## ETHIRAJ COLLEGE FOR WOMEN

(AUTONOMOUS)

**CHENNAI - 600 008** 



## **DEPARTMENT OF CHEMISTRY**

Syllabus for

M.Sc. CHEMISTRY

2018 - 2019

ETHIRAJ COLLEGE FOR WOMEN (AUTONOMOUS) CHENNAI – 8

DEPARTMENT OF CHEMISTRY MASTER OF SCIENCE IN CHEMISTRY

## CBC System (Syllabus effective from the academic year 2018 -2019)

Department of Chemistry is revising the syllabus under CBC system with effect from the academic year 2018-2019, as specified by the Government of Tamil Nadu. Electives-(Major) components will enrich the knowledge of the students in the currently developing fields of Chemistry and Electives-(Non-major) will enable the students to be entrepreneurs. In the syllabus there are four Soft skills courses one each in every Semester.

The duration of the course is two academic years. Every academic year is divided into two semesters. Each semester will have a minimum of 90 working days and each day will have 5 working hours. Teaching is organized into a modular pattern of credit courses. Credit is related to the number of lecture, tutorial and practical hours (LTP) for a particular subject. It is also related to the number of hours a student spends learning a subject or carrying out an activity

#### REGULATIONS

## 1. ELIGIBILITY FOR ADMISSION:

Candidates for admission to the first year of the Degree of Master of Science in Chemistry course shall be required to have passed the B.Sc degree examination with Chemistry as the major subject of study of this University or an equivalent examination of some other University accepted by the syndicate. The candidate should have taken Mathematics and Physics as the allied subjects in their undergraduate course.

## 2. ELIGIBILITY FOR THE AWARD OF DEGREE:

A candidate shall be eligible for the award of the Degree only if she has undergone the prescribed course of study for a period of not less than two academic years, passed the examinations of all the four semesters prescribed and earned a total of 93 credits.

#### 3. COURSE OF STUDY:

The main subject of study for Master's Degree in Chemistry shall consist of the following:

Courses	Number	Credit per course	Total Credits
Core Course			
Theory	11	4	44
Project	1	4	4
Practicals	3	4	12
Elective Cou	rses:		
Major	5	3-4	17
Non major	2	3	6
Soft Skill Courses	4	2	8
Internship	1	2	2
	Tota	I	93

### 4. PASSING MINIMUM:

A candidate shall be declared to have passed in each Theory / practical of the Core, Elective (Major and Non Major) subject of study wherever prescribed, if she secured not less than 50 % of the marks prescribed for the end semester examination and also 50% in the sum of end semester examination and continuous assessment. There is no passing minimum for Continuous Assessment (CA).

The maximum marks for CA is 40 and for End Semester examination is 60 (for theory, practicals and Project). The aggregate mark for each paper is 100.

## 5. CLASSIFICATION OF SUCCESSFUL CANDIDATES:

Successful candidates passing the examination and securing the marks

- (i) 60 % and above and
- (ii) 50 % and above but below 60 % in the aggregate shall be declared to have passed the examination in the FIRST CLASS and SECOND CLASS respectively.

Candidates who pass all the examinations prescribed for the course in the First appearance itself alone are eligible for ranking.

## 6. QUESTION PAPER PATTERN:

## CORE and ELECTIVE (Major) Courses:

COMPONENT NATURE OF THE QUE		MAXIMUM MARK
Part A	Definition/Short answers	20
Part B	Understanding, Descriptions / Problems	40 .
Part C	Application / Analysis /	
	Synthesis / Evaluation	40

Part A: All 10 questions to be answered each carrying 2 marks with 2 questions from each unit

 $[10Q \times 2 = 20 \text{ MARKS}]$ 

Part B: All 5 questions to be answered [5Q  $\times$  8 = 40 marks] with an internal choice choosing one semester from each unit

Part C: 2 questions to be answered out of 4 questions covering all the 5 units with a maximum of 4 subdivisions (a,b,c,d) [2Q x 20 = 40 marks]

## **ELECTIVE COURSE (Non Major):**

COMPONENT	NATURE OF THE QUESTION	MAXIMUM MARKS
Part A	Understanding, Descriptions / Problems	40
Part B	Application / Analysis / Synthesis / Evaluation	60

Part A: 8 questions to be answered out of 10 questions covering all the 5 units

[  $8 \, \text{Q x } 5 = 40 \, \text{marks}$  ]

Part B: 6 questions to be answered out of 9 Questions covering all the 5 units

[ 6 Q X 10 = 60 marks ]

#### M.Sc. CHEMISTRY

(Syllabus effective from the year 2018-2019)

#### 1. OBJECTIVES OF THE COURSE:

- (i) To provide an advanced knowledge in Chemistry and also expose the students to research.
- (ii) To have a career in the following areas after completion of the course with a M.Sc degree in Chemistry
  - (a) a teaching career in a college for science and engineering courses.
  - (b) a job in a scientific laboratory / R&D Departments / Chemical industry.
  - (c) a research career in an academic institution or a National Institute / Laboratory.
  - (d) one's own industry and be an entrepreneur.
- (iii) All the topics in the NET/SLET syllabus for Chemistry are incorporated as passing the NET/SLET is a pre-requisite for UGC/CSIR Research Fellowship, for recruitment of college teachers and an added qualification for many research positions.

## 2. PREAMBLE:

- Modification of course contents in few courses based on feedback from students and report given by Academic audit members.
- 5 Elective (Major) –courses on the current topics.
- Project based on current topics.
- Practical Examination conducted at the end of even semester
- Internship at the end of the II semester.
- Four soft skills courses one in each semester
- Two non major electives courses one each in II and III semester.

#### 3. COURSE PROFILE:

Total Credits: 93

Core	:	60
Major Elective	:	17
Non major elective	:	06
Soft skills	:	08
Internship	:	02

Semester	Ι	$\Pi$	$\mathbf{m}$	$\mathbf{IV}$
Credits	18	30	20	25

#### M.Sc. CHEMISTRY

## CHOICE BASED CREDIT SYSTEM (CBCS)

## From 2018-2019 Batch onwards

## Preamble

- Modification of course contents in few courses based on feedback from students and report given by Academic audit members.
- 5 Elective (Major) –courses on the current topics.
- Project based on current topics.
- Practical Examinations are conducted once in an academic year ie at the end of semester II, and IV
- Internship at the end of the II semester.
- Four soft skills courses one in each semester
- Two non major electives courses one each in II and III semester.

## COURSE PROFILE

	COURSE PROFILE									
				SEM	ESTER –I					
Course code	Course title	L	T	P	Total	Credit	Exam		MARK	S
		S		359	Hours /week		Hrs	CA	SE	TOTAL
6P18/1C/OC1	Core 1- Organic Chemistry – I	4	1	0	5	4	3	40	60	100
6P18/1C/IC1	Core 2 -	4	1	0	5	4	3	40	60	100
	Inorganic Chemistry – I									
6P18/1C/PC1	Core 3 - Physical Chemistry – I	4	1	0	5	4	3	40	60	100
6P18/1E1/NAC	Major Elective 1-	4	1	0	5	4	3	40	60	100
	Nano Chemistry									
	*Core Practical- 1-Organic Chemistry	-	-	-	4	-			-	1 5
, a	*Core Practical - 2- Inorganic Chemistry	-	-	-	4	-		-	×-	- 2
PG18/1S/PEW	Soft skill 1 –	2	0	0	2	2	2		50	50
	Personality Enrichment for Women				20	10				
	Total				30	18	-			

	SEMESTER – II									
Course code	Course title	L	Т	P	Total	Credit	Exam		MA	RKS
	-				Hours		Hrs	CA	SE	TOTAL
		G			/week					
6P18/2C/OC2	Core 4 - Organic	3	1	0	4	4	3	40	60	100
	Chemistry – II									
6P18/2C/IC2	Core 5 -Inorganic	3	1	0	4	4	3	40	60	100
	Chemistry – II									
6P18/2C/PC2	Core 6 - Physical	3	1	0	4	4	3	40	60	100
	Chemistry – II									
6P18/2E2/SPE	Major Elective 2 -	3	1	0	4	3	3	40	60	100
	Spectroscopy									
6P18/2E/COS	Non Major Elective 1	3	1	0	4	3	3	40	60	100
	- Cosmetology									
6P18/2C/PR1	*Core 7 - Practical –1	-	-		4	4	6	40	60	100
	Organic Chemistry									
6P18/2C/PR2	*Core 8 - Practical -2	-	-	-	4	4	6	40	60	100
	-Inorganic Chemistry			i.						
6P18/2C/INT	Internship	-	-	-	-	2	-	-	-	-
	0.0.131.0.1		0	0	2	2			50	<b>7.0</b>
DC10/00/LOE	Soft skill- 2 Language	2	0	0	2	2	2	-	50	50
PG18/2S/LCE	and Communication									
	in English/Soft Skill									
PG18/2S/FRE	in French/Soft Skill									
PG18/2S/FRE PG18/2S/GER	in German									
FG18/28/GER	Company Street S									
							,			
						20				
	Total				30	30				

	SEMESTER – III								
Course Code	Name of the Course	LTP	Hours/ Week	Credits	Exam Hours	M	Marks		
			WCCK		Hours	CA	SE	Total	
6P18/3C/OC3	Core 9 - Organic	3 1 0	4	4	3	40	60	100	
	Chemistry – III								
6P18/3C/IC3	Core 10 - Inorganic	310	4	4	3	40	60	100	
	Chemistry – III								
6P18/3C/PC3	Core 11- Physical	310	4	4	3	40	60	100	
	Chemistry – III								
6P18/3E3/PHC	Major Elective 3-	310	4	3	3	40	60	100	
	PhotoChemistry					Land Company			
6P18/3E/FDP	Non Major Elective -2	310	4	3	3	40	60	100	
	Fibre Fabrics, Dyeing and								
	Printing of Textiles								
	*Core Practical III –	-	4	-	-	40	60	100	
	Physical Chemistry								
	*Core - Project	-	4	-	= ;	40	60	100	
6P18/3S/LSS	Soft Skill 3- Laboratory	200	2	2	2	_	50	50	
	Safety Skills		-						
	Total		30	20					
							<u></u>		

	SE	MESTE	R – IV		8			
Course Code Name of the Course	Name of the Course	LTP	Hours/	Credits	Exam	Marks		
			Week		Hours	CA	SE	Total
6P18/4C/OC4	Core 12 - Organic Chemistry – IV	410	5	4	3	40	60	100
6P18/4C/IC4	Core 13 - Inorganic Chemistry - IV	410	5	4	3	40	60	100
6P18/4E4/ECC	Major Elective 4 - Electrochemistry and Computational Chemistry	410	5	4	3	40	60	100
6P18/4E5/POC	Major Elective 5 -Polymer Chemistry	310	4	3	3	40	60	100
6P18/4C/PR3	*Core 14 Practical III - Physical Chemistry	-	4	4	6	40	60	100
6P18/4C/PRO	*Core 15 - Project	=	5	4	ing <del>t</del> em	40	60	100
6P18/4S/SRP	Soft Skill 4- Scientific Research and Presentation Skills	200	2	2	2	-	50	50
		Total	30	25				×
		Total (	Credits	93				

L = Lecture hours, T = Tutorial hours, P = Practical hours

The above highlighted courses of the pg programme enriche the Skills in employability skill Development/entreprenuership which caters the needs of the students.

CA = Continuous Assessment marks, SE = End semester Marks

<sup>\*</sup>Practical Examinations are conducted once in a Academic year ie at the end of II & IV Semester

#### **EVALUATION PATTERN**

#### Theory & Practicals

CA Marks : 40 End Semester Examination Marks : 60 Total Marks : 100

Theory: Continuous Assessment (CA)

#### **Pattern for Continuous Assessment**

			CA marks
Test I	2hrs.	50 marks	10
П	2hrs.	50 marks	10
Quiz/ Assignment/	10		
Participatory Learni	ng		10
	To	tal .	40

## Practical Continuous Assessment (CA):

(a)	One Test	-	10 marks
(b)	Skill in practical	-	10 marks
(c)	Viva -Voce	-	10 marks
(d)	Record	-	10 marks
			40 Marks

End Semester Examination questions are to be chosen from the question bank by the External Examiner and evaluated by both Internal and External Examiners.

## **Rubrics for Continuous Assessment**

**Assignment:** Appearance, contents, originality, presentation, schematic representation and diagram, bibliography.

Seminar: Organization, subject knowledge, visual aids, confidence level, presentation.

Participatory learning: Answering questions, clearing doubts, participation in discussion, attendance, communication and language.

Field trip: Participation, Preparation, respect, attitude, leadership.

Project: Preliminary work, design, content, presentation.

End Semester Examination question papers are to be set by the External Examiners and evaluated by both Internal and External Examiners.

Duration of end semester examination is 3 hours and maximum mark is 100.

#### SEMESTER - I

Title of the Course: Core 1- Organic Chemistry- I

Teaching hours:  $15 \times 5 = 75$  Credits: 4

Course Code: 6P18/1C/OC1 LTP 4 1 0

## **Objectives:**

1. To study the concepts in Optical isomerism and Asymmetric synthesis

- 2. To study the concepts of Prochirality Prostereoisomerism
- 3. To study the conformation and stereoisomerism of cyclohexane, decalins and their relationship with reactivity
- 4. To study Linear free energy relationships and Neighbouring group participation
- 5. To study the mechanisms and stereochemistry of Elimination reactions.

#### COURSE OUTLINE

UNIT I: Optical isomerism: Sterochemistry and conformational analysis: Optical activity and chirality, classification of chiral molecules as asymmetric and dissymmetric. A brief study of dissymmetry of allenes, biphenyls, spiro compounds, trans-cyclooctene, cyclononene and molecules with helical structures- hexahelicene. Absolute configuration – D. L and R, S- notations of biphenyls and allenes. Saw horse, Newmann and Fischer projection representations and interconversion (restricted to molecules with one to five asymmetric carbon atom). Erythro and threo nomenclature, Asymmetric synthesis and Absolute asymmetric synthesis - Principle Categories of asymmetric synthesis - Chiral substrate, Chiral reagents-Asymmetric hydroboration, Chiral auxillary -derived from Proline, Menthol, modification of Lithium Aluminium Hydride - BINAL - H- application in reduction of enantiotopic ketone . Chiral catalyst - Sharpless asymmetric Wilkinson catalyst enantioselectivity. enoxidation Chiral diastereoselectivity, Optical Purity, Cram's rule and Prelog's rule.

15 hrs

- UNIT II: Geometrical isomerism: E, Z nomenclature of olefins. Geometrical and optical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentane. Identification- enantiotopic, homotopic, diastereotopic ligands and faces and prochiral carbons and nomenclature of enantiotopic hydrogens.

  Stereospecific and stereoselective synthesis. Chemoselectivity, regioselectivity and regiospecificity.

  15 hrs
- <u>UNIT III</u>: Conformational analysis: Conformational analysis of cyclohexane and mono, di-substituted cyclohexanes and their stereochemical features (Geometrical and optical isomerism if shown by their derivatives) conformation and reactivity of substituted cyclohexanols (oxidation and acylation) and cyclohexane carboxylic acid derivates (esterification and hydrolysis) conformation and stereochemistry of cis and trans decalin and 9-methyldecalin, decalones

- <u>UNIT IV</u>: Reaction Mechanism: Kinetic and non kinetic methods of determining organic reaction mechanisms. kinetic and thermodynamic controlled products. Neighbouring group participation Substitution in norbornyl and bridge head systems, Reactivity, structural and solvent effects in substitution reactions. Hammett equation- simple problems and Taft equation, substitution at allylic and vinylic carbons, substitution by ambident nucleophiles-such as CN, NO<sub>2</sub>, phenoxide and ambident dianions. Williamsons reaction, Von-Braun reaction, Dieckman condensation and Claisen condensation. 15 hrs
- <u>UNIT V</u>: Elimination: E<sub>1</sub>-E<sub>2</sub>-E<sub>1cb</sub> spectrum orientation of the double bond- Hofmann and Saytzeff rule. Competition between elimination and substitution. Sterochemistry of E<sub>2</sub> eliminations, Elimination in cyclohexane ring system. Mechanism of Pyrolytic eliminations. Examples- Chugaev reactions and Cope elimination, Hofmann degradation, pyrolysis of esters.

  15 hrs

#### RECOMMENDED TEXTBOOKS:

- 1. Jerry March, Advanced organic Chemistry, 6<sup>th</sup>edn. John Wiley and Sons, Inc.1992
- 2. Ernest Eliel, Sterochemistry of carbon compounds, 1st John Wiley and Sons
- 3. I.L. Finar, Organic Chemistry Vol I, 5<sup>th</sup> edn ELBS
- 4. I.L. Finar, Organic Chemistry Vol II, 5<sup>th</sup> edn ELBS

## **REFERENCE BOOKS:**

- 1. Neil Isaac, Physical organic Chemistry, ELBS publication. 2<sup>nd</sup> edn Longmann 1995
- 2. Stanley H.Pine, Organic Chemistry, 5<sup>th</sup> edn Mac Graw Hill 1987
- 3. E.S.Gould, Mechanism and Structure in Organic Chemistry
- 4. Francis A.Carey and Richard, Advanced organic Chemistry, Part A & B by 5<sup>th</sup> edn J.Sundberg Plenum Press
- 5. P.S.Kalsi, Sterochemistry, conformation and mechanism, 7<sup>th</sup>Wiley Eastern Ltd., Chennai
- 6. D.Nasipuri, Sterochemistry of organic compounds, principles and applications, 3<sup>rd</sup> Wiley Eastern Ltd.,
- 7. Petersykes, A Guide book to mechanism in organic Chemistry 5<sup>th</sup>edn John Wiley 1981
- 8. Y.R.T.Morrison, R.N.Boyd, Organic Chemistry VI edition, Prentice- Hall of India Pvt, New Delhi
- 9. G.Solomon, Organic Chemistry, C.B.Fryhle 8<sup>th</sup> edn Wiley 2003

## PERIODICALS:

- 1. Journal of Organic Chemistry
- 2. Indian Journal of Chemistry B
- 3. Current Science
- 4. Organic Letters
- 5. Tetrahedron Letters

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http://swayam.gov.in
- 6. http://search.ebscohost.com

#### SEMESTER-I

Title of the course: Core-2 Inorganic Chemistry - I

Teaching hours:  $15 \times 5 = 75$  Credits: 4

Course Code: 6P18/1C/IC1

L T P 4 1 0

### **Objectives:**

1. To impart detailed knowledge in different aspects of coordination Chemistry.

- 2. To understand the concepts of spin orbit coupling, micro states and term symbols of free ion
- 3. To show the importance of electronic transitions in metal complexes and their absorption spectra.
- 4. To understand the outer and inner sphere reactions in coordination complexes
- 5. To impart the knowledge about the mechanism involved in substitution reaction in coordination complexes

#### COURSE OUTLINE

- <u>UNIT I:</u> Crystal field theory and its limitations: Application to octahedral and tetrahedral systems-Measurement of 10Dq. Factors affecting crystal field splitting. Strong and weak field-Evidence in support of crystal field effect-Octahedral Vs Tetradehdral. Octahedral site stabilization energy-Jahn Teller distortion- Square planar complexes-Nephelauxetic effection favour of metal ligand oribital overlap.

  15hrs
- <u>UNIT II:</u> Molecular orbital theory: Octahedral and tetrahedral systems- construction of ligand group orbitals- site inspection –use of symmetry pi-bonding in octahedral system. Molecular orbital picture of square planar systems. Spin Orbit coupling RS and jj coupling micro states and term symbols. Terms of free ions.
- UNIT III: Splitting in octahedral and tetrahedral fields: Orgel and Tanabe Sugano diagrams- Electronic transitions in metal complexes- Analysis of electronic absorption spectra of complexes- selection rule-vibronic coupling-dp mixing-spin spin and spin orbit coupling- charge transfer spectra.

  15 hrs
- <u>UNIT IV:</u> Electron transfer reactions: Outer sphere-exchange and cross reactions-Marcus equation-complementary and Non complementary electron transfersinner sphere- Bridging ligand-role-Resonance and radical mechanisms.

15 hrs

<u>UNIT V:</u> Substitution reactions- Classification A, D and interchange mechanisms. Substitution in square planar complexes- influence of nature of leaving, entering groups and other ligands present on rate. Trans effect, cis effect, parallel path mechanisms-Evidence –substitution in octahedral complexes— anation-acid catalysed hydrlysis- Based catalysed- CB mechanism Evidence.

15 hrs

#### RECOMMENDED TEXTBOOKS:

- 1. Inorganic Chemistry, F.Purcell and J.C.Kotz, W.B.Sounders & Co (1980)
- 2. Coordination Chemistry D Banerjea Tata McGraw Hill 1994
- 3. Inorganic Chemistry: Principles of Structure and Reactivity (4th Edition), 1997 by James, Ellen, Richard L. Keiter
- **4.** Advanced inorganic Chemistry FA Cotton & G.W.Wilkinson, John Wiley & sons 1988
- 5. Coordination Chemistry –S.F.A.Kettle., ELBS 1973.
- 6. Coordination Chemistry Basalo & Johnson
- 7. Inorganic Chemistry Shriver & Atkins, oxford University press- 3<sup>rd</sup>edn 1999

#### REFERENCE BOOKS:

- Mechanisms of Inorganic reactions- Basalo F.and R.G.Pearson, 2<sup>nd</sup> edn 1967, John Wiley
- 2. Inorganic reaction Mechanism, Tobe M.L.Nelson, London 1972
- 3. Ligand substitution processes, Langford C.H.and H.B.Gray, Benjamin Newyork 1965
- 4. Mechanisms of inorganic reactions in solution, Benson D McGrawHill London 1968
- 5. E.J.Corey and J.C.Bailar Jr- J.Am chem.Soc. 81, 2620 (1959)
- 6. J.R.Gollogly, C.J.Hawkins and J.K.Beattle, Inorg. chem., 10, 317 (1971)
- 7. Complexes of I row transition elements D. Nicholos
- 8. Introduction to ligand fields- B.N.Figgis- John Wiley- New york 1966
- 9. Introduction to ligand field theory, Ballhausen C.J, McGrawHill, New york 1962

#### PERIODICALS:

- 1. Coordination Chemistry review.
- 2. Inorganica Chimica acta
- 3. J.Coordination Chemistry
- 4. Current Science
- 5. Journal of Indian chemical society
- 6. Chemical society review
- 7. Polyhedron

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http://swayam.gov.in
- 6. http://search.ebscohost.com

## **SEMESTER-I**

Title of the course: Core 3-Physical Chemistry-I

Teaching hours:  $15 \times 5 = 75$  Credits: 4

Course code: 6P18/1C/PC1 L T P 4 1 0

## **Objectives:**

1. To provide a significant knowledge in theories of chemical reactions, and its applications.

- 2. To study the kinetics of reactions and the effect of experimental parameters on it
- 3. To understand the significance and applications of Radiation Chemistry
- 4. To study the concepts of molecular and crystallographic symmetry
- 5. To apply the concepts of symmetry for the study of molecular bonding and spectroscopy.

#### COURSE OUTLINE

- <u>UNIT I:</u> Chemical Kinetics-I: Theories of reactions-effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindemann and Christiansen hypothesis- molecular beams, collision cross sections, effectiveness of collisions, potential energy surfaces. Transition state theory —based on thermodynamic and statistical mechanics-partition functions and activated complex- Eyring equation estimation of free energy, enthalpy and entropy of activation and their significance.

  15hrs
- UNIT II: Chemical Kinetics-II: Reactions in solutions, reactions in ideal solutions, effect of pressure, di-electric constant, ionic strength on rate of reactions in solution primary salt effect and secondary salt effect, kinetic isotope effects, linear free energy relationships- Hammett and Taft equations- Homogeneous catalysis- acid- base catalysis-mechanism of acid base catalysed reactions-Bronsted catalysis law, enzyme catalysis-Michaelis-Menten catalysis, Line Weaver Burk method, influence of pH and temperature.
- <u>UNIT III</u>: Radiation Chemistry: Range of radiations, interaction of γ radiation with matter -photoelectric effect, Compton effect and pair production, neutrons through matter-elastic and inelastic scattering, significance, radiation dosimetry-Fricke dosimeter, ceric sulphate dosimeter, conversion of dose values, radiolysis of water, hydrated electron-methods of generation, properties, structure and uses. Radiometric titrations and applications. Radiation precautions

15 hrs

- **UNIT IV**: Group Theory: Symmetry elements and symmetry operations, point groupsidentification and determination, comparison of molecular symmetry with crystallographic symmetry, reducible and irreducible representations, direct product representation, Great Orthogonality theorem and its consequencescharacter tables-C2V & C3V
- **Applications of Group Theory:** Hybrid orbitals in non-linear molecules (Examples H<sub>2</sub>O, NH<sub>3</sub>, BF<sub>3</sub>, determination of representations of UNIT V vibrational modes in non-linear molecules (H2O, NH3 BF3, XeF4, PCl5 and SF<sub>6</sub> symmetry selection rules for infra red and Raman spectra – electronic spectra of ethylene and formaldehyde. SALC principle (H<sub>2</sub>O, NH<sub>,3</sub>)

  15 hours

#### RECOMMENDED TEXT BOOKS:

- 1. K.J.Laidlar Chemical Kinetics, Harper and Row, Newyork, 1987 J.Rajaram
- 2. J.C.Kuriacose- Kinetics of Mechanism of Chemical Transforantions, Macmillan India Ltd., 1983
- 3. V. Ramakrishnan and M.S.Gopinathan Group Theory in Chemistry, Vishal Publications, 1988
- 4. K.V.Raman- Group theory and its applications to Chemistry, Tata Mc Graw Hill Publishing Co., 1990
- 5. Essentials of Nuclear Chemistry, Arnikar, Hari Jeevan, ISBN: 978-81-224-3203-9 (2011)

#### **REFERENCE BOOKS:**

- 1. W.J.Moore- Physical Chemistry, Orient Longmann, London, 1972
- 2. G.M.Barrow-Physical Chemistry, Mc Graw Hill, 1988R.
- 3. G.Frost and Pearson-Kinetics and Mechanism, Wiley Newyork, 1961.
- 4. C.Capellos and B.H.J.Bielski- Kinetic systems, Wiley inter science, Newyork 1972
- 5. G.M.Harris- Chemical Kinetics, D.C.Heath and Co., 1966
- 6. F.A.Cotton Chemical Applications of Group theory, John Wiley and Sons Inc., Newyork 1971.
- 7. N.Tinkham- Group Theory and Quantum Mechanics, Mc Graw Hill Book Company, Newyork, 1964
- and 8. D.S.Schonland Molecular symmetry Group Programmed introduction to chemical application, Wiley, Newyork (1977)
- 9. Paul L Houston- Chemical Kinetics and Reaction dynamics, Dover publications (2006)
- 10. E.T.Denisov,O. M. Sarkinov and GI. Likhlenshtein,Chemical Kinetics Fundamentals and new Development by Elsevier publication 2003
- 11. B S Garg Chemical applications of molecular symmetry and group theory. Macmillan 2013

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education
- 6. Journal of American chemical society
- 7. Bulletin of material science

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com
- 7. http://www.ch.ic.ac.uk/vchemlab/symmetry/
- 8. http://www.reciprocalnet.org/edumodules/symmetry/intro.html
- 9. http://www.win.tue.nl/~amc/ow/gpth/reader.pdf

#### SEMESTER - I

Title of the course: Major Elective 1- Nano Chemistry

Teaching hours:  $15 \times 5 = 75$  Credits: 4

Course Code: 6P18/1E1/NAC LTP 410

## **Objectives:**

1. To introduce and give an insight into the fascinating area of nanoscience & its development.

2. To learn the experimental techniques of nonoscale synthesis.

- 3. To understand the tools of characterization of nano scale features.
- 4. To understand the variation of properties upon size
- 5. To study the applications of Nano materials
- UNIT I: Background to nanoscience and nanotechnology: Scientific revolutionsnanosized effects- surface to volume ratio-atomic structure-molecules &
  phases- energy at the nanoscale molecular and atomic size-quantum effectstypes of nanotechnology and nano machines. Definition of nano systemdimensionality and size dependent phenomena, Quantum dots, Nanowires
  and Nanotubes, 2D films; self assembly systems NanotechnologyNanomaterials-Fillers, fibres, Wires, Fluids, tubes-CNT, Graphene,
  Nanoclays-types.
- UNIT II: Experimental Techniques and Separation: Mechanical methods: grinding-high energy ball milling-types of balls-WC and ZrO<sub>2</sub>-material-ball ratio-medium for grinding. Physical methods: Vapour deposition and different types of epitaxial growth techniques-Pulsed laser deposition, magnetron sputtering-micro Lithography, photolithography, soft lithography, e-beam writing, -laser ablation-RF/DC magnetron sputtering-microwave plasma evaporation control of grain size-scale up process. Chemical methods: Sol-gel technique-Solvo thermal methods-control of grain size-Co-precipitation hydrolysis- Sonochemical method combustion technique-colloidal precipitation template process.
- UNIT III: Characterization using Analytical tools: Applications of UV-Vis, NIR, FTIR, FT-Raman, Photoluminescence, NMR, ESR and Light scattering methods. X-ray techniques: X-ray power diffraction- Crystallite size determination- Sherrer equation, structure analysis, use of JCPDS, determination of crystal systems-accurate lattice parameters. Electron Spectroscopy: X-ray Photoelectron Spectroscopy, Auger electron spectroscopy, X-ray characterization of nanomaterials. SEM, TEM, AFM 15hrs

<u>UNIT IV</u>: Properties at the Nano scale: Electrical properties- electrical conductivity,

Optical properties absorption and luminescence, Magnetic Properties- Para,
Dia, Ferro and Ferri magnetism, Super paramagnetism- SPIONS, Mechanical properties micro hardness fracture toughness, plastic nature of nanoceramics

15 hrs

<u>UNIT V</u>: Applications: Ceramics and Composites: membranes for purification of water, catalysis-tooth and bone substitute-hydroxyappetites-inductive bone-replacements of ceramic valves. Capping and caging system-dendrimers-functionalisation of CNT. Environmental applications-nanotoxicology-biomediation-removal of microbes, sensors for DNA, proteins, detection of malignancy and biological applications
 15 hrs

## **RECOMMENDED TEXTBOOKS:**

- 1. Nanoscale materials in Chemistry, Kenneth, J. Klabunde willey Interscience, 2001
- 2. Nano: The essentials, T. Pradeep Tata McGraw-Hill Publishing Company Limited, 2007.

## **REFERENCE BOOKS:**

- 1. Nano and Microelectromechanical Systems: Fundamentals of Nano and microengineering, Sergy Lyshevski, Vallabh publications 2/e 2005.
- 2. Nanotechnology Environmental application and Solutions, Lious Theodore, Robert g.Kunz palgrave macmillan 2005.
- 3. Nanostructure & Nanomaterials: Synthesis, Properties & Applications, G. Cao, Imperial College Press, 2004.
- 4. Nanomaterials, Nanotechnologoes and Design: An introduction for Engineers and Architects, Micheal F. Ashby. P.J. Ferria. D.L. Schodekpalgrave macmillan 2005.

### PERIODICALS:

- 1. Current Science
- 2. Journal of nanotechnology
- 3. Journal of nanomaterials

- 1. http://search.ebscohost.com
- 2. http://nisenet.org/
- 3. http://www.nanoparticles.org/nano%20links/
- 4. http://www.nsti.org/
- 5. http://nanozone.org/
- 6. http://www.understandingnano.com/
- 7. http://www.nanoparticles.org/nano%20links/
- 8. http://www.nanotechweb.org/
- 9. http://www.pjonline.com/pdf/forum/pj\_20060318\_apsgb.pdf

## SEMESTER - II

Title of the course: Core 4-Organic Chemistry-II

Teaching hours:  $15 \times 4 = 60$  Credits: 4

Course Code: 6P18/2C/OC2 LTP 310

## **Objectives:**

- 1. To provide an understanding of the mechanisms of important oxidation reactions using different reagents .
- 2. To study the reactions of reactive intermediates viz carbenes and nitrenes,
- 3. To study some important rearrangements in organic chemistry.
- 4. To study the generation of free radicals and aromatic radical substitution reactions
- 5. To study the mechanism of reduction reaction using different reducing agents.

#### COURSE OUTLINE

- UNIT I: Oxidation: Mechanism of oxidation of alcohols & aldehydes with Cr (VI) & Mn (VII) oxidants; Oxidation of C=C and C-H bonds; Uses of PCC, PDC and Collin's reagent. Peroxy oxidations-Alkene epoxidation by peracids and metal/alkyl hydroperoxides. oxidation of methylene to carbonyl, oxidation of arylmethanes- allylic oxidation of olefins, Oppenauer oxidation; Prevost and Woodward hydroxylation of alkenes; Oxidative cleavage of C-C single and double bonds; Periodates, LTA and Osmium tetraoxide.
   12hrs
- WNIT II: Reduction: Selectivity in reduction of 4-t-butylcyclohexanone using selectrides-hydride reductions, Clemmensen, Wolf-Kishner reductions-Modification of Wolff-Kishner reduction, Birch reduction, MPV reduction, Catalytic hydrogenation and selectivity in reduction Reduction with LiAlH<sub>4</sub>, NaBH<sub>4</sub> tritertiarybutyoxyaluminium hydride, sodium cyanoborohydride, trialkyltin hydride, Acyloin condensation.
- <u>UNIT III:</u> Reactive Intermediates Carbenes: Stability, structure and spin states of carbenes; Cyclopropanation-spin dependence and stereoChemistry; Carbene insertion to C-H bonds; Rearrangement to alkenes, Wolff rearrangement .Simmon Smith reaction. Nitrenes: Stability, structure and spin states of nitrenes; C-H bond insertions and aziridine formation; Rearrangement of acylnitrenes (Hoffmann, Curtius and Schmidt reactions with applications in organic synthesis).

12hrs

<u>UNIT IV</u>: Free radicals: Long lived and short lived free radicals, methods of generation of free radicals. Addition of free radicals to the olefinic double bonds. The following aromatic radical substitutions are to be studied. Sandmeyer reaction, Gomberg-Bachmann reaction, Pschorr reaction Ulmann

reaction, Mechanism of Hunsdieker reaction and Barton deoxygenation. **Aryne** -Methods of generation of benzyne intermediate, and trapping of aryne intermediate

12hrs

<u>UNIT V:</u> Molecular Rearrangements: Migratory aptitudes: A detailed study of the molecular rearrangements mechanism of the following rearrangements: Wagner Meerwein Rearrangements, Demjanov, dienone-phenol, Baeyer-Villeger, Favorski, Steven, and Von-Richter re-arrangements, Sommlet-Hauser, (A few examples in each re-arrangement are to be studied). 12hrs

#### RECOMMENDED TEXT BOOKS:

- 1. Organic Chemistry V Edition (1986) 5<sup>th</sup> Vol I by I.L.Finar, ELBS Publication
- 2. Advanced Organic Chemistry, 4<sup>th</sup> Edition by Jerry March, Wiley Eastern Ltd., New Delhi
- 3. Principles of organic synthesis R.O.C. Norman, Chapman and Hall, London. 2<sup>nd</sup> edition 1980.
- 4. Peter Sykes, A guide book to mechanism in organic Chemistry 5<sup>th</sup> edn John Wiley 1981

## **REFERENCE BOOKS:**

- 1. Advanced Organic Chemistry by Francis A.Carey and Richard J.Sundberg, 5<sup>th</sup> Edition plenum press, New york (1990), Part A& B
- 2. Organic Chemistry, 6<sup>th</sup> edn(1992), Y.R.T.Morrison, R.N.Boyd, prentic-Hall of India Pvt.. New Delhi
- 3. Mechanism and Structure in organic Chemistry by E.S.Gould
- 4. Carbenes, Nitrenes and Arynes by T.L. Gilchrist and C.W. Rees, Thomas Nelson and Sons Ltd., London 1<sup>st</sup> edition
- 5. Organic Reaction Mechanism by S.M. Mukherji and S.P. Singh, MacMillan India Ltd., 3 rd Chennai (1990)
- StereoChemistry and Mechanism through solved problems by P.S. Kalsi.7<sup>th</sup> Wiley Eastern Ltd., (1994)

## PERIODICALS:

- 1 Journal of Organic Chemistry
- 2. Indian Journal of Chemistry B
- 3. Current Science
- 4. Organic Letters
- 5. Tetrahedron Letters

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com

## SEMESTER-II

Title of the course: Core-5 Inorganic Chemistry-II

Teaching hours:  $15 \times 4 = 60$  Credits: 4

Course Code: 6P18/2C/IC2 LTP 310

## Objective:

1. To introduce different boranes and carboranes and important aspects of structural Inorganic chemistry.

- 2. To study the important aspects of solid state chemistry
- 3. To bring out the significance of solid state defects
- 4. To study the magnetic properties of transition metal complexex
- 5. To study novel inorganic compounds

#### **COURSE OUTLINE**

- <u>UNIT I</u>: Structural aspects of boranes: Different types of Boron hydrides-Nido, arachno and closo- Lipscomb's rule- structure and bonding in polyboranes-Reactions of polyboranes-carboranes and metallo carboranes-structure.12hrs
- UNIT II: Structural aspects of metallic clusters and poly anions of important compounds. Poly organophosphazenes, poly sulphur-nitrogen compounds structure-properties correlation. Iso and hetero poly anions of Vanadium, chromium, molybdenum and tungsten- structural aspects only. Metal clusters Binuclear and trinuclear clusters of Rhenium, Chromium, Molybdenum and Tungsten- Octahedral clusters- Metal only clusters structure and bonding only.
- <u>UNIT III</u>: Solid state Chemistry I: The Bravais Lattices simple, body centered, face centered and end centered arrangements-slide axis-Glide planes- Space groups- Miller indices- Interplanar distances-Bragg's equation, x-ray powder data in identifying inorganic crystalline solids- details for cubic systems. Van Lane equation- Determination of structure.

  12 hrs
- <u>UNIT IV</u>: Crystal Structure and defects NaCl, CsCl, ZnS (Wurtzite & sphalarite), Diamond, Graphite, Nickel arsenide NiAs, Rutile, cadmium iodide, perovskite, spinels (normal and inverse). Stoichiometric and Non stoichiometric defects- Schottky, Frenkel, Metal excess, Metal deficiency, line, plane defects- Shear planes, F centers, Defect spinels. Non stoichiometric compounds. Photo Conductors: Principle and application-Liquid Crystals-Types and Applications
- <u>UNIT V</u>: Diffusion in solids: Diffusion mechanisms- phase transitions, solid solutions, order disorder transformations and super structure formations, solid state electrolytes, solid state reactions- Band theory of solids- Semi conductors-p-n

junctions- rectifiers, super conductivity-Meissner state-Type I & II super conductors-Magnetic properties of solids-para, ferro and antiferro magnetism-ferrites structure significance. Hysterisis-spin only magnetic moment- orbital contribution- systems with A,E and T ground terms. Determination of magnetic susceptibility by Guoy and Faraday methods- Optical properties of solids- Inorganic phosphors, Garnets, solid state Lasers. 12hrs

## RECOMMENDED TEXT BOOKS:

- Principles of electronics V.K.Mehta & Rohit Mehta, Sultan chand & sons, 9<sup>th</sup> edn 2006
- 2. Solid State Chemistry and its Applications, 2nd Edition, Student Edition, Anthony R. West, 2014 Wiley
- 3. Fundamentals of crystal Chemistry- TRN Kutty & JAK Tareen Universities Press (2001)
- 4. Introduction to solids L.V.Azaroff MacGraw Hill New york 1960
- 5. Elements of x-ray crystallography L.V.Azaroff, Mc.Graw-Hill Inc, New york (1968)
- 6. Inorganic solids D.M.Adams Wiley (new york) 1974
- 7. Inorganic Chemistry: Principles of Structure and Reactivity (4th Edition), 1997by James E. Huheey, Ellen A. Keiter, Richard L. Keiter
- 8. Advanced Inorganic Chemistry- A comprehensive text- F.A.Cotton & G.Wilkinson- John- Wiley V edn 1988
- 9. Structural principles in Inorganic compounds W.E.Addison John Wiley & Sons, Newyork (1961)
- 10. Modern aspects of inorganic Chemistry, H J Emeléus; A G Sharpe 4<sup>th</sup> edn (1973)

## REFERENCE BOOKS:

- 1. Structural inorganic Chemistry A.F.Wells., 5<sup>th</sup> edition, 2014 Clarendon press, oxford (1985)
- 2. Inorganic structural Chemistry. A. Miller Wiley, New york 1993
- 3. New directions in solid state Chemistry, CNR Rao and J.Gopalakrishnan, Cambridge University press (1997)

## PERIODICALS:

- 1. Inorganica Chimica acta
- 2. Polyhedron
- 3. Chemical reviews
- 4. Current Science
- 5. Journal of Indian chemical society
- 6. Journal of American chemical society
- 7. Bulletin of material science

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com

### SEMESTER-II

Title of the course: Core-6 Physical Chemistry-II

Teaching hours:  $15 \times 4 = 60$  Credits: 4

Course Code: 6P18/2C/PC2 L T P 3 1 0

## **Objectives:**

1. To study the concepts and applications of quantum Chemistry.

- 2. To study the approximation methods in quantum chemistry
- 3. To study chemical bonding in diatomic molecules and HMO theory
- 4. To study the kinetics of complex reactions and methods to study fast reactions
- 5. To study various adsorption isotherms and mechanisms of Heterogeneous catalytic reactions

#### **COURSE OUTLINE**

- UNIT I: Quantum Chemistry I: wave equation for electrons, the wave function and its physical meaning. Functions and operators- eigen function, eigen values, Hamiltonian operator, angular momentum operator- commutation of operators. Hermitian property of operators. Basic postulates of quantum mechanics. Application of quantum mechanics-particle in a 1Dbox, three dimensional box and simple harmonic oscillator. Application of quantum mechanics- particle in a ring, rigid, rotator, hydrogen atom. Complete wave function of hydrogen like atoms, significance of quantum numbers n,l.m, physical representation of the orbitals, radial distribution, points of maximum probability, angular probability distribution.
- <u>UNIT II</u>: Quantum Chemistry II: Approximation methods-variation method and perturbation method-application to hydrogen and helium atom. Symmetric and anti-symmetric wave function, general principles of setting up of wave function for many electron atoms- Pauli's principle -Slater type orbitals. Hartree and Hartree Fock SCF method.

12hrs

- <u>UNIT III</u>: Quantum Chemistry III: Chemical Bonding-Born-Open Heimmer approximation. VB and MO treatment of H<sub>2</sub> and H<sub>2</sub><sup>+</sup>, MO theory for homo nuclear and hetero nuclear diatomic molecules. HMO calculations for simple molecules like ethylene, butadiene and cyclobutadiene. Evaluation of co-efficients and eigen values for simple molecules, electron density, bond order an free valence index.
- <u>UNIT IV</u>: Chemical Kinetics III: Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. General treatment of chain reactions-chain length, kinetics of H<sub>2</sub> Cl<sub>2</sub> & H<sub>2</sub> Br<sub>2</sub> reactions Rice Herzfeld mechanism, explosion limits. Study of fast reactions-relaxation methods-temperature and pressure jump methods electric and magnetic field jump methods -stopped flow and flash photolysis methods.

  12 hrs
- UNIT V: Chemical kinetics IV: Adsorption isotherms-Freundlich, Langmuir and BET

adsorption isotherms, surface area-determination, sticking probability, adsorption co-efficient and its significance Mechanism of heterogeneous catalytic reactions-Langmuir-Hinshelwood, Langmuir-Rideal mechanism-unimolecular and bimolecular surface reactions. Catalysis by metals and semiconductor oxides.

#### RECOMMENDED TEXT BOOKS:

- 1. Quantum Mechanics in Chemistry, R.K. Prasad Wiley Eastern, New Delhi 1992
- 2. Quantum Mechanics in Chemistry, M.W.Hanna W.A.Benjamin Inc., London,
- 3. K.J.Laidlar Chemical Kinetics, Harper and Row, Newyork, 1987 J.Rajaram
- 4. J.C.Kuriacose- Kinetics of Mechanism of Chemical Transforamtions, Macmillan India Ltd., 1983

## **REFERENCE BOOKS:**

- 1. A.K.Chandra- Introductory Quantum Chemistry, Tata Mc Graw Hill.
- 2. Quantum Chemistry, D.A.Mc Quarrie University Science Books, Mill Valley California, 1983
- 3. Molecular Quantum Mechanics, P.W.Atkins Oxford University Press, Oxford, 1989
- 4. W.J.Moore- Physical Chemistry, Orient Longmann, London, 1972
- 5. Physical Chemistry Volume 1: Thermodynamics and Kinetics, Peter Atkins, Julio de Paula, 9<sup>th</sup> edition.
- 6. Physical Chemistry, G.W. Castellan, 3<sup>rd</sup> Edition, Narosa Publishing House, 2004

#### PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education
- 6. Journal of American chemical society
- 7. Bulletin of material science

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. Mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com
- 7. http://antoine.frostburg.edu/chem/senese/101/quantum/index.shtml

#### SEMESTER-II

Title of the course: Major Elective 2 Spectroscopy

Teaching hours: 15 x 4 = 60 Credits: 3

Course Code: 6P18/2E2/SPE LTP 310

## **Objectives:**

1. To understand the concepts of IR, UV, Raman, Mass, PES, NMR, EPR, Mossbauer spectroscopy.

- 2. To learn the principles of the techniques.
- 3. To apply the fundamentals to various systems.
- 4. To study the applications of the tools.
- 5. To determine the structure of organic and inorganic compounds.
- UNIT I: Infrared Spectroscopy: Introduction-Origin- Fundamental modes, overtones combination and difference bands Fermi resonance. Selection rule-anharmonicity of vibrations-Normal coordinate analysis (brief outline)- choice of solvents-Base line correction-standard for calibration of the instrument Application of IR to complexes of metals with isocyanides, carbonyls and nitrosyls. Different modes of binding of acetate, thioacetate and DMSO. Urea (amides) and amino acids, DMG as a ligand. Ethylene and acetylene complexes, Evidence for extensive pi bonding in these complexes. Isotopic labeling D<sup>2</sup>, N<sup>15</sup> and C<sup>13</sup> and applications.

12hrs

UNIT II UV absorption Spectroscopy: Electronic spectra of diatomic and polyatomic molecules – Franck – Codon principle – determination of dissociation energy – predissociation spectra – selection rules- types of electronic transitions – effect of conjugation and solvent – chromophores. Auxochromes, Bathochromic and Hypsochromic Shifts. Applications in organic structure determination – Woodward – Feiser rules for conjugate systems and unsaturated ketones. Raman Spectroscopy: Stokes- Antistokes lines classical theory- selection rule, polarisibility ellipsoids-quantum theory-polarization of scattered radiation-depolarization ratio-Assignment of bands-Laser Raman-Ruby Laser- Instrumentation –Resonance Raman effect- Application- Study of solution equilibria-Detection of dimeric species like Hg2<sup>2+</sup>, N2O2.

12 hrs

UNIT III:Mass Spectroscopy: Basic principles. Theory- Instrumentation -ion production. Electron Impact technique- CI Mass spectrometry-Field desorption-FAB and SIMS-Mass analyzer,-Mass spectrometers Molecular ion, Fragment ions, Meta stable peaks-McLafferty rearrangement-Fragmentation pattern in alkanes, alkenes, alkynes, alcohols & aromatic alcohols, phenols, Toluene, aldehydes and ketones. Photo electron spectroscopy: Introduction-UV/XPES Instrumentation. Ionization from bonding, antibonding and non bonding MO-UVPES data/spectrum of H<sub>2</sub> N<sub>2</sub> and O<sub>2</sub>-XPES data/spectrum of O<sub>2</sub>, N<sub>2</sub> and application of Koopman's

theorem Spin Orbit coupling-photo electron spectrum of Xe, Kr, Ar etc and UV PES of HCl, HBr and HI. Spin spin coupling O<sub>2</sub>, NO molecules- Jahn Teller & Renner Teller distortions- NH<sub>3</sub>, CH<sub>4</sub>, UVPES data, Satellite signals- Auger lines- Binding energy- Oxidation state correlation-Errors in binding energy data-correction.

12hrs

UNIT IV: Nuclear Magnetic Resonance: Origin chemical shift- dependence on filed-spin spin coupling. One bond, two bond, three bond and higher order coupling constants. Sample data from <sup>31</sup>p-<sup>31</sup>p, <sup>13</sup>C- <sup>1</sup>H, <sup>31</sup>p-<sup>19</sup>F coupling. Dependence of coupling constant on 's' electron density. Decoupling and off Resonance-NOE effect-factors contributing to it. Systems like PF<sub>3</sub>(CH<sub>3</sub>)<sub>2</sub>, PF<sub>3</sub>(CF<sub>3</sub>)<sub>2</sub> NMR temperature variation- time scale- Relaxation, effect of Quadrupolar nuclei Fluxional behaviour as applied to allyl, cyclopentadienyl systems-Inter and Intra molecular exchange.

12hrs

<u>UNIT V</u>: Electron spin resonance: Introduction-Electron Zeeman effect, Hyperfine interaction, structural information, EPR of Benzylanion, pyrazylanion, BH<sub>3</sub>, Nephalauxetic effect-Data on simple complexes. Factors affecting EPR spectrum – Low symmetry fileds- Anisotropic 'g' and hyperfine constants. Zerofield splitting. Mossbauer Spectroscopy Origin-Isomer shift-correlation with S electron density, Quadrupolar splitting- <sup>57</sup>Fe and <sup>119</sup>Sn data. Time scale- Line width- Instrumentation- iron complexes, Low & high spin-iron carbonyls-prussiates- Turnbull's blue-structure –MB data correlation

12hrs

#### **RECOMMENDED TEXT BOOKS:**

- 1. Structural Methods in Inorganic Chemistry- EAV Ebsworth, D.Will Rankin, S.Cradock, Blackwell scientific publ(1987)
- 2. Physical methods in Inorganic Chemistry- Drago R.S.-Reinhold –1965
- 3. Infrared spectra of Inorganic and coordination compounds Nakamoto k 2<sup>nd</sup> edn Wiley 1970
- 4. Basic principles of spectroscopy R.Chang, McGraw Hill, New york (1971)
- 5. Complexes of I row transition elements D. Nicholas
- 6. Introduction to Ligand field B.N.Figgis, John Wiley (Newyork) 1966
- 7. Fundamental of molecular spectroscopy, C.N.Banwell McGraw Hill Newyork 1966 Organic spectroscopy by William Kemp 3<sup>rd</sup> edn W.H.Freeman & Co, 1991 Spectroscopic methods in organic Chemistry by Silverstein Bassler
- 8. Instrumental method of analysis by H.Willard, W.Merrit, J Dean. 6th edn Van Nostrand 1981

## **REFERENCE BOOKS:**

- 1. Inorganic Electronic spectroscopy-A.B.P.Lever-Elsevier, Amsterdam (1984)
- 2. Physical methods in advanced inorganic Chemistry, H.A.O Hill and P.Day, John Wiley (1968)
- 3. Coordination Chemistry Experimental methods, J.K.Burger butterworths (1973)

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Applied Spectroscopy
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education
- 6. Journal of American chemical society
- 7. Bulletin of material science

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- 3. MATLAB
- 4. mooc.org
- 5. http://swayam.gov.in
- 6. http://search.ebscohost.com
- 7. www.spectro.com

# SEMESTER – II Common to I M.A /M.Sc/M.Com

Title of the course: Non Major Elective 1-Cosmetology

Teaching hours:  $15 \times 4 = 60$ 

Credits: 3

Course Code: 6P18/2E/COS

LTP 3 1 0

### **Objectives:**

- 1. To improve one's own personal appearance and develop self confidence.
- 2. To develop skill in cosmetology.
- 3. To acquire knowledge about chemicals in cosmetics
- 4. To learn the facial procedures in cosmetology
- 5. To understand the usage of cosmetics and Quality control of cosmetics.

#### COURSE CONTENT

<u>UNIT I</u>: Personality development: Self analysis, grooming, professional behavior, personality development. Skin care-theory of massage, facials, facial manipulate one, skin treatment, Infect control for esthetics. Make-up-purpose and types, corrective make-up, optical illusion.

12hrs

<u>UNIT II:</u> Face creams: Types of face creams-cold, vanishing, cleaning and bleaching creams-preparation and application. Hand lotions and creams-simple method of preparation. Bleaching:

Bleach, facial, facial massage- Herbal and synthetic applications, manicure, pedicure, waxing,

12hrs

- <u>UNIT III:</u> Powders: Face powders, constituents in alcum powders-preparation and application. Nail care: Nail preparation-nail lacquer, nail enamels and nail bleach. Oils: Importance of Essential oils: Rose oil, almond oil, Ecalyptus oil, sandal wood oil in cosmetic industries.

  12hrs
- UNIT IV: Hair caring: Hair oils and hair creams, hair conditioning, hair cut, hair style,. hair colouring, hair dye. Shampoos and shampooing: Types of shampoos, liquid, emulsion, paste or powder, ingredients.
   12hrs
- <u>UNIT V</u>: Hair removing techniques: temporary removal of hair- depilation processs and epilation process-permanent removal of hair. . Hazards of cosmetics and quality control of cosmetics.

  12hrs

## RECOMMENDED BOOKS:

- 1. Reagents/Prentice Hall –Text book of Cosmetology by Mary Healy Eastern Economy Edition.
- 2. The complete book of beauty care Aruna Anand

#### SEMESTERS I & II

## Title of the Course: Core 7: Practical 1 - Organic Chemistry (Qualitative and Quantitative Analysis)

Teaching hours:  $30 \times 4 = 120$  Credits: 4

Course Code: 6P18/2C/PR1

# I Spectral Interpretation of Organic Compounds. UV, IR, PMR and Mass Spectra of 15 Compounds.

- 1. 1,3,5-Trimethylbenzene
- 2. Pinacolone
- 3. Propyl amine
- 4. p-Methoxybenzyl alcohol
- 5. Benzyl bromide
- 6. Phenyl acetone
- 7. 2-Methoxyethyl acetate
- 8. Acetone
- 9. Isopropyl alcohol
- 10. Acetaldehyde diacetate
- 11. 2-N, N-Dimethylamino ethanol
- 12. Pyridine
- 13. 4-Picoline
- 14. 1, 3 dibromo-1, 1-dichloropropene
- 15. Cinnamaldehyde

## II Qualitative Analysis

Qualitative analysis of an organic mixture containing two components – Separation, identification and preparation of derivatives. Determination of melting point/Boiling of the purified components and melting point of the derivatives.

## III Quantitative Analysis

- 1. Estimation of Aniline.
- 2. Estimation of Phenol.
- 3. Estimation of Glucose.
- 4. Estimation of Ketone.
- \*5. Saponification value of an oil.
- \*6. Iodine value of an oil.

## \*IV Two stage preparations

- 1. Preparation of para bromo Acetanilide from Aniline.
- 2. Preparation of Benzanilide from Benzophenone.
- 3. Preparation of m-nitro Benzoic acid from Methyl Benzoate.
- 4. Preparation of symmetrical tri-Bromo Benzene from Aniline.
- **\*V Extraction of natural products**-purification and spectroscopic identification by UV-visible and FTIR.
  - 1. Isolation of Citric acid from lemon.
  - 2. Isolation of Caffeine from tea leaves.
  - 3. Isolation of Lactose from milk.

<sup>\*</sup>For internal assessment only.

<sup>\*</sup>Note: Characterization by UV & IR spectra for the preparation

#### END SEMESTER PRACTICAL EXAMINATION

### I M.Sc CHEMISTRY SEMESTERS I & II

#### **QUESTION BANK**

Title of the Course: Core 7 Practical 1- Organic Chemistry -

(Qualitative & Quantitative analysis)

Max: 60 marks

Course Code: 6P18/2C/PR1

Time: 6 hrs

## Total marks: 100 (40 CA+60 End semester)

- 1. Analyse the given spectra with the data given.
- 2. Analyze systematically the given organic mixture and report the nature of the two components after pilot separation.

Analyze the two components separately and report the following.

- a. Aromatic/aliphatic
- b. Presence/absence of elements nitrogen, sulphur and halogens.
- c. Saturated/unsaturated.
- d. Functional group
- e. Melting point or Boiling point of separated components

f.Melting points of the derivatives

Exhibit the color reactions and the derivatives.

- 3. Estimate the amount of aniline present in the whole of the given solution. You are provided with an approximately decinormal solution of sodium thiosulphate.
- 3. Estimate the amount of phenol present in the whole of the given solution. You are provided with an approximately decinormal solution of sodium thiosulphate.
- 4. Estimate the amount of glucose present in the whole of the given solution. You are provided with an approximately decinormal solution of potassium permanganate.
- 5. Estimate the amount of ethyl methyl ketone present in the whole of the given solution. You are provided with an approximately decinormal solution of sodium thiosulphate.

#### Scheme of valuation

Total Marks 100- (CA 40 and End Semester 60)

Systematic analysis - 20 marks

Estimation

- 20 marks

Spectral Interpretation – 10 marks

Record

-5 marks

Viva voce

-5 marks

Total

- 60 marks

1. Systematic analysis

20 marks (Pilot separation -4 marks +

Components - 16 marks)

Analysis:

(8 marks for component I and 8 marks for component II)

1. Aromatic/Aliphatic

1 marks

2. Saturation/Unsaturation

1 marks

3. Elemental detection

2 marks

4. Functional group

2 marks

5. Derivative

1 marks

6. Derivative melting point

1 marks

Total

8x2=16 marks

2. Estimation - 20 marks

up to 2% - 20

2.1-3% - 15

3.1-4% - 10

> 4% - 5

#### SEMESTERS I & II

## Title of the Course: Core: 8 -Practical 2 - Inorganic Chemistry (Qualitative & Quantitative Analysis)

Teaching hours:  $30 \times 4 = 120$  Hrs Credits: 4

Course Code: 6P18/2C/PR2

I Qualitative Analysis of a mixture containing two rare and two common cations.

Rare ions

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

Common ions Pb, Cu, Bi, Cd, Al, Zn, Co, Ni, Mn, Ba, Ca, Sr, & Mg

## II Quantitative Analysis of mixtures

i. Mixture containing Cu & Ni

Copper Volumetrically and Nickel

gravimetrically

ii. Mixture containing Cu & Zn

Copper Volumetrically and Zinc

gravimetrically

iii. Mixture containing Fe & Zn

Iron Volumetrically and Zinc

volumetrically

iv Calorimetric Analysis-Spectrophotometric methods-Estimation of Fe, Ni, Mn & Cu

## III \*Analysis of Alloys and Ores

- i. Analysis of Dolomite, Pyrolusite
- ii. Analysis of Brass

## IV \*Preparations

- i. Bis acetylacetonato copper (II)- Characterisation by IR, UV-VIS absorbtion studies in CHCl<sub>3</sub>
- ii. Hexammine nickel (II) chloride-Study of electronic spectrum to calculate 10 Dq & Racah parameter.
- iii. Tris thiourea copper (I) sulphate.

Note- \* For Internal Assessment only

<sup>\*</sup> Only for internal assessment

## **End Semester Practical Examination**

## I M.Sc Chemistry SEMESTERS I & II

## **Question Bank**

Title of the Course: Core 8- Practical 2 - Inorganic Chemistry

Max Marks: 60

(Qualitative & Quantitative Analysis)

Course Code: 6P18/2C/PR2

Time: 6hrs

- 1. Analyze the given mixture systematically and report two common and two rare cations.
- 2. Estimate the amount of copper volumetrically and nickel gravimetrically, present in the whole of the given solution.

or

3. Estimate the amount of copper volumetrically and zinc gravimetrically, present in the whole of the given solution.

or

- 4. Estimate the amount of iron volumetrically and zinc also volumetrically, present in the whole of the given solution.
- 5. Estimate the amount of metal ions Cu /Ni /Mn /Fe colorimetrically

## SCHEME OF VALUATION

## Total Marks 100 (CA -40 marks and End semester - 60 marks)

Qualitative Analysis 5 x 4 (20 marks)

Quantitative Analysis 2 x 10 (20 marks) (Gravimetric 10 marks + Volumetric 10 marks) or Calorimetric Analysis (20 marks)

Viva

10 marks

Record

10 marks

Total marks

60 marks

## Volumetric /Gravimetric Estimation

10 marks	UPTO 2 %	ERROR
8 marks		2.1-3
6 marks		3.1-4
5 marks		>4

## SEMESTER - III

Title of the Course: Core 9 - Organic Chemistry-III

Teaching hours:  $15 \times 4 = 60$ 

Course Code: 6P18/3C/OC3 LTP 310

Objectives:

1. To study the structure, properties and synthesis of natural products like alkaloids proteins, flavonoids, steroids, and terpenoids

- 2. To study the structure and role of nucleic acids
- 3. To introduce the basics of supra molecular chemistry
- 4. To study the synthesis and properties of heterocyclic compounds like Pyrazole,Oxazole and Thiazole and its derivatives
- 5. To study the Biosynthesis of Nucleotides.

#### **COURSE OUTLINE:**

<u>UNIT I:</u> Heterocyclic Compounds: Nomenclature, synthesis and properties of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, benzimidazole, benzoxazole, benzthiazole.

12hrs

UNIT II: Alkaloids and Proteins: Total synthesis of quinine, morphine reserpine. (No Structural elucidation). Peptides and their synthesis-(Synthesis of any tripeptide using glycine, alanine, lysine, cystine, glutamic acid and argenine). Solid Phase Peptide synthesis-Merrified synthesis, Determination of primary structure of a protein, secondary tertiary and quaternary structure of proteins 12hrs

**UNIT III:** Flavanoids-Synthesis of the following (synthesis of parent compounds and simple hydroxy and methoxy substituted derivatives only) and products obtained on fusion with KOH or boiling with ethanoic KOH or Ba(OH)<sub>2</sub>

- Flavones- Flavone, Chrysin, Apigenin and Luteolin
- Flavonols- Flavonol, Quercetin
- Isoflavones- Isoflavone, Daidzein
- Cyanidin Chloride and Cyanin Chloride
- Delphinidin Chloride and Delphin Chloride
- Malvidin Chloride and Malvin chloride and
- Hirsutidin Chloride and Hirsutin Chloride
- Distinction of Flavonoids by using characteristic colour reactions and absorption spectra (UV and visible)

Credits: 4

Relationship between Quercetin and Cyanidin Chloride

12hrs

<u>UNIT IV:</u>Terpenoids: Synthesis of Vitamin A (Reformatsky and Wittig reaction methods only) and carotenes- biological functions. Steroids-Elucidation of structure of Cholesterol and Oestrone. Conversions of Cholesterol to Progesterone, Testosterone and Oestrone. 12hrs

UNIT V: Bio-organic Chemistry: Structure and role of (genetic code) DNA and RNA. Structure, name and representation of Nucleotides and Nucleosides (Structural Elucidation not necessary). Structures of products of hydrolysis of DNA and RNA- Action of dilute acid and alkali. Replication and protein synthesis. Nucleotide monophosphate (NMP), diphosphate (NDP) and triphosphate (NTP). ATP as currency of energy. Bio Synthesis of Nucleotides (No chemical synthesis)-DeNovo and salvage synthesis and synthesis of pyridimine and purine derivatives-Adenine, Guanine, Cytosine, Uracil and Thymine (Chemical synthesis only). Biosynthesis of cholesterol. Supramolecules-General methods of synthesis and application of supramolecules.

## **RECOMMENDED TEXT BOOKS:**

- 1. Organic Chemistry- Volume I and II, L.L.Finar, 5<sup>th</sup> Edition, ELBS publication
- 2. Organic Chemistry of natural products by Gurdeep Chatwal Volume I and II
- 3. Chemistry of organic natural products by Agarwal, Geol Publishing House
- 4. Chemistry of natural products by P.S. Kalsi

#### **REFERRENCE BOOKS:**

- 1. Stanley H.Pine, Organic Chemistry, 4th edn Mac Graw Hill
- 2. Outlines of Biochemistry V Edition by Eric E. Conn, Paul. R. Stumpf, George Bruening and Roy H. Dole, John Wiley and Sons.
- 3. Principles of Biochemistry General aspects by L. Smith, Robert L. Hill I. Robert Lehman, Robert J. Let Rowitz, Philip Handlar and Abrahim white. McGraw Hill Int. (7th Edition)
- 4. Biochemistry by Lubert Stryer, WH. Freeman and Co., New York
- 5. Chemistry of alkaloids by Pelletier...
- 6. Introduction to Alkaloids by G.A. Swan
- 7. Introduction to Chemistry of Heterocyclic compounds by R.M.Acheson, interscience publishers
- 8. Heterocyclic Chemistry by T.L.Gilhrist, Longman Scientific and Technical (1991)
- 9. Heterocyclic Chemistry by Raj Bansal, Wiley Eastern Ltd.Jonathan W. Steed, Jerry. L. Atwood, Supramolecular Chemistry, John Wiley & Sons, 2002

# PERIODICALS:

- 1. Journal of Organic Chemistry
- 2. Indian Journal of Chemistry B
- 3. Current Science
- 4. Organic Letters
- 5. Tetrahedron Letters

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com

#### SEMESTER - III

Title of the course: Core -10 Inorganic Chemistry-III

Teaching hours:  $15 \times 4 = 60$  Credits: 4
Course Code: 6P18/3C/IC3 LTP 3 1 0

## **Objectives:**

- 1. To focus on Electro analytical chemistry as applied to metal complexes
- 2. To study in detail the Analytical separation techniques
- 3. To create awareness to carry out qualitative and quantitative estimation of ions using modern instrumentation techniques
- 4. To focus on macrocyclic ligand systems with special emphasis on bioinorganic chemistry
- 5. To introduce research mind in the field of coordination chemistry

## **COURSE OUTLINE**

- <u>UNIT 1:</u> Analytical Chemistry: Polarography- Theory apparatus, DME, Diffusion, Kinetic and catalytic current, Voltage curve for reversible and irreversible systems, Qualitative and Quantitative-inorganic analysis. Amperometric titration-theory, apparatus, types of titrations and two indicator electrodes. Application-cyclic voltametry-theory, application to inorganic systems. Complexometric titrations- Types of EDTA titrations, direct and back titrations, replacement titrations. Masking and demasking agents. Coulometry: Coulometry-Theory, Apparatus, Different types, Applications -Coulometric titrations.
- UNIT II: Analytical techniques: Chromatography- Gas liquid chromatography, principles, retention volumes, instrumentation, carrier gas column, preparation, stationery phases, detectors, thermal conductivity, flame ionization, electron capture application of GLC. High performance in liquid chromatography, scope column efficiency, instrumentation- ion pumping system, column packing detectors- applications. Flame Photometry-Atomic absorption spectroscopy, theory, atomizers, flames atomically and electron thermal, instrumentation, spectral and chemical methods analysis. interferences applications. Thermal Thermogravimetric analysis, differential thermal analysis, thermometric 12 hrs analysis.
- <u>UNIT III:</u> Macrocyclic ligands: Schiff's bases, Crown ethers, Cryptates, tetraaza ligands, catenands and spherands. Macrocyclic effect- template effect.

  12 hrs
- <u>UNIT IV:</u> Transport proteins & Oxygen carriers-haemoglobin, hercrythrin-cytochromes, caroxy peptidase, carbonic biochemistry of Zn, Iron, Sulphur proteins.

  myoglobin, anhydrase, 12 hrs

<u>UNIT V:</u> Photosynthesis- Chlorophyll, discussion on photosystems I & II. Vitamin B<sub>12</sub>- Structure of corrin ring, function of vitamin. Role of Na, K, Ca, Mg & Cu. Fixation of nitrogen and nitrogenase enzymes.
 12 hrs

#### RECOMMENDED TEXT BOOKS:

- 1. K.F.Purcell and J.C.Kotz, Inorganic chemistry, SWB Saunders Co (1977)
- 2. J.E.Huheey, Harper and Collins, Inorganic chemistry, Ny IV edn
- 3. J.R.Chatwal, A.K.Bhogi, Bioinorganic chemistry, Himalaya publishers.
- 4. D.F.Shrivers and P.W.Atkins, Inorganic chemistry, oxford university press, 3<sup>rd</sup> edn 1999
- 5. D.Banerjea, Coordination chemistry, Tata McGraw Hill 1993
- 6. P.K.Bhattacharya, Metal ions in Bio chemistry, Narosa publishing House (2005)
- 7. D.A.Skoog, Principles of instrumental methods of analysis, Saunders coillage publication III Edition (1985)
- 8. Wilard Merrit, Dean and Settle, Instrumental methods of analysis, CBS Publ, VI Edition (1986)
- 9. Vogal, Text book of qualitative inorganic analysis, ELBS III Edition, (1976) and IV Edition (1985)
- 10. D.O.Halls, K.K.Rao, Photosynthesis, Vedn Cambridge University press
- 11. Bertini, H.B.Gray, S.J.Lippard, Bio inorganic chemistry, J.S.Valentine (ed) University Science Books, mill valley (1994)
- 12. Bioinorganic enzymology, Chem.Rev.7 (1996)

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education
- 6. Journal of American chemical society
- 7. Bulletin of material science

- 1. www.virtlab.com
- 2. http://nptel.ac.in
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- 4. mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com

#### **SEMESTER - III**

Title of the course: Core 11-Physical Chemistry-III

Teaching hours:  $15 \times 4 = 60$  Credits: 4

Course code: 6P18/3C/PC3 LTP 310

## **Objectives:**

1. To understand the theory of relationship between microscopic and macroscopic phenomena.

- 2. To study the thermodynamic properties of single molecules and their interaction with their bulk counterparts.
- 3. To study the thermodynamic aspects and applications.
- 4. To study the Phase equilibria of three component systems.
- 5. To study the thermodynamic aspects of Phase Transitions

#### COURSE OUTLINE

- UNIT I: Statistical Thermodynamics I: Objectives of statistical thermodynamics-concept of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell- Boltzmann, Fermi-Dirac & Bose-Einstein Statistics- comparison and applications. Modes of contribution to energy, Maxwell's law of distribution of molecular speeds, graphical representation, experimental verification, derivation of expressions for average, most probable and root mean square velocity.

  12hrs
- <u>UNIT II:</u> Statistical Thermodynamics II: Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions- calculation of equilibrium constants from partition functions, isotope exchange and dissociation of diatomic molecules. 12hrs
- <u>UNIT III:</u> Statistical Thermodynamics III: Applications of partition function to heat capacities of ideal gases-heat capacity of solids-Einstein and Debye theory of heat capacity of solids. Thermodynamics of black body radiation, Wein's-Stefan-Boltzmann law.

  12hrs
- <u>UNIT IV:</u> Phase Equilbria I: Phase, Component, Degrees of freedom- Gibbs phase rule-derivation. Roozeboom plots, Scheme of triangular plot-method of parallel lines, direct method & Lever rule method, Systems of three liquid components exhibiting partial miscibility Formation of one pair, two pairs and three pairs of partial miscibility, effect of temperature. Ternary systems

of two solid components and a liquid - Crystallization of pure components only. 12hrs

UNIT V: Phase Equilbria II: Formation of binary compounds - hydrates and double salt-Congruently saturating and incongruently saturating, formation of ternary compounds, solid solutions, solid solutions with partial miscibility, Salting out phenomena, Thermodynamic aspects of phase transitions, dependence of stability-temperature and pressure. Phase boundaries — solid-liquid, liquid-vapour and solid-vapour boundaries. The Ehrenferst classification of phase transition-I order II order phase transitions and lambda transitions.

## **RECOMMENDED TEXT BOOKS:**

- 1. Chemical Thermodynamics: Classical, Statistical and Irreversible, Rajaram and Kuriakose, 2013 edition, Pearson Publications
- 2. M.C.Gupta- Statistical Thermodynamics, Wiley Eastern, New Delhi 1990
- 3. A Textbook of Physical Chemistry K.L.Kapoor, Vol. 3, 2012 edition.

## **REFERENCE BOOKS:**

- 1. Statistical Thermodynamics, M.Dole, Prentice Hall, Newyork, 1954.
- 2. Statistical Thermodynamics, N.O.Smith B.J.Clelland Chapman and Hall, London 1973 Elementary
- 3. Statistical Thermodynamics, a problems approach, Plenum Press, Newyork, 1980
- 4. The Phase rule and its applications: Alex Fixdlay, 3<sup>rd</sup> editions Longman Green and Co.
- 5. Physical Chemistry by Peter Atkins and Jullio de Paula, 10<sup>th</sup> edition Oxford press
- 6. Physical Chemistry, I.N. Levine, 5<sup>th</sup> Ed., Tata McGraw Hill Pub. Co. Ltd., New Delhi.

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. Mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com
- 7. e book Introductory Physical Chemistry by David Ronis, McGill University 2011

## SEMESTER-III

Title of the Course: Major Elective 3 - Photochemistry

Teaching hours: 15 x 4=60 Credits: 3

Course Code: 6P18/3E3/PHC LTP 310

## **Objectives:**

1. To study the principles of photochemistry,

2. To study the fate of excited molecules – Jablonski diagram

- 3. To study the different types of Photochemical reactions and its applications.
- 4. To study the photochemistry of ketones and a few re- arrangement reactions
- 5. To study the principles of orbital symmetry for different organic reactions

#### **COURSE OUTLINE:**

<u>UNIT I:</u> Fundamentals of Photochemistry: Interaction of electromagnetic radiation with matter. Absorption and emission of radiation, sources of irradiation and filters, internal and external methods of irradiation. Photochemical excitation-types of excitation, quantum yields and chemical actinometry.

12 hrs

<u>UNIT II:</u> Fate of the excited molecules: exited state life time, singlet and triplet statesallowed and forbidden transitions. Jablonski diagram- radiative and nonradiative processes- internal conversion, inter system crossing, fluorescence and phosphorescence. Energy transfer process- sensitization, excimer and exciplex, Stern Volmer analysis -static and dynamic quenching.

12 hrs

- <u>UNIT III:</u> Applications of Photochemistry: Photophysical processes and kinetics of photochemical reactions-photoredox reactions, photo substitution reactions, photosensitized reactions- photo isomerisation reactions. Photo voltaic and photo galvanic cells, photo electrochemical cells, photo assisted electrolysis of water. Aspects of solar energy conversions.

  12hrs
- UNIT IV: Organic Photochemistry: Examples for direct photolysis involving the singlet excited state and sensitized photolysis involving the triplet state. Introduction of a quencher to a photochemical reaction proceeding from the triplet state. Photochemistry of alkene-cis-trans isomerization. Study of photochemistry of ketones Photoreduction of Ketones , Intramolecular reactions- Norrish Type-I and Norrish Type-II cleavages, saturated acyclic and cyclic carbonyl compounds. Re-arrangements of 1,4-dienes-di-pimethane re-arrangement. Re-arrangement of β-γ unsaturated ketones-oxa-di-pimethane rearrangement. Intermolecular cycloaddition reaction of ketone-Paterno- Buchi reaction, Barton reaction, Photo-Fries reaction.

<u>UNIT V:</u> Pericyclic reactions: classification-orbital symmetry- Woodward Hoffmann rule- conrotation and disrotation. Electrocyclic reactions- thermal and photochemical cyclisations and ring openings- stereochemistry of electrocyclic reactions- FMO method and correlation diagram for butadiene-

cyclobutene and 1,3,5- hexatriene-1,3 cyclohexadiene systems. Cycloadditions- thermal and photochemical-sterochemistry- FMO method and correlation diagrams of [2+2] and [4+2] cycloadditions and 1,3-dipolar addition Sigmatropic rearrangements- stereochemistry-thermal and photochemical- FMO method. Cope re-arrangement- stereochemistry-oxy-cope rearrangement, degenerate Cope re-arrangement-fluxional molecules-homotropylidene, barbarlone, bullvalene, Claisen rearrangement. 12 hrs

## **RECOMMENDED BOOKS:**

- 1. K.K.Rohatgi Mukherjee- Fundamentals of Photo Chemistry, Wiley Eastern Limited
- 2. Advanced Organic chemistry by J.March 5<sup>th</sup>edn Wiley Interscience 2001
- 3. Pericyclic reactions by Jagdamba Singh

#### REFERENCE BOOKS:

- 1. N.J.Turro- Modern Molecular Photo chemistry, Menio Park, California 1991
- 2. J.G.Calvert&J.N.Pitts- Photo Chemistry, Wiley, London 1996
- 3. R.P.Wayne- Photo Chemistry, Butterworths, 3 rdednLondon Oxford univ press, 2000
- 4. R.P.Gundell&A.Gilbert- Photo chemistry, Thomas Nelson, London
- 5. Molecular Reaction and Photo chemistry by Charles H.Depuy and Orvill E.L.Chapman, Prentice Hall of Indian Ltd., New Delhi
- 6. Organic Photo chemistry by Coxon and Halton 2<sup>nd</sup>edn Cambridge univ press, 1974
- 7. Pericyclic reactions by Mukherjee Mac Millan
- 8. Organic Photochemistry and Pericyclic reactions by Dr. Shankar Raman

## PERIODICALS:

- 1. Journal of Organic Chemistry
- 2. Indian Journal of Chemistry B
- 3. Current Science
- 4. Organic Letters
- 5. Tetrahedron Letters
- 6. Journal of Indian chemical education
- 7. Journal of American chemical society

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   6. http://search.ebscohost.com

## **SEMESTER-III**

#### Common to II M.A/M.Sc/M.Com

Title of the Course: Non Major Elective 2 - Fibres, Fabrics,

**Dyeing and Printing of Textiles** 

Teaching hours:  $15 \times 4 = 60$  Credits: 3

Course Code: 6P18/3E/FDP LTP 310

## **Objectives:**

- 1. To impart basic knowledge in Textile production from fibre to fabric stage
- 2. To stress the importance of Natural fibres and their applications
- 3. To give the students a theoretical knowledge in dyeing and printing
- 4. To gain knowledge on weaving & spinning methods
- 5. To inculcate entrepreneur skills in the students

#### COURSE OUTLINE

- <u>UNIT I:</u> Textile fibres: Classification Based on the origin of fibres- natural fibres of vegetable and animal origin- Manmade fibres- semi synthetic and synthetic fibres. Classification based on the thermal properties –thermoplastic and nonthermoplastic fibres. Man made fibresSemi synthetic fibres-characteristics and uses of cellulose acetate and cellulose triacetate Arnel. Synthetic fibres-characteristics and uses of polyamides- Nylon 6,6 and Nylon 6-finishing nylon fabrics.

  12hrs
- UNIT II: Natural fibres of vegetable origin: Cotton-types-cultivation-transformation of raw cotton to yarn- By products- mercerization, slack mercerization, Ammoniating-yarn twist, yarn count-composition and characteristics. Natural fibres of animal origin. Silk-silk producing countries, sericulture-cultivation of cocoons composition. Transformation of cocoons to silk yarn, degumming, weighting, spun silk, pure dye silk and wild silk, compostion and characteristics.
  12hrs
- <u>UNIT III:</u> Fabrics: Classification of yarn Fabric construction-Spinning methods-Melt, dry and we spinning. Weaving-basic weaves-plain, variations of plain-basket, rib-twill and satin weaves. Identification of weaves and designs. 12hrs
- <u>UNIT IV:</u> Dyes: Classification main types of synthetic dyes and their characteristics basic methods and principles of dyeing. Dyeing cotton fabrics with Naphtha, direct, sulphur and vegetable dyes-wool-silk-nylon.
   12hrs
- <u>UNIT V:</u> Basic methods of printing and its applications: direct printing, discharge printing and resist printing. Printing Block, roller, screen, transfer, Batik, resist, kalamkari, Tie and dye.

  12hrs

## RECOMMENDED BOOKS:

1. Textile - Fabric to Fabrics - Dr. Bernad P. Lorbman.

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education
- 6. Journal of American chemical society
- 7. Bulletin of material science

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- 5. http://swayam.gov.in
- 6. http://search.ebscohost.com

## SEMESTER-III

Title of the course: Soft Skill 3- Laboratory Safety Skills

Teaching hours: 15 x 2=30 Credits: 2

Course Code: 6P18/3S/LSS L T P 2 0 0

## **Objectives:**

1. To study the safety measures involved in handling of chemicals.

- 2. To develop an awareness in first aid techniques.
- 3. To create an awareness in waste and fume disposals.

#### COURSE OUTLINE

- UNIT I: Storage and handling of chemicals: carcinogenic chemicals, glove box, handling of ethers, toxic and poisonous chemicals, safe limits of vapour concentrations. Precautions for avoiding accidents, laboratory safety measures.

  10 hrs
- UNIT II: First aid techniques: eye injuries, fire and burns, cuts, electric shock, poisoning treatment for specific poisoning, conc.H<sub>2</sub>SO<sub>4</sub>, carcinogens, hazards in laboratory, LPG-composition, characteristics, handling -gas leakage detector -fire extinguisher-principle and usage. 10 hrs
- UNIT III: Waste disposal- fume disposals, Fume cupboard. Nuclear reactor management-low level wastes, intermediate level wastes, high level wastes, ultimate disposal. Radioactive waste disposal: Radioactive wastes: sources of radioactive wastes-classification of wastes-treatment techniques for solid, liquid and gaseous effluents-permissible limits for disposal of wastes. Disposal of radioactive wastes: General method of disposal-management of radioactive in medical, industrial and research establishment.

## **RECOMMENDED BOOKS:**

- 1. Elements of Analytical Chemistry, Gopalan R, Rangarajan K, Subramanian P.S. 3<sup>rd</sup> edition, 2013
- 2. Source book on Atomic Energy, Samuel Glasstone, 3<sup>rd</sup> edition, 1979.

## SEMESTER-IV

Title of the Course: Core 12-Organic Chemistry-IV

Teaching hours:  $15 \times 5 = 75$  Credits: 4

Course Code: 6P18/4C/OC4 LTP 410

## **Objectives:**

1. To study the concept of Retro synthesis and synthetic strategies of organic compounds

- 2. To study the principles of Green chemistry and Sonochemistry
- 3. To study the various important Name reactions in organic chemistry
- 4. To study the Synthesis of some important Target molecules .
- 5. To study the aromaticity of annulenes and the different type of aromatic compounds.

## COURSE OUTLINE

<u>UNIT I:</u> Modern Synthetic Methodology-1: Formation of C-C bond using alkylation and acylation of enamines, enolates, active methylene compounds and organo metallic compounds-RMgX, R<sub>2</sub>LiCu, RLi, Pd complexes, O-alkylation vs C-alkylation. Protection and deprotection of functional groups (R-OH, R-CHO, RCOR, R-NH<sub>2</sub> and R-COOH). Uses of the following reagents in organic synthesis: Trimethyl silyl chloride, 1,3-dithiane (umpolung), (DIBAL). 9-BBN, tributyl tin hydride, LDA.

15 hrs

- <u>UNIT II</u>: Modern Synthetic Methodology-2: An introduction to Retrosynthesis-Disconnections- Synthon- Nucleophilic, electrophilic and neutral and their Synthetic equivalent, Target molecule, Functional groupinterconversion Retro synthesis of simple molecules alcohols, alkenes, carbonyl compounds, 1,2, 1,3, 1,4,1,5 & 1,6 dicarbonyl compounds. Formation of C-C bond using Pd & Ni catalyst Heck reaction ,Sonogashira coupling ,Suzuki coupling , Kumada coupling , Negishi coupling and Stille coupling 15 hrs
- WNIT III: Modern Synthetic Methodology-3: Synthesis of Target molecules- 5-hexenoicacid, bicycloheptan [4,1,0]-2-one, Cubane, Longifolene, Brufen, trans-9-methyl-1-decalone. Green chemistry- need for green chemistry, twelve principles, choice of starting materials, choice of reagents, choice of catalysts-bio catalysts and polymer supported catalysts (examples), choice of solvents Sonochemistry-principles, instrumentation applications in esterification, hydrolysis, substitution and addition reactions. Microwave assisted synthesis-Principles, instrumentation, limitations and precautions. Applicatons- deprotection of esters, C- and N-alkylation.

UNIT IV: Synthetic Applications of Name reactions: Mannich, Darzen, Reformatsky reaction, Wittig reaction- Stabilisedand non- stabilized ylides, Diels Alder reaction,1,3-Dipolar addition, Hydroboration, Michael addition, Robinson annulation reaction (Stereochemical aspects to be studied wherever applicable). Typical formylation reactions-Gattermann-Koch, Gattermann, Vilsmeyer Haack and Riemer-Tiemann and Houben Hoesch reactions, Chichibabin reaction and Zeigler alkylation, Shapiro reaction.

<u>UNIT V</u>: Aromaticity- Benzenoid, heterocyclic and non-benzenoid compounds, diatropic behaviour in NMR. Huckel's rule- aromatic systems with pi electron numbers other than six-anulene. Non aromatic (cyclooctatetraene) and anti aromatic systems- paratropic behaviour in NMR (cyclobutadiene) systems with more than 10 pi electrons- annulene-(18)-annulene. (Synthesis of all these compounds is not expected). Homoaromatic compounds. 15 hrs

## **RECOMMENDED BOOKS:**

- 1. Guide book to Organic Synthesis by Raymond K.Mackie and David M.Smith, ELBS Publication
- 2. W. Carruther, Jain Coldham, Modern Methods of organic synthesis, 4th Edition

#### REFERENCE BOOKS:

- Advanced Organic Chemistry by Francis A. Carey and Richard J. Sundberg -Part A and Part B
- 2. Advanced Organic Chemistry by Pine, Cram and Hammond.
- 3. Organic synthesis by R.E. Ireland, Prentice Hall of India, Geol Publishing House.
- 4. Principles of Organic synthesis by R.O.C. Norman, Champan and Hall, NY, 1980
- 5. Stuart Warren, Work book for organic synthesis, The Disconnection Approach John Wiley & Sons (Asia) Pvt. Ltd.

## PERIODICALS:

- 1. Journal of Organic Chemistry
- 2. Indian Journal of Chemistry B
- 3. Current Science
- 4. Organic Letters
- 5. Tetrahedron Letters

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- 6. http://search.ebscohost.com

#### SEMESTER -IV

Title of the course: Core 13-Inorganic Chemistry- IV

Teaching hours: 15 x 5=75 Credits: 4

Course Code: 6P18/4C/IC4 L T P 4 1 0

## **Objectives:**

1. To study some important aspects of organmetallic chemistry

- 2. To study the industrial applications of organometalic catalyst
- 3. To introduce the principles and applications of Nuclear chemistry
- 4. To obtain knowledge about fission, fusion reactions and nuclear reactors
- 5 To introduce environmental problems and possible treatment Procedures

## **COURSE OUTLINE**

UNIT I: Organo metallic chemistry: Carbon donors: alkyls and aryls: metallation, bonding in carbonyls and nitrosyls: Chain and cyclic donors. Olefin acetylene and allyl systems: synthesis: structure and bonding: metallocenesferrocene, Reactions: Fluxional molecules-study of allyl, allene, cyclooctatetraene, and cyclopentadienyl η¹ & η⁵ systems-NMR evidence.Organometallic compounds of Litium.Beryllium, Megnesium,Boron and Alluminium.

15 hrs

- UNIT II: Catalysis: hydrogenation of olefins (Wilkinsons catalyst) hydroformylation of olefins using cobalt or rhodium catalysts (oxo process), oxidation of olefins to aldehydes and ketones. (Wacker process): polymerization (zeigler natta catalyst): stereospecificity mechanisms, cyclo oligomerization of acetylene using nickel catalyst (Reppe's catalyst): polymer bound catalysts.

  15 hrs
- UNIT III: Nuclear Chemistry I: Nuclear properties- Nuclear spin and moments, origin of nuclear forces, salient features of liquid drop and the shell models of nucleus. Models of radioactive decay:-Orbital electron capture nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M. Scintillation and Cherenkov counters.
- <u>UNIT IV:</u> Nuclear Chemistry II: Nuclear reaction: Types, reaction, cross section, Q-value, threshold energy, compound nucleus theory, high energy nuclear reaction, nuclear fission and fusion reactions as energy sources, direct

reaction, photonuclear and thermonuclear reaction, Nuclear reactors- Breeder technology, reactions involved. Application relating to nuclear chemistry:

Neutron activation analysis, radiopharmacology, autoradiography, isotope dilution analysis.

15 hrs

UNIT V: Environmental Chemistry: Water treatment-primary, secondary and teriary stages in detail BOD-COD Ambient air quality standard- Allowed level, permissible limit, oxides of nitrogen, photochemical smog. Toxic chemicals in environment LD Toxicity of Hg, Pb, Cu. Analytical methods in environmental toxins- soil pollution-contamination of soil due to excess use of fertilizers-pH of the soil- Remedy.

15hrs

## **RECOMMENDED TEXT BOOKS:**

- 1. Text book of environmental chemistry by O.D.Thiyagi and M.Mehta, Anmol Publications Pvt Ltd (1996).
- 2. H.J.Arniker, Nuclear Chemistry, Wiley Eastern Co., II edition Wiley-Blackwell (1987)
- 3. F.A.Cotton and G.Wilkinson, Advanced inorganic chemistry, John wiley & sons (2007) VI edition
- 4. K.F.Purcelle and J.C.Kotz, Inorganic Chemistry, SWB sauders co., (1980)

#### REFERENCE BOOKS:

- 1. Comprehensive environmental studies by Dr.J.P.Sharma Laxmi Publications (2006)
- 2. Environmental chemistry by B.K.Sharma, 13 edition, Krishna's Educational Publications (2014)
- 3. Source books on atomic energy, S.Glasstone, Van Nostr and Co, Krieger Pub Co; 3 edition (1979)
- 4. Nuclear and Radiochemistry, G.Friedlander, J.W.Kenedy, J.M.Miller, John Wiley and sons (1981).
- 5. Principles of Organometallic chemistry, P. Powell, Springer Netherlands (1988)
- Reaction Mechanism of Inorganics and organometallic Systems, R.B.Jordan, Oxford University Press (2007).
- 7. Organometallic chemistry, R.C.Mehrothra, A.Singh, New Age International Publishers Ltd.-New Delhi (2000)

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education
- 6. Journal of American chemical society
- 7. Bulletin of material science

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http://swayam.gov.in
- 6. http://search.ebscohost.com

#### SEMESTER - IV

Title of the course: Major Elective 4 - Electrochemistry and

## **Computational Chemistry**

Teaching hours: 15 x 5 = 75 Course Code: 6P18/4E4/ECC Credits: 4

LTP 410

## **Objectives:**

1. To understand the concepts, principles and theories of ionic and electronic interactions in solutions

2. To explore thermodynamic models of electrode-electrolyte interface

- 3. To study the working and applications of electro chemical systems Cells and Batteries
- 4. To derive the kinetics and the parameters affecting them.
- 5. To understand first principles atomic structure using computational methods.

## **COURSE OUTLINE**

<u>UNIT I:</u> Electrochemistry I: Ionics: Ions in solutions, true and potential electrolytes, ion — solvent , ion —ion interactions ,ionic strength—concept and calculations, Debye Huckel theory of strong electrolytes , Poisson equation, Poisson—Boltzman equation, activity co-efficient and mean ionic activity efficient of electrolytes, Debye Huckel limiting law — Derivation verification and its extensions, Debye Huckel Onsager equation—derivation and verification.

15 Hrs

- UNIT II: Electrochemistry II: Electrodics: Electode-electrolyte interface, adsorption at electrified interface-electrical double layer, Structure of double layer-Helmholtz-Perrin, Guoy Chapmann and Stern models of electrical double layers. Thermodynamic derivation of electrified interfaces— Lippmann capillary equation—electro capillary phenomenon, Polarizable and Non Polarizable electrodes. Electrokinetic phenomenon—explanation of these phenomenon with the concept of forces and flux-Onsager reciprocity. 15 hrs
- UNIT III: Electrochemistry III: Electrodics- Butler Volmer equation for one step and multi step electron transfer reactions. Limiting cases- Tafel and Nernst equation. Significance of equilibrium exchange current density and symmetry factor, transfer co-efficient. Electrochemical (inorganic and organic) reactions of technological interest (one example each). 15 hrs
- <u>UNIT IV:</u> <u>Electrochemistry IV:</u> Mechanism of electrode reactions-polarizations and over potential –Corrosion and passivation of metals- Pourbaix (Iron and Lead

systems only) and Evans diagrams, Theories of corrosion. Prevention from corrosion—anodic and cathodic protection, corrosion inhibitors. Electrochemical energy systems -primary and secondary batteries- dry cells, lead acid storage batteries, silver zinc cell, nickel cadmium battery, mercury cell, fuel cells. Electrodeposition - principles and applications. 15 hrs

UNIT V: Computational Chemistry: A brief outline of molecular mechanics, semiempirical approximations, *ab initio* methods, basis sets and Z-matrix; Gaussian, Slater type. Density Function Theory- overview- Kohn Hohenberg and Kohn Sham equation (no derivation) Hartree -Fock calculations for determining electronic energies. Basic concepts of molecular dynamics and simulations.

#### RECOMMENDED TEXT BOOKS:

- S. Glasstone- Introduction to Electrochemistry, Affiliated East West press, New Delhi
- 2. D. R.Crow-Principles and Applications of Electrochemistry, Chapman and Hall.
- 3. Frank Jensen, Introduction to computational chemistry, 2<sup>nd</sup> edition, John Wiley & Sons Ltd. (2007)
- 4. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, 2002.
- 5. D. Young, Computational Chemistry: A practical Guide for applying Techniques to Real World Problems, Wiley Interscience, 2001.
- 6. A.R.Leach, Molecular Modelling: Principles and Applications, Pearson Education, 2001.
- 7. J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods. Gaussian Inc., 1996.
- 8. M. P. Allen and D. J. Tildesley, Computer Simulations of Liquids, Oxford, 1987

#### REFERENCE BOOKS:

- 1. J.O.M.Bockris and A.K.N.Reddy-Electrochemistry-Vol I & II, Plenum, Newyork 1977
- P.Delhay Electrode Kinetics and structure of double layer interscience, New york, 1965
- 3. J.Robbins-Ion in solution-an introduction to electro chemistry, Clarendon press, Oxford (1972)
- 4. C.M.A.Brett and A.M.O.Brett –Electrochemistry principles, methods and applications, OUP,Oxford, 1993.
- 5. P.H.Rieger-Electrochemistry, Chapman and Hall, Newyork (1994)
- 6. R.L.De Koch and H.B.Gray Chemical structures and Bonding, Benjamin/Cummings, Menlo Park, California.

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 5. Journal of Indian chemical education

## WEBSITES & e-LEARNING SOURCES:

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. Mooc.org
- 5. http://swayam.gov.in
- 6. http://search.ebscohost.com
- 7. http://ccl.osc,edu/ccl.cca.html
- 8. http://www.chem.swin.esu.au/chem ref.html
- 9. http://www.colby.edu/chemistry/PChem/Lecture1.html
- 10. http://hyperphysics.phy-astr.gsu.edu/hbase/chemical/electrode.html#c3

# Computational chemistry software

- 11. SPARTAN
- 12. http://www.wavefun.com
- 13. GAUSSIAN
- 14. www.gaussian.com
- 15. MOLPRO
- 16. www.tc.bham.ac.uk/morpro

#### SEMESTER- IV

Title of the course: Major Elective-5 Polymer Chemistry

Teaching hours: 15 x 4=60 Credits: 3

Course Code: 6P18/4E5/POC L T P 3 1 0

## **Objectives:**

1. To learn the theoretical concepts in polymer chemistry

- 2. To appreciate their significance and applications of polymers
- 3. To motivate the students to pursue research in polymer chemistry
- 4. To study the techniques for characterization of polymers
- 5. To study the mechanism of polymerisation

#### **COURSE OUTLINE**

- UNIT I: Introductory Survey: Concept of Polymers, common terms used in Polymers-Classification of Polymers-natural and synthetic Polymers-condensation polymers, addition polymers, co-polymerization, polymerization of cyclic compounds- Inorganic Polymers-Techniques of polymerization-bulk polymerization-solution polymerization, suspension polymerization, emulsion polymerization, melt poly condensation-interfacial condensation-solid and gas phase polymerization and plasma polymerization. Polymer Structure-Co-polymers, Tacticity, Geometrical isomerism.
- <u>UNIT II</u>: Mechanism and Kinetics of Polymerisation: Step Growth Polymerisation or Polycondensation Chain Polymerisation- Radical polymerization Anionic polymerization, Cationic polymerization, coordination polymerization, with respect to Ziegler Natta catalyst, co-polymerization, composition of co-polymers-block and graft co-polymers,-ring opening-polymerisation.
   12hrs
- UNIT III: Structure and Properties: Primary and secondary bond forces in Polymers.

  Coherence energy-structure property relationship. Mechanical propertiesTensile strength, Compressive, Flexural strength, fatigue resistance and impact resistance Relationship between molecular weight and mechanical properties.

  Glass Transition Temperature Degradability-Degradation by a. Oxidative degradation b. Mechanical, c. Ultrasonic wave. d. Photo degradation bio degradation Chain flexiblity. Electrical Conductivity. Flow properties of polymer melts and solutions.

  12hrs
- UNIT IV: Polymer Analysis and Characterisation: Identification-Physical testing, IR, NMR, (spectral methods) Identification of typical plastic materials eg. ABS, Acrylics, polyfluorocarbons pvc,. Other examples polystyrene, poly vinyl acetate, polyvinyl alcohol. Testing Thermal, electrical and chemical. Characterization Molecular weight distribution in polymers. Determination of molecular weight, fractionation-gel permiation chromatography, number average molecular weight-osmometry. Weight average molecular weight light scattering measurements, ultracentrifugation, viscosity and DLS method.

12hrs

UNIT V: Polymer Processing and Applications: Plastics-thermosetting and thermoplastics, Rubber-the composition of rubber latex- the processing of rubber Natural and Synthetic fibres criteria for fibre formation. Basic Processing Operations-Extrusion, Moulding, Calendering, Coating Membrane Application for Polymeric Materials. Biomedical Applications-Artificial Organs, Controlled Drug Delivery, Homodialysis and Hemofiltration. Application in Electronics-Electrically conductive polymers, electronic shielding, encapsulation. Polymers in Photonics applications, Drag Reduction and Dentrimers.

#### RECOMMENDED TEXT BOOKS:

- 1. F.W.Billmeyer- Textbook of Polymer science, Wiley intersicence
- 2. A.Rudin- The elements of Polymer Science and Engineering- An introductory text for engineers and chemists, Academic Press, Newyork
- 3. Polymer Science- V.R.Gowarikar, N.V.Viswanathan & Jayadev Sreedar
- 4. Principles of Polymer Science- P.Bhadur, N.V.Sastry, Warosa Publishing House
- 5. Introductory Polymer Chemistry-G.S.Mishra

## REFERENCE BOOKS:

- 1. C.E.H.Bawn- The chemistry of high polymers, Butterworth and Co., London
- 2. E.A.Collins, J.Bares and E.W.Billmeyer- Experiments in Polymer Science, Wiley Inter Science, New york
- 3. G.S.Krishenbaum-Polymer Science study guide, Gordon Breach Science Publishing, New york
- 4. G.Odien Principles of Polymerisation, Mc Graw Hill book co, Newyork
- 5. P.H.Flory- Principles of Polymer Chemistry, Cornell Press, Ithaca
- 6. Polymer Science and Technology- Joel and Fried
- 7. Polymer Chemistry- An introduction, Malcolm P.Stevens.

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com

#### SEMESTERS III & IV

## Title of the Course: Core 14-Practical III - Physical Chemistry

Teaching hours:  $30 \times 4 = 120$  Credits: 4

Course Code: 6P18/4C/PR3

## I Kinetics:-

- 1. Study of the kinetics and determination of the Arrhenius parameters, activation energy Ea and frequency A factor graphically for the acid catalysed hydrolysis of methyl acetate.
- 2. Comparision of acid strengths of hydrochloric acid for hydrolysis of methyl acetate catalysed by acid
- 3. Determination of the rate constant and order of reaction for the reaction between potassium persuphate and potassium iodide
- 4. Study of the primary salt effect on the kinetics of ionic reactions Bronsted Bjerrum relationship for the reaction between Potassium Iodide and Potassium persulphate
- II Adsorption: Study of the adsorption of acetic acid or oxalic acid on charcoal and verification of Freundlich adsorption isotherm and determination of concentration of given acid.

## III Conductivity:-

- 1. Determination of the equivalent conductance of a weak acid at different concentrations and determination of dissociation constant of the acid.
- 2. Study of the saponification of ethyl acetate and determination of the order of the reaction conductometrically
- 3. Comparison of the strengths of acetic acid and monochloro acetic acid by conductance method.
- 4. Determination of equivalent conductivity of strong electrolyte at infinite dilution and testing the validity of Onsager's theory as limiting law at high dilutions.

### 5. Conductometric titrations:-

- b. Standardisation of sodium hydroxide using standard hydrochloric acid and determination of strengths of hydrochloric acid and acetic acid in a mixture.
- c. Standardisation of Silver Nitrate using Standard KCl and determination of strengths of KCl and KI in the mixture.

## IV Potentiometry:-

- 1. Determination of the strength and hence the dissociation constant of weak acid by potentiometric method.
- 2. Determination of the strengths of KCl & KI in the given mixture by titration against silver nitrate potentiometrically.
- 3. Determination of pH of three given buffer solutions by emf method using quinhydrone electrode and the influence of added alkali or acid on them, provided with a standard buffer solution.
- 4. Determination of the strength of HCl and CH<sub>3</sub>COOH in the given mixture by titration against NaOH using quinhydrone electrode.
- 5. Determination of the strength of the given solution of Fe<sup>2+</sup> by potentiometric titration against standard potassium dichromate.
- 6 Determination of the strength of the given solution of KI by potentiometric titration against standard potassium permanganate.

## V Phase study:

Construction of a phase diagram for binary system.

a. Simple Eutectic Naphthalene - Biphenyl

Naphthalene – p-dichlorobenzene

Naphthalene – diphenylamine

- \* b. With Compound formation Naphthalene m-dinitrobenzene
- \*Determination of solubility product of a sparingly soluble salt Potentiometrically- Chemical Cell method

<sup>\*</sup>For Internal valuation only

# END SEMESTER PRACTICAL EXAMINATION SEMESTERS III & IV QUESTION BANK

Title of the Course: Core 14- Practical III - Physical Chemistry
Course Code: 6P18/4C/PR3
Time: 6hrs

Max. Marks: 60

1. Studies the kinetics of acid catalysed hydrolysis of methyl acetate and compare the given acid strengths.

- 2. Study the kinetics of acid catalysed hydrolysis of methyl acetate at three different temperatures differing by 10°C and hence evaluate the Arrhenius parameters Ea and A graphically. You are provided with 0.5 N HCl
- 3. Study the kinetics of reaction between 0.1 M KI and 0.05M K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> aqueous solutions in the absence and presence of three different concentrations of KNO<sub>3</sub>-A, B, C and arrange the rate constants in the order of increasing ionic strength.
- 4. Determine the strength of the given acetic acid solution and verify Freundlich adsorption isotherm.
- 5. a. Determine the  $\Lambda_{\infty}$  value for the given strong electrolyte conductometrically. The cell constant for the cell is given.
  - b. Determine the strengths of the strong acid and weak acid present in the given mixture conductometrically
- 6. a. Determine the strength and hence the dissociation constant of the given weak acid by potentiometric method.
  - b. Determine the pH of three given buffer solutions A, B, C using D as standard by emf method using quinhydrone electrode and the influence of added alkali or acid on it.
- 7. a. Determine the strength of given solution of KI by potentiometric titration against standard potassium permanganate.
  - b. Determine the strength of the given solution of Fe<sup>2+</sup> by potentiometric titration against standard potassium dichromate.
- 8. a. Determine the strength of the given silver nitrate solution by potentiometric titration against std. KCl.
  - b. Determine the strengths of KCl and KI in the given mixture by potentiometric titration against std. silver nitrate.
- 9. Construct the freezing point percentage composition diagram for the system of two given solids A and B. Use the diagram to fix the composition of the unknown mixture of A and B.

## **SCHEME OF VALUATION**

## Total Marks 100 (CA-40 + End Semester -60)

Record		10
Viva voce	• -	10
Manipulation		10
Skill	-	30.
Total	_	60

## 1. Ester hydrolysis

 $k_1 = 4 + 4$  [calculation + graph]

 $E_a=3$  marks

 $k_2 = 4 + 4$  [calculation + graph]

A = 3 marks

 $k_3 = 4 + 4$  [calculation + graph]

Below a factor of 10 =

Full marks

Upto a factor of 10

Reduce 2 marks

Above a factor of 10 =

Reduce 4 marks

## 2.K<sub>2</sub> S<sub>2</sub> O<sub>8</sub> & KI reaction

For each k value -6 marks [3+3] [calculation + graph]

 $6 \times 4 = 24 \text{ marks}$ 

Arranging the rate constants in increasing order – 6 marks

## 3.Adsorption

Verification of Adsorption isotherm by Graph -10 marks

Up to 5% -

20 marks

Above 5–10% % - 15 marks

>10% -

5 Marks

## 4.Conductometry

a)Determination of strength of the acid-15 marks

Verification and determination of the constants

Error	Marks
Upto 10 %	15
Above 10-15%	10
Above > 15%	5

b) Determination of  $\Lambda_{\infty}$  for strong electrolyte conductometrically

 $\Lambda_{\infty}$  of strong electrolyte

15 marks

Upto 10% error = 15 marks

Above 10% to 15% = 10 marks

Above 15% = 5 marks

c) Determination of strength of weak acid – 7.5 marks

Determination of strength of strong acid -7.5 marks

Error	Marks
Upto 5%	7.5
Above 5-10%	. 5
Above 10%	2

## **POTENTIOMETRY**

## 1. Potentiometric Titration

Error	Marks	For mixtures
Upto 5%	15	7.5 + 7.5 marks each
Above 5-10%	10	5 + 5 marks each
Above 10-15%	6	3 + 3 marks each

5a) Determination of strength of weak acid - 10 marks

Error	Marks
Upto 5 %	5
> 5-10 %	5
> 10 %	5

Determination of K<sub>a</sub> of weak acid - 5 marks

Below a factor of 10 - 5 marks

A factor of 10 - 3 marks

Above a factor of 10 - 2 marks

5b) Determination of pH of three buffer solutions:  $5 \times 3 = 15$  marks

Determination of  $E_{cal}$  - 5 marks

Interpretation of results - 10 marks

8. Phase Diagram -20 marks [8+4+4]

Unknown composition – 10 marks

Phase diagram – 8 marks

Freezing point of components A and B = 4 marks [2+2]

Eutectic temperature – 4 marks

Eutectic composition – 4 marks

Total - 30 marks

# Eutectic temperature

Error	Marks
+/- 2°	4 marks
+/- 3°	2 marks
> 3°	1 marks

# Eutectic composition – 4 marks

Error	Marks
+/- 5%	. 4
6-10%	2
> 10%	1

# Unknown composition

Error	Marks
+/- 5%	10
6-10%	8
> 10%	5

## SEMESTER IV

Title of the course: Soft Skills 4-Scientific Research and Presentation Skills

Teaching hours:  $15 \times 2 = 30$  Credits: 2

Course Code: 6P18/4S/SRP L T P 2 0 0

## **Objective:**

1. To develop the skills needed for analysis and presentation of research data

2. To create awareness towards research problem.

3. To introduce computational skills required for research.

## **COURSE OUTLINE**

UNIT I: Selection of research problems and writing- Project proposal-funding agencies-Survey of scientific literature-Primary and secondary sources. Impact factor and citation index. Thesis and Assignment writing. Conventions of writing-General format-page and chapter format-use of quotations and foot notes-preparation of tables and figures-referencing-appendices-revising, editing and evaluating the final material- proof reading -meanings and examples of commonly used abbreviations. Plagiarism, copy right and patent laws.

UNIT II: Statistical treatment: Precision and Accuracy-Reliability-Determinate and random errors-Distribution of random errors-Normal distribution curve. Statistical treatment of finite samples-the student's T test and F test-criteria for rejection of an observation Q test. Significant figures and computational rules. Data plotting-Least square analysis-significance of correlation coefficient. Publication of research paper—manuscript preparation Referencing-endnote

UNIT III: Computer and their application to Chemistry: Computer binary language, introduction-hardware, software-programming-C. Language-variables, constants, operators-input, output functions- control statements, loop, functions arrays and pointers. Programming to calculate pH of a solution, solubility product, standard deviation and correlation coefficient for a straight line. Microsoft Word, Excel, Power point presentation, Internet.

#### **RECOMMENDED TEXT BOOKS:**

- 1. K.V.Raman, Computers in chemistry, Tata McGraw Hill, New Delhi 1993
- 2. Thesis and Assignment writing, J. Anderson, B.H. Durston and M.Poole, Wiley EasteLtd (1970)
- 3. Ramesh Kumari Computers and their applications to chemistry: Narosa publications.

#### REFERENCES:

- 1. Advanced organic chemistry: Reactions, Mechanism and structure, J. March, McGraw Hill International Student edition, 1977.
- 2. Instrumental methods of chemical analysis (4th edition), G.W. Ewing, McGraw Hill International Student edition, 1975.
- 3. Quantitative Analysis (3rd edition), R.A. Jr. and A.L. Underwood, Prentice Hall of India Pvt. Ltd. (1977).
- 4. Techniques of Organic Chemistry, Ed. A. Weissberger (series of volumes) Wiley —Inter sciences.
- 5. Statistical Analysis Chemistry and Chemical Industry, C.A Bennett and N.L.Franklin, John Wiley (1954).
- 6. Correlation Analysis in organic chemistry An introduction to linear free energy relationships, J. Shorter, Olarendon Press. Oxford (1973) [Oxford chemistry series11].
- 7. The way they learn Siendia Ulrich Tobiah-Pindole house Inc. U.S.A.
- 8. Tactist Rosemary Napper and Trudy Newton, TA resources, U.K 2003.
- 9. Hand book for Authors Journal of the American Chemical Society Publications
- 10. Chemical Publications-Their nature and uses.

## PERIODICALS:

- 1. Resonance- Journal of science education
- 2. Span
- 3. Indian academy of sciences-proceedings- Chemical Sciences
- 4. Current Science
- 6. Journal of Indian chemical education
- 7. Journal of American chemical society
- 8. Bulletin of material science

- 1. www.virtlab.com
- 2. http://nptel.ac.in
- 3. MATLAB
- 4. Mooc.org
- 5. http:/swayam.gov.in
- 6. http://search.ebscohost.com

## ETHIRAJ COLLEGE FOR WOMEN [Autonomous] CHENNAI- 8

## END SEMESTER EXAMINATION

## TEMPLATE OF THE QUESTION PAPER

## M.Sc Chemistry

## Common to all Core theory and Major Elective papers

Title of the course Paper Code

Max Marks: 100

Time: 3hrs

#### Section A

Answer all the Questions

10Qx2=20 marks

Question Numbers 1 to 10 Equal weight age to be given for all the 5 units in the syllabus. 2 Questions from each unit.

#### Section B

Answer all the Questions

5Qx8=40 marks

Question numbers 11 to 15 (5 Questions)

5 Questions to be given with an internal choice choosing one question from each unit ie 11a or 11b

## Section-C

Answer any two questions

2Qx20=40 marks

Question Numbers 16-19 (4 Questions)

4 questions to be given with a maximum of 4 subdivisions (a, b, c, d) giving equal weightage to all the five units in the syllabus.

Note: Equal weightage to be given to all the 5 units in the syllabus

Section A =  $10Q \times 2$  marks = 20 marks

Section  $B = 5Q \times 8 \text{ marks} = 40 \text{ marks}$ 

Section  $C = 2Q \times 20$  marks = 40 marks

Total = 100 marks

## ETHIRAJ COLLEGE FOR WOMEN [Autonomous] CHENNAI- 8

#### END SEMESTER EXAMINATION

## TEMPLATE OF THE QUESTION PAPER

Common to all Non Major Electives I & II year MA/M.Sc/M.Com

Title of the Course: Cosmetology/ Fibre, Fabrics, Dyeing and printing of Textiles

Course Code: 6P18/2E/COS // 6P18/3E/FDP

Max.Marks:100

Time: 3hrs

**SECTION A** 

 $(8Q \times 5 = 40)$ 

## ANSWER ANY EIGHT QUESTIONS

Question numbers 1-10.

8 Questions to be answered out of 10 Questions choosing two from each unit

**SECTION-B** 

 $(6Q \times 10 = 60)$ 

# ANSWER ANY SIX QUESTIONS

Question numbers 11-19 (9 Questions).

6 Questions to be answered out of 9 Questions choosing not more than two questions from each unit. Each question can have a maximum of two subdivisions (a, b)

Note: Equal weightage must be given to all five units of the syllabus.

Section A -8Q x 5 marks= 40 marks.

Section B - 6Q x 10 marks=60 marks

## ETHIRAJ COLLEGE FOR WOMEN [Autonomous] CHENNAI- 8

## END SEMESTER EXAMINATION

## TEMPLATE OF THE QUESTION PAPER

# Common to all Soft Skill Papers

PG18/1S/PEW

Soft skill 1 – Personality Enrichment for Women

6P18/3S/LSS

Soft Skill 3- Laboratory Safety Skills

6P18/4S/SRP

Soft Skill 4- Scientific Research and Presentation Skills

Time -2 Hrs,

Max. Marks - 50

SECTION A

(10 Q X 5 = 50 Marks)

10 Questions to be answered out of 12 Questions