c. Fe and Ni d. Zn and Cu.

#### **IV. Project based learning:**

- a. Synthesis of a metal complex and determination of its composition.
- b. Estimation of the components of an alloy by green method.
- c. Estimation of an inorganic component in a real sample by spectrophotometric method.
- d. Separation of inorganic cations by paper chromatography.
- e. Synthesis of a photo-sensitive complex and study of its application.

## V. Quantitative analysis of the following (any two):

a. Brass, b. Bronze, c. Solder & d. Pyrolusite

## TEXTBOOKS

- 1. Shriniwas L Kelkar, Dilip D Dhavale and Prabodh G Pol, Microscale Experiments in Chemistry The Need of the New Millenium, Resonance (2001) 14-22
- G H Jeffery, J Bassett, J Mendham and R C Denney, Vogel's textbook of Quantitative Chemical Analysis, 5th Edition, Longman Group Limited, London, 1989
- 3. S K Agarwala and Keemti Lal, Advanced Inorganic Analysis, 10<sup>th</sup> Edition, Pragati Prakashan, Uttar Pradesh, 2008

## REFERENCES

1. Anil J Elias, A Collection of Interesting General Chemistry Experiments, Sangam Books Ltd, 2002

## SUGGESTED READING

1. Gurdeep Raj, Advanced Practical Inorganic Chemistry, 27th Edition, Goel Publishing House, Uttar Pradesh, 2016

## **ONLINE RESOURCES**

- 1. https://www.ias.ac.in/article/fulltext/reso/006/02/0014-0022
- 2. https://www.youtube.com/watch?v=uNhHotinlOg

#### PHYSICAL CHEMISTRY PRACTICAL II (Semester III and IV) (120 hours)

Course code: For EO use onlyNumber of hours/cycle: 4Nature of course: Core PracticalCredits: 4LearningTo apply the theoretical concepts of physical chemistry in determining andObjectiveunderstanding various physical parameters

CO	Course Outcomes	PSO's	CL
No	Upon completion of this course learners will be able	Addressed	
	to		
CO-1	Prepare required solutions by meticulous planning and	PSO-1,	Ap
	execution of experiments.	PSO-5	
CO-2	Acquire skills to determine and evaluate various	PSO-1,	Е
	physical parameters through conductometry and study	PSO-5	
	kinetics of reactions.		
CO-3	Utilize emf measurements as a tool to study titrations	PSO-1,	Ар
		PSO-5	
CO-4	Use analytical techniques for detection and separation	PSO-5	Ар
	of metal ions.		_
CO-5	Summarize their findings in writing in a clear and	PSO-5,	Ар
	concise manner	PSO-6	-

- 1. Verification of Job's continuous variation method for complex formation.
- 2. Determination of critical micelle concentration by conductometry method.
- 3. Comparison of acid strength hydrolysis of methyl ethanoate.
- 4. Determination of energy of activation for hydrolysis of methyl ethanoate.
- 5. Study of kinetics of iodination of acetone.
- 6. Evaluation of rate constant for ester hydrolysis using Guggenheim's method.
- 7. Potentiometric titration strong acid vs strong base.
- 8. Potentiometric titration mixture of strong acid and weak acid vs strong base.
- 9. Potentiometric titration mixture of halides vs silver nitrate.
- 10. Potentiometric titration ferrous ion vs potassium dichromate.
- 11. Determination of thermodynamic parameters by potentiometry.
- 12. Determination of hydrolysis constant of a weak salt from emf measurements.
- 13. Study of kinetics of hydrolysis of ethyl ethanoate by NaOH using conductance method.
- 14. Determination of concentration of sodium ions by flame photometry.

- 15. Electrogravimetry separation of copper and nickel.
- 16. Study of kinetics of oxidation of alcohols by photometry.
- 17. Verification of Freundlich adsorption isotherm.
- 18. Study of effect of ionic strength on the reaction between persulphate and iodide.

#### **TEXTBOOKS**

- 1. A. Findlay, J.A. Kitchener, Findlay's Practical Chemistry, 8th Edition, Prentice Hall Press, 1954.
- 2. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books, 2012.

#### REFERENCES

1. R.C. Das and B. Behera, Experimental Physical Chemistry, McGraw-Hill Education, 1984.

#### SUGGESTED READING

1. Farrington Daniels, Experimental Physical Chemistry, 7<sup>th</sup> Edition, McGraw-Hill Inc., US, 1970.

# SEMESTER-III & IV COURSE TITLE: PROJECT

Course Code : ( will be filled by EO)Credits: 6Number of hours/cycle: 5

Lear	rning Objective
(i)	Disseminate fundamental concepts/knowledge in their field of research effectively, both in written and oral form.
(ii)	Ethical and moral responsibility in their research and publication will be developed.
(iii)	Enables proficiency in the laboratory, theoretical and computational techniques necessary to contribute to knowledge in their field of research.
(iv)	Identify a new area of research, planning of effective strategies, conduct research, and contribute to the knowledge in their area of work.

CO No.	<b>Course Outcomes</b> Upon completion of this course, students will be able to	PSO's addressed	CL
CO-1	Assess the current status of the area of the research	PSO-1, PSO-5, PSO-6	E
CO-2	Describe concisely about the area of research with relevant studies	PSO-1, PSO-5, PSO-6	E
CO-3	Gain in-sight into deeper knowledge, understanding, capabilities and attitudes in the context of the research work	PSO-1, PSO-5, PSO-6	C

The project work in M.Sc program develop and inculcate a better understanding of research work which improves the skills and decision-making capabilities of the students. It also provides them opportunities to learn with hands-on experience about the various techniques in their respective fields which will give them an insight for pursuing research oriented higher studies also an exposure to the industry-oriented career programs.

# END OF SEMESTER – EXTERNAL ASSESSMENT FOR THEORY COURSES QUESTION PAPER PATTERN & MARK DISTRIBUTION

#### MAXIMUM MARKS: 100

SECTION-A

(10x2=20 marks)

I. Answer all the questions (total 10 questions-2 questions from each unit) Q.No: 1 to 10

**SECTION-B** 

(4x10=40 marks)

**II.** Answer any four questions

Q.No: 11 to 16

SECTION-C

(2x20=40 marks)

**III.** Answer TWO questions (Either Or type)

Q. No: 17 (Or) 18 & Q.No: 19 (Or) 20

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