

Avinashilingam Institute for Home Science and Higher Education for Women

(Deemed to be University Estd. u/s 3 of UGC Act 1956, Category A by MHRD)

Re-accredited with A++ Grade by NAAC. CGPA 3.65/4, Category I by UGC

Coimbatore - 641 043, Tamil Nadu, India

## Department of Chemistry M.Sc. Chemistry

## **Programme Outcomes**

- 1. Demonstrate holistic core competencies in classical, contemporary and Applied Chemistry
- 2. Ability to apply core knowledge and understanding in Chemistry and exhibit problem solving skills
- 3. Comprehensive communication of concepts and techniques in Chemistry
- 4. Expertise in handling sophisticated equipment for identification and analysis of materials
- 5. Capability to integrate knowledge and skills to solve societal and environmental problems
- 6. Suitability to be employable in industries and R&D organizations

## **Programme Specific Outcomes**

- 1. Firm foundation in fundamentals and in-depth knowledge in Chemistry
- 2. Ability to synthesize, evaluate, classify, interpret and utilize principles, phenomena, processes and reaction mechanisms involved in the various domains of Chemistry
- 3. To acquire research aptitude and adaptability to sustainable environmental practices and socio economic awareness

# Scheme of Instruction and Examination (For students admitted from 2025 – 2026 & onwards)

Pa	Subjec Code	Name of Paper/Component	Inst	ours of tructions week	S	cheme	Scheme of Examination						
	= .		T	P	Duration of exam	CIA	CE	Total	Credi				
	1.	First S	emeste	r				1					
	25MCHC0	Barno Chemistry-1	4		3	40	60	100					
	25MCHC0	2 Inorganic Chemistry-I	4	+ +	3			100	4				
т	25MCHC0	Physical Chemistry-I	4			40	60	100	4				
I	25MCHC04		3	1	3	40	60	100	4				
	25MCHC05		3		3	40	60	100	3				
	25MCHC06	- Built Chemistry Tractical-1		6	6	40	60	100	3				
		Barre Chemistry Flactical- II		6	6	40	60	100	3				
П		CSS/Adult Education / Community Engagement and Social Responsibility	2	-	-	-	-	-					
		Library	1										
		Second S	emeste	r									
	25MCHC07	Organic Chemistry-II	4		3	40							
	25MCHC08	Inorganic Chemistry-II	4			40	60	100	4				
	25MCHC09	Physical Chemistry-II	4		3	40	60	100	4				
	25MCHC10	Spectroscopy-I			3	40	60	100	4				
	25MCHC11		3		3	40	60	100	3				
-	25MCHC12	Physical Chemistry Practical-I		4	6	40	60	100	2				
-	251/10/10/12	Inorganic Chemistry Practical-I		4	6	40	60	100	2				
-		Interdisciplinary Course	4	-	3	100	-	100	4				
		Professional Certification Course							2				
	25MXCSS1 / 25MXAED1/ 25MXCSR1	CSS / Adult Education / Community Engagement and Social Responsibility	2	-	2	-	-	100	2				
		Library	1										

		Third Ser	mest	er					
	25MCHC13	Organic Chemistry-III	3		3	40	60	100	3
	25MCHC14	Inorganic Chemistry-III	3		3	40	60	100	3
	25MCHC15	Physical Chemistry-III	3		3	40	60	100	3
	25MCHC16	Spectroscopy-II	3		3	40	60	100	3
	25MCHC17	Computational Chemistry	3		3	40	60	100	3
İ	25MCHC18	Inorganic Chemistry Practical-II		6	6	40	60	100	3
	25MCHC19	Physical Chemistry Practical- II		4	6	40	60	100	2
	25MCHC20	Environmental Chemistry (Self-study)	2		3	100	-	100	2
	25MCHC21	Mini Project	1	-	-	100	-	100	2
	25MCHC22	Internship				-		100	2
П		Multidisciplinary Course	2		3	100	_	100	2
		Fourth Ser	nest	er		4			
I	25MCHC23	Research - Thesis/ Project/ Patent		30		100	100	200	20
						Tot	tal Cre	dit	96

Other courses to be undergone by the student:

MOOC courses- 2 to 4 Credits - Credit transfer may be claimed.

## Minimum 96 + 2 Credits to earn the degree

Students who exit at the end of 1st year with 40 credits shall be awarded a Postgraduate Diploma.

## Courses offered by the department

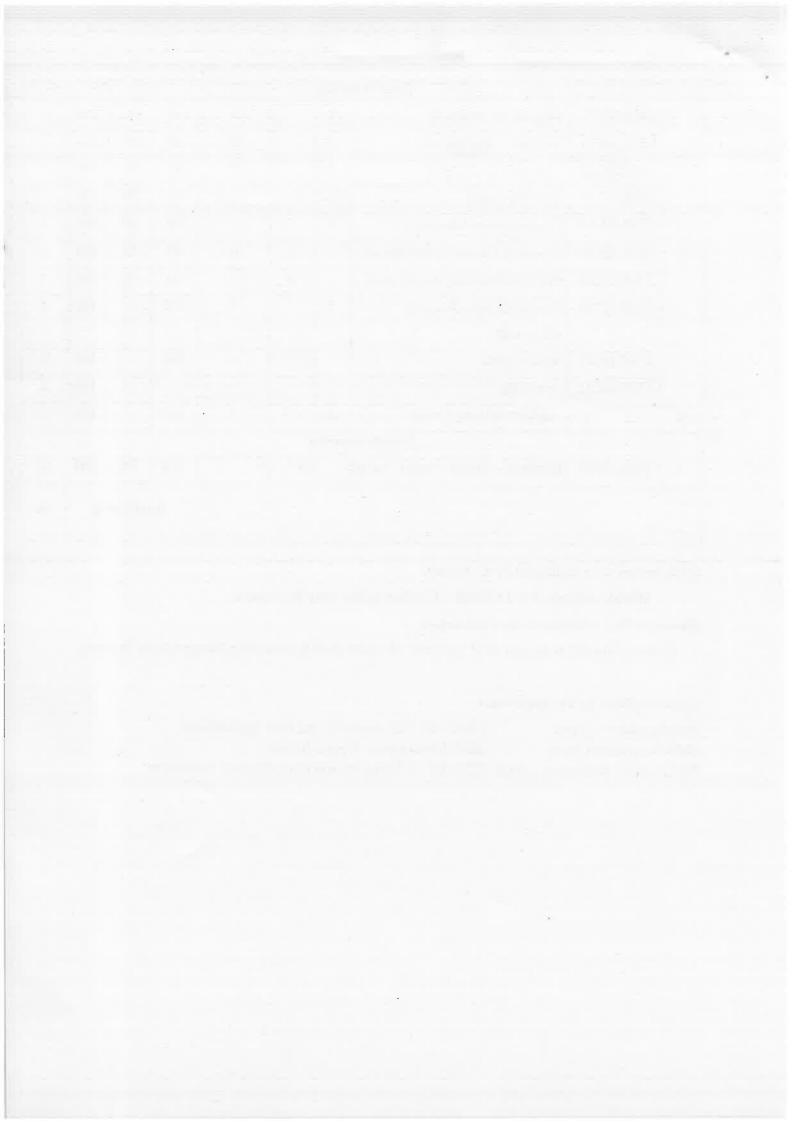
Interdisciplinary Course

25MCHI01 Nanomaterials and their Applications

Multidisciplinary Course

25MCHM01 Green Aspects in Life

Professional Certification Course 25MCHPC1 Analytical and Phytochemical Techniques



#### Organic Chemistry-I

Semester I 25MCHC01

Hours of Instruction/Week: 4

No. of Credits: 4

#### **Objectives**

1. To recall the concepts of field effects

2. To impart advanced knowledge in stereochemistry

3. To comprehend on reaction intermediates and determination of reaction mechanism

4.To gain knowledge on free radical reactions

Unit 1 Concepts in Organic Reaction Mechanism, Aromaticity and Tautomerism

Field effects- inductive, inductomeric, electromeric and resonance effects, hyperconjugation-aromaticity in benzenoids and non-benzenoid systems- tautomerism: keto, enol, amido, imido, nitro and acinitro systems (self-study)- fullerenes- bonding in fullerene- applications- hydrogen bonding-inter and intramolecular hydrogen bonding- applications (self-study)- bonds weaker than covalent bond – addition compounds - crown ether complexes and cryptands - inclusion compounds, catenanes and rotaxanes - molecular switches- calixarenes

Unit 2 Stereochemistry I

Optical isomerism- elements of symmetry and chirality (self-study)- R-S convention, E-Z convention-optical activity in the absence of asymmetric atoms (allenes, spiranes, biphenyls) (self-study)-stereoselective and stereospecific synthesis- prochirality—enantiotropic and diastereotopic groups-chirality due to helical shape- conformational analysis of acyclic compounds- conformations of cyclohexanes and decalin

**Unit 3 Stereochemistry II** 

Circular dichroism and optical rotatory dispersion- axial haloketone rule, octant rule and their application to simple decalin systems- asymmetric synthesis- chiral auxiliaries- methods of asymmetric induction— substrate, reagent and catalyst- controlled reactions- determination of enantiomeric and diastereomeric excess- enantio-discrimination- resolution: optical and kinetic

Unit 4 Reactive Intermediates and Reaction Mechanism

Reaction intermediates- Classical and non-classical carbocations, carbanions, radical- anions, radical-cations, carbenes, arynes and nitrenes- general methods of generation (self-study), detection of reaction intermediates- isotope effects and kinetic effects- reactivity, effect of structure on reactivity – Hammett and Taft equations, singlet oxygen - generation and reactions- determination of reaction mechanism of kinetically and thermodynamically controlled reactions- energy profile diagrams- hard and soft acids and bases

**Unit 5 Free Radical Substitution** 

Types of free radical reactions- mechanism of free radical reaction- mechanism at an aromatic substrate- reactivity in aliphatic substrate- alkenes, olefins, alkyl side chain aromatic compound and bridgehead, effect of solvent on reactivity, reactivity in aromatic substitution, reactivity in the attacking free radicals, allylic halogenation (NBS)

Total hours: 60

#### **Textbooks**

- Mukherji, S. M., and Singh, S. P., Reaction Mechanism in Organic Chemistry, Macmillan, ISBN 9780333904619 (1984)
- 2. Carey, F.A., and Sundberg, R.J., Advanced Organic Chemistry, Parts A and B, 5th Ed., Springer, Germany (2007)

#### Reference Books

- 1. Jerry March, Advanced Organic Chemistry, Reaction Mechanisms and Structure, 6th Ed., John Wiley & Sons (2011)
- 2. Kalsi, P. S., Stereochemistry, Wiley Eastern Limited, New Delhi (1993)

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- 3. Clayden, J., Greeves, N., Warren, S., and Wothers, P., Organic Chemistry, 1st Ed., Oxford University Press, UK (2000)
- 4. Eliel, E.L., and Wilen, S. H., Stereochemistry of Carbon Compounds, John Wiley, Newyork, (1994)
- 5. Pine, S.H., Henrickson, J.B., Gram, D.J., and Hammon, G.S., Organic Chemistry, 3rd Ed., McGraw-Hill Kogakusha
- 6. Nasipuri, D. Stereochemistry of Organic Compounds-Principles and Applications, 2nd Ed., New Age International, New Delhi (1994)

#### **Course Outcomes**

At the end of the course the student will be able to

- 1. Describe and explain the influence of field effects, tautomerism, aromaticity, fullerenes, hydrogen bonding, and supramolecular assemblies
- 2. Assign stereochemical descriptors (R/S, E/Z), analyze chirality and symmetry, and evaluate conformational preferences in organic molecules.
- 3. Apply principles of asymmetric synthesis and chiral discrimination to determine and control stereochemistry and optical activity in organic compounds
- 4. Identify and analyze the structure, generation, detection, and reactivity of key organic reaction intermediates, and to predict and rationalize reaction mechanisms and outcomes
- 5. Explain the mechanisms and factors influencing free radical reactions and predict reactivity and selectivity based on substrate structure and reaction conditions

CO PO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	Н	M	M		L	M	M	H	
CO2	H	М	L				M	M	
CO3	Н	Н	L				H	H	
CO4	L	M	L				M	H	
CO5	M	M	L		M	H	M	H	L

#### Inorganic Chemistry-I

Semester I 25MCHC02

Hours of Instruction/Week: 4

No. of Credits: 4

#### **Objectives**

- 1. To acquire thorough understanding of concepts and theories of coordination chemistry
- 2. To comprehend on stability constants and mechanistic pathways of reactions in complexes

3. To gain knowledge of solid-state chemistry

#### Unit 1 Coordination Chemistry I

Nature of metal-ligand bonding in complexes- crystal field theory (CFT) crystal field splitting in octahedral, tetrahedral, square planar complexes and tetragonal complexes – distribution of delectrons in octahedral and tetrahedral complexes, crystal field stabilization energy and its applications in stereochemistry, stability of oxidation states, trends in heats of hydration & lattice energy and colour & magnetic properties- weak and strong fields – pairing energy, Jahn-Teller theorem- tetragonal distortion from octahedral symmetry, conditions for distortion- Jahn Teller stabilization energy-limitations of CFT

Self-study - Spectro chemical series and Spinels

#### **Unit 2 Coordination Chemistry II**

Molecular orbital theory- LCAO-MO model, TASO, LUMO-HOMO concepts in bonding – homo diatomic molecules, MO theory for hetero poly atomic molecules and ions (CO, NO, HCl, CO<sub>3</sub><sup>2-</sup>, NO<sub>3</sub><sup>2-</sup>, SO<sub>3</sub>, O<sub>3</sub>, NO<sub>2</sub>, CO<sub>2</sub>, N<sup>3-</sup>), comparison between VBT and MOT, term states for d ions - characteristics of d-d transitions - charge transfer spectra - selection rules for electronic spectra - Orgel correlation diagrams for d<sup>1</sup> to d<sup>9</sup> ions- Sugano-Tanabe energy level diagrams - nephelauxetic series - Racha parameter and calculation of inter-electronic repulsion parameter

Self-study - Quantum numbers of multi-electron atoms - Russell-Sanders coupling - L-S coupling and micro states - ground state terms for  $d^1 - d^{10}$  ions

## Unit 3 Stability of Complexes Kinetics and mechanisms of substitution reactions

Stability of complexes in solution- thermodynamic and kinetic stability- labile and inert complexes – factor influencing the stability of complexes- determination of stability constant, ligand substitution reaction in octahedral complexes- types of substitution reactions –  $S_N1$  and  $S_N2$  and  $S_E$  mechanism – hydrolysis reaction – aquation and base hydrolysis-  $S_N1$ cb mechanism- anation reactions- ligand substitution reaction in square planar complexes- trans effect series- uses and theories of trans effect- mechanism of substitution reaction in square planar complexes- electron transfer reaction in coordination compounds – types of electron transfer reaction- mechanism of one – electron transfer reaction – bridge or inner sphere mechanism and outer sphere mechanism, factors affecting the rates of direct electron transfer reactions

Self-study- two electron transfer reaction -complementary and non-complementary electron transfer reaction

#### Unit 4 Solid State -I

Crystalline and amorphous solids-polymorphism-isomorphism- Mitcherlich's law of isomorphism-isopolymorphism-close packing of spheres, packing efficiency, hexagonal Close packed (hcp) and cubic close packed (ccp) structures, coordination number, Interstitial sites in closely packed arrangement of atoms- trigonal sites, tetrahedral and octahedral sites, radius ratio rule and its effect on

12h

12h

12h

the shape of ionic crystals, Coordination number of cubic lattice—Structure of ionic crystals of AB type-Caesiumchloride, Zinc Blende, Wurtzite, AB2 type-Rutile, Fluorite

#### Unit 5 Solid State -II

Stoichiometric defects – Schottky and Frenkel defects, Non-stoichiometric defects – metal excess and metal deficiency defects – Extended defects – line and plane defects, band theory – semiconductors – intrinsic and extrinsic type, p and n type semiconductors, crystal growth methods: from melt and solution (hydrothermal, sol-gel methods) – principles and examples- X-ray diffraction technique: powder diffraction method – principle and Instrumentation; interpretation of XRD data – ICDD files, phase purity, Scherrer formula, lattice constants calculation; systematic absence of reflections

Total hours: 60

#### **Recommended Text**

- 1. J E Huheey, EA Keiter, RL Keiter and OK Medhi, Inorganic Chemistry Principles of structure and reactivity, 4th Edition, Pearson Education Inc., 2006
- 2. G L Meissler and D A Tarr, Inorganic Chemistry, 3rd Edition, Pearson Education Inc., 2014
- 3. D. Bannerjea, Co-ordination Chemistry, TATA Mcgraw Hill, 1993.
- 4. B. N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd, 1976.
- 5. F. A. Cotton, G. Wilkinson.; C. A. Murillo; M. Bochmann, Advanced Inorganic Chemistry, 6<sup>th</sup> Ed.; Wiley Interscience: New York, 1988.
- 6. Malik, W.U., Tuli G.D. and Madan, R.D. Selected Topics in Inorganic Chemistry, 17th Ed., S. Chand Company Ltd, (2010)
- 7. A R West, Solid state Chemistry and its applications, 2<sup>nd</sup>Edition (Students Edition), John Wiley & Sons Ltd., 2014.
- 8. L Smart, E Moore, Solid State Chemistry An Introduction, 4th Edition, CRC Press, 2012.

#### Reference Books

- 1. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, Saunders Publications, USA, 1977.
- 2. Peter Atkins and Tina Overton, Shriver and Atkins' Inorganic Chemistry, 5th Edition, Oxford University Press, 2010
- 3. Inorganic Chemistry, D. F. Shriver, P. W. Atkins, W. H. Freeman and Co, London, 2010.
- 4. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994.
- 5. C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2<sup>nd</sup> Edition, Cambridge University Press, 199.
- 6. G. H. Stout and L. H. Jenson, X-Ray Structure Determination; 2nd ed.; John Wiley & Sons: New York, 1989.
- 7. Solid-state Chemistry and its application, D.K. Chakrabarty, New Age International Private Publications, 2010.

#### **Course Outcomes**

- 1. Ability to apply theories of coordination compounds to understand structure
- 2. Predict the physical/electronic properties, bonding and reactivity of inorganic complexes specially coordination complexes containing transition metals
- 3. Explain the stability of complexes and various experimental methods to determine the stability of complexes
- 4. Ability to analyze crystal systems and identify class of defects in crystals
- 5. To understand the principles of diffraction techniques and microscopic techniques

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PS O 1	PSO 2	PSO 3
CO 1	M	L			M	·M	M		
CO 2	M	M	L			M	M	M	
CO 3	M	M	L				M	M	M
CO 4	M	M	M	M		M	M	M	M
CO 5	M	M	M	M	M	M	H	M	M

10h

12h

14h

#### Physical Chemistry-I

Semester I 25MCHC03

Hours of Instruction/Week: 4 No. of Credits: 4

#### **Objectives**

- 1. To widen knowledge on the essential concepts of thermodynamics
- 2. To acquire knowledge on statistical thermodynamics
- 3. To understand the principles of partition functions and concepts in non-equilibrium thermodynamics

#### Unit 1 Thermodynamics I

A brief resume of thermodynamics (confined form of first and second laws) – concept of entropy – definition of entropy – entropy changes – Carnot efficiency, Helmholtz and Gibb's functions, criteria of equilibrium (Self-study), Maxwell relation, Partial molar properties—chemical potential – significance - Gibbs—Duhem equation - variation of chemical potential with temperature and pressure

Unit 2 Thermodynamics II

Third law – need for third law, Nernst heat theorem, statements of third law - thermodynamics quantities at absolute zero, calculation of absolute entropies - apparent exception to third law, thermodynamic properties of real gases- fugacity – definition determination of fugacity of gases by graphical method and from equations of state – variation of fugacity with temperature and pressure, fugacity of gases in a mixture

## **Unit 3 Statistical Thermodynamics**

Basic concepts – phase space, ensembles-micro canonical, canonical, grand canonical ensembles, microstates and macro states, Stirling's theorem, thermodynamic probability classical Maxwell Boltzmann statistics - quantum Statistics - Bose Einstein distribution law- derivation – entropy of boson applications - derivation of Planck's black body radiation law - Bose Einstein condensation - helium at low temperature - Fermi-Dirac distribution law - derivation, entropy of fermions, applications - electron gas, Fermi energy of free electrons at absolute zero - comparison of Maxwell Boltzmann, Bose Einstein, Fermi-Dirac statistics - heat capacity – Einstein theory and Debye theory, Debye T cube law

#### **Unit 4 Partition Function**

Definition - physical significance, rotational, translational, vibrational and electronic partition functions for diatomic molecules, relation between the total partition function and the individual partition functions, application of partition in the calculations of thermodynamic functions - internal energy, heat content, entropy, work function, heat capacities and equilibrium constants- <u>numerical problems (self-study)</u>

## Unit 5 Non Equilibrium Thermodynamics

Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes, transformations of the generalized fluxes and forces — non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocal relations, electro kinetic phenomena, diffusion, electric conduction, <u>irreversible</u> thermodynamics for biological systems (self-study), coupled reactions

12h

#### **Textbooks**

- 1. Gurdeep Raj, Advanced Physical Chemistry, 42<sup>nd</sup>Ed., Goel Publishing House, (2018)
- 2. John M. Bockris and Amulya K.N. Reddy, Modern Electrochemistry, Volume I & II, 2<sup>nd</sup> Ed. (2008)
- 3. Gupta and Sharma, K. Advanced Physical Chemistry, Nath & Co. Educational Publishers, (2011)
- 4. Gurtu, J. N., and Gurtu, A., Advanced Physical Chemistry, 18th Ed., Pragati Prakashan (2015)

#### Reference Books

- 1. Lewis and Randall, Thermodynamics (2000)
- 2. Cerasimov, Y.A., Physical Chemistry, Volume II (2001)
- 3. Peter Atkins, Julio DePaula and James Keeler, Physical Chemistry,11th Ed., Oxford University Press, (2018)
- 4. Gupta, R.K.A Textbook of Physical Chemistry, Latest Ed., Arihant Publication (2018)

#### **Course Outcomes**

After the completion of the course students will be able to

- 1. Understand the concepts of first and second law of thermodynamics
- 2. Explain the applications of third law of thermodynamics
- 3. Distinguish the various thermodynamic statistics and partition functions
- 4. Describe the applications of partition functions
- 5. Apply the concepts of non equilibrium thermodynamics to biological reactions

CO/PO	PO1	PO 2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO 3
CO 1	M	M				M	M	M	
CO 2	M	M				M	M		
CO 3	M	M	M		M		M	M	
CO 4	M	M	M				M		
CO 5	M	M	M	M	M	M	M	M	M

#### Research Methodology

Semester I 25MCHC04

Hours of Instruction/Week: 3

No. of Credits: 3

#### **Objectives**

- 1. To understand concepts of research and
- 2. To develop skills in formulating various research designs
- 3. To gain knowledge on statistical tools and analysis
- 4. To acquire various techniques used in research
- 5. To learn the application of technology in research

#### **Unit 1 Concept of Research**

Objectives and characteristics of research, criteria of good research, qualities of a good researcher, types of research – basic, applied, action, experimental, diagnostic and exploratory research importance of research in science (self-study)

**Unit 2 Components of Research Design** 

Sampling –random and non random sampling, Formulation of hypotheses-Testing of hypotheses and tests of significance, Null and alternative hypotheses. Primary and secondary data, Primary and Secondary references (self-study)

Unit 3 Techniques of Analysis

Mean, median, mode, standard deviation, correlation analysis- definition, types, regression analysis – definition, linear regression - types, Student t test, ANOVA-assumptions, one way and two ANOVA Chi square-test and goodness of fit – characteristics, assumptions, degree of freedom and applications

**Unit 4 Research Reporting** 

Tabulation of data, parts of a table, types of diagram-line, bar, pie and pictogram-chapterisation of research, preparation of synopsis of a research - scope of research in higher education- current status of research in chemistry in India (self-study)

Unit 5 Application of Technology in Research

Use of technology in chemistry research – computer packages for data analysis – SPSS package, ISIS draw, sources of funding in scientific research (self-study)

Reference Books

1. Gurumani, N. An introduction to Biostatistics, 2<sup>nd</sup> Ed., MJP publishers (2004)

- 2. Kothari, C.R. Research Methodology: Methods and Techniques, 2<sup>nd</sup> Ed., New Age International (P) Ltd., New Delhi (2000)
- 3. Gupta, S.P. Statistical Methods, 43rd Ed., Sultan Chand & Sons Publications, New Delhi, (2014)
- 4. Jerrold H. Zae, Biostatistical Analysis, 4th Ed., Pearson Education (2006)

9h

9h

9h

9h

Total hours: 45

#### **Course Outcomes**

After the completion of course students will be able to

- 1. Familiarize various research concepts
- 2. Formulate research designs
- 3. Apply statistical analysis to research
- 4. Write a good research report
- 5. Apply latest technology in research and get to know of funding openings for research

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1		M			M	M	M		M
CO 2	M	M			Н	M			
CO 3	M	M	L		Н	M	M	M	M
CO 4	M				Н	M			
CO 5	M				M	M		M	

#### Organic Chemistry Practical-I

Semester I 25MCHC05

Hours of Instruction/Week: 6

No. of Credits: 3

#### **Objectives**

1. To acquaint with the binary separation of a binary mixture and qualitative analysis of organic compounds

2. To get acquainted with practical skills in finding boiling point, melting point of organic compounds and laboratory techniques for crystallization

#### Unit 1 Qualitative Analysis

Analysis of binary mixture- comprising of acidic and neutral, basic and neutral or weakly acidic and neutral mixture

Compounds to be given: monocarboxylic acids, dicarboxylic acids, monoamides, diamides, hydrocarbons, sugars, anilides, aldehydes, ketones, simple phenol, phenolic compounds, esters, primary, secondary, tertiary amines, nitro compounds

Preliminary pilot analysis

- Pilot reporting
- Bulk separation

Purification of separated compounds- recrystallization

- Systematic analysis of each component inclusive of preliminary identification, confirmatory tests, derivative preparation
- Recording melting point/boiling point of components

Total hours: 90

#### Reference Books

- 1. Furniss, B.S., Hannaford, A.J., Rogers, V. Smith, P.W.G. and Tatchell, A.R. Vogel's Text Book of Practical Organic Chemistry, (ELBS) (2005)
- 2. Venkateswaran, V., Veraswamy, R. and Kulandaivelu, A.R. Basic Principles of Practical Chemistry, Sultan Chand & Sons, ISBN: 9788180547768, 8180547760 (2012)
- 3. Mann and Saunders, Practical Organic Chemistry, 4th Ed., 2009, Pearson Publication
- 4. Clarke, H. T. A Handbook of Quantitative and Qualitative Analysis, 4th Ed. (2007)

- 1. Skill in carrying out laboratory techniques for purification, crystallization, and distillation
- 2. Formulate strategies for binary mixture separation
- 3. Ability to identify organic compounds by qualitative analysis
- 4. Plan synthetic procedures in derivatization of organic compounds
- 5. Identification of organic compounds for synthetic procedures in derivatization of organic compounds

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	Н	Н	M	M	Н	M	Н	L	Н
CO 2	H	H	M	L	H	Н	Н	M	Н
CO 3	H	H	H	H	H	H	Н	M	Н
CO 4	H	Н	M	M	H	Н	Н	M	Н
CO 5	H	Н	Н	M	H	L	Н	M	M

50 h

40h

#### **Organic Chemistry Practical-II**

Semester I 25MCHC06

Hours of Instruction/Week: 6
No. of Credits: 3

#### **Objectives**

- 1. To develop skills in the estimation and preparation of selected organic compounds
- 2. To get acquainted with isolation and chromatographic techniques
- 3. To develop skills in extraction of selected natural products

#### **Unit I Quantitative Analysis**

Estimation of phenol

Estimation of aniline

Estimation of Glucose

Estimation of Ascorbic acid

Estimation of ethyl methyl ketone

Estimation of lactose from milk

Determination of saponification value of oil

Determination of iodine value of oil

Isolation of casein from milk (Class Work)

Isolation of piperine from black pepper (Class Work)

Experiments involving TLC (o-nitro phenol and p-nitro phenol and L-lecuine, DL-Alanine, L-Lysine) and paper chromatography(sugars) for separation and identification of organic compounds

#### **Unit II Organic Preparations**

Two stage preparation of organic compounds involving synthetic methods like oxidation, acylation, nitration, bromination, hydrolysis and condensation and cyclization

Preparation of aspirin (methyl salicylate -salicylic acid-aspirin)

Preparation of p-nitro aniline (acetanilide-p-nitro acetanilide-p-nitro aniline)

Preparation of 1,3,5 tribromo benzene(aniline-2,4,6 tribromoaniline-1,3,5 tribromo benzene)

Preparation of anthranilic acid (pthalic anhydride-pthalimide-anthranilic acid)

Preparation of phenyl indole(acetophenone-acetophenone phenyl hydrazone-2-phenyl indole)

#### Multi stage preparation

Preparation of Benzilic acid (benzaldehyde-benzoin-benzil-benzilic acid) (Class work)

**Total hours: 90** 

#### **Textbooks**

- 1. Furniss, B.S., Hannaford, A.J., Rogers, V., Smith, P.W.G., and Tatchell, A.R. Vogel's Text Book of Practical Organic Chemistry, (ELBS) (2005)
- 2. Hill, P.J. Small Scale Organic Preparations (2001)

#### **Reference Books**

- 1. Dupont Durst, George, H. and Gokel, W. Experimental Organic Chemistry, McGraw Hill Book Co., New York (2000)
- 2. Shrnier, R.L., Fusen R.C. and Curtin, D.V. The Systematic Identification of Organic Compounds (2002)
- 3. Cheronis, N.D., Entrikin, J.B. and Hodnett Semlmicro, E.M. Qualitative Organic Analysis (2001)

- 1. Skills in estimation of organic compounds
- Skills in extraction of selected natural products
   Familiarization on oil analysis
   Know chromatographic techniques

- 5. Ability to prepare organic compounds

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	M	M	Н	M	Н	M	Н	Н	Н
CO 2	M	M	H	M	Н	M	Н	M	Н
CO 3	M	M	H	L	Н	Н	Н	M	H
CO 4	M	M	M	L	M	H	H	H	H
CO 5	M	M	L	Н	Н	H	H	M	H

12h

12h

12h

#### Organic Chemistry-II

Semester II 25MCHC07

Hours of Instruction/Week: 4
No. of Credits: 4

#### **Objectives**

1. To gain knowledge on pericyclic reactions

2. To familiarize the concepts of photochemical reactions

3. To get acquainted with the use of synthetic reagents and name reactions for applications in organic synthesis

#### Unit 1 Pericyclic Reactions I

Symmetry of molecular orbital, Frontier orbitals of ethylene, 1.3 butadiene, 1,3,5 hexatriene, allyl system, classification of pericylic reactions FMO method, Woodward –Hoffman rule, molecular orbital correlation diagram method and perturbation of molecular orbital (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions, electrocyclic reactions – conrotatory and disrotatory motions (4n), (4n+ 2), allyl systems- simple problems in pericyclic reactions (self-study)

### Unit 2 Pericyclic Reactions II

Cycloadditions antarafacial and suprafacial additions, 1,3 dipolar cycloadditions and chelotropic reactions- sigma-tropic rearrangements – suprafacial and antarafacial shifts of H- sigmatropic shifts involving carbon moieties- retention and inversion of configuration- detailed treatment of Claisen and Cope rearrangements- fluxional tautomerism- Aza cope rearrangements (self-study)

#### Unit 3 Photochemistry I

Photochemical energy- experimental method of photochemistry, Jablonski diagram, singlet and triplet state, dissipation of photochemical energy, intersystem crossing, internal conversion, photosensitization, quenching, quantum efficiency and quantum yield (self-study), Norrish, type I and Norrish type II cleavages, Paterno-Buchi reaction, photo reduction, photo chemistry of enones, hydrogen abstraction, rearrangement of  $\alpha$ ,  $\beta$  unsaturated ketone and cyclohexadienones

**Unit 4 Photochemistry II** 

Photochemistry of carbonyl compounds,  $n-\pi$  and  $\pi-\pi^*$  transition (**self-study**), photochemistry of unsaturated system, olefins cis-trans isomerisation, dimerization – hydrogen abstraction and addition, Dienes –photochemistry of 1, 3 butadiene (2+2) additions leading to cage structures, photochemistry of benzene derivatives (**self-study**)- photosubstitution- Barton reactions, Photo Fries reaction, photochemistry of vision

Unit 5 Synthetic reagents and Name Reactions

Lithium diisopropylamine (LDA), Azobisisobutyronitrile (AIBN). Sodium cyanoborohydride (NaBH<sub>3</sub>CN), meta-Chloroperbenzoic acid (m-CPBA), Dimethyl aminiopyridine (DMAP), n-Bu<sub>3</sub>SnD/Bu<sub>3</sub>SnH, Triethylamine (TEA), Diazobicyclo[5.4.0]undec-7-ene (DBU), Diisopropylazodicarboxylate (DIAD), Diethylazodicarboxylate (DEAD), Trifluoroacetic acid (TFA), Tetramethyl piperiridin-1-oxyl (TEMPO), Phenyltrimethylammonium tribromide (PTAB). Diazomethane and Zn-Cu couple, Diethyl maleate (DEM), Copper diacetylacetonate (Cu(acac)<sub>2</sub>), TiCl<sub>3</sub>, NaIO<sub>4</sub>

Name reactions: Robinson annulations, Suzuki Coupling, Heck reaction, Negishi reaction, Baylis-Hillman reaction, Wittig reaction, Stark enamine synthesis, Shapiro reaction, Sandmeyer reaction, Hunsdiecker reaction, Arndt-Eistert Homologation, Bischler-Napeiralski reaction, Oppenaeur oxidation, Willgerodt reaction, Sommelet reaction, Darzen condensation, Elbs persulphate oxidation, Periodic acid oxidation, Vilsmeir-Haack reaction, Reimer Tiemann reaction, Pechmann and Houben

Hoesch reaction, Gattermann-Koch reaction, Diazonium coupling, Scholl reaction and Bradsher reaction

Total hours: 60

#### Reference Books

- 1. Jagadamba Singh, Photochemistry and Pericyclic reactions, New Age Int.Pvt.Ltd. (2003)
- 2. W.M.Horspool, Aspects of Organic Photochemistry, Academic Press (1976)
- 3. Depuy and Chapman, Photochemistry, (2000)
- 4. DePuy, C.H. and Chapman, O.L. Molecular Reactions and Photochemistry, Prentice-Hall, New Delhi (1987)

#### **Course Outcomes**

The students will acquire knowledge of

- 1. Concerted organic reactions and their mechanisms
- 2. Sigmatropic rearrangements & fluxinol tautomerism
- 3. Photochemistry of carbonyl compounds
- 4. Photochemistry of unsaturated systems
- 5. Synthetic uses of reagents in organic chemistry and name reactions

CO PO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	Н	М	М		L	М	М	Н	
CO <sub>2</sub>	Н	M	L				M	M	
CO <sub>3</sub>	Н	Н	L				Н	Н	
CO4	L	M	L				M	Н	
CO5	M	M	L		M	Н	М	Н	L

#### Inorganic Chemistry-II

Semester II 25MCHC08

Hours of Instruction/Week: 4
No. of Credits: 4

#### **Objectives**

- 1. To understand the significance symmetry in molecules, symmetry operations and point groups
- 2. To gain in-depth knowledge of inorganic spectroscopy
- 3. To analyze structure of molecules

#### **Unit 1 Symmetry Elements and Symmetry Operations**

Importance of symmetry- VSEPR theory to predict geometry of molecules, symmetry elements and symmetry operation- classification of groups- mathematical rules for the formation of a group- group multiplication table – properties of groups – order classes and similarity transformations- sub groups, isomorphic groups, Abelian group and non Abelian group, molecular point groups- classification, identification of molecular point groups- flow sheet for the identification of point groups by Yes-No method – Optical activity and dipole moment on the basis of point group symmetry (Self-study)

**Unit 2 Group Theory** 

Introduction to matrix- matrix representation of symmetry operation – identity, rotation, reflection, inversion and improper axis of rotation- characteristics of matrix representation- character representation of point group – matrix representation for  $C_{2V}$  and  $C_{3V}$  point groups- reducible and irreducible representation, properties of irreducible representation applied to  $C_{2V}$  and  $C_{3V}$  – Orthogonality theorem – significance of the Orthogonality theorem, consequences of the Orthogonality theorem- construction of character table for point groups, explanation for complete character table for  $C_{2V}$  and  $C_{3V}$  point group- Isomorphism and direct product representation (Self-study)

Unit 3 Inorganic spectroscopy -I

Spectroscopy: effect of coordination on the stretching frequency- sulphato, carbonato, sulphito, aqua, nitro, thiocyanato, cyano, thiourea, DMSO complexes; NMR spectroscopy- introduction, applications of <sup>1</sup>H, <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P-NMR spectroscopy in structural identification of inorganic complexes, fluxional molecules, quadrupolar nuclei- effect in NMR spectroscopy

Unit 4 Inorganic spectroscopy-II

ESR introduction - Zeeman equation, g-value, nuclear hyperfine splitting - interpretations of the spectrum, simple carbon centered free radicals- anisotropy- g-value and hyperfine splitting constant - McConnel's equation - Krammer's theorem - spin-orbit coupling - dipolar contribution - dipole-dipole interaction, ESR spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II), Cu(II) complexes, bis(salicylaldimine)copper(II) and [(NH<sub>3</sub>)<sub>5</sub>Co-O<sub>2</sub>-Co(NH<sub>3</sub>)<sub>5</sub>]<sup>5+</sup>

Mossbauer spectroscopy – Mossbauer effect, recoil energy, Mossbauer active nuclei, Doppler shift, isomer shift, quadrupole splitting and magnetic interactions, applications of Mössbauer spectra to Fe and Sn compounds, molecular magnetism - bioinorganic compounds

#### **Unit 5 Photo Electron Spectroscopy**

.

12h

12h

12h

Theory, types, origin of fine structures - shapes of vibrational fine structures - adiabatic and vertical transitions, PES of homonuclear diatomic molecules ( $N_2$ ,  $N_2$ ) and heteronuclear diatomic molecules ( $N_2$ ,  $N_3$ ) - evaluation of vibrational constants of the above molecules- Koopman's theorem- applications and limitations, applications of Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) in inorganic complexes

Total hours: 60

#### **Recommended Text:**

- 1. Ramakrishnan, V. and Gopinathan, M.S. Group Theory in Chemistry, 2<sup>nd</sup> Ed., Vishal Publications (2013)
- 2. Gurdeep Raj, Ajay Bhagi and Vinod Jain, Group Theory and Symmetry in Chemistry, 3<sup>rd</sup> Ed., Krishna Prakashan Media (P) Ltd., Meerut (2010)
- 3. Raman, K.V. Group Theory and Its Applications to Chemistry, 4<sup>th</sup> Ed., Tata McGraw-Hill Publishing Company Ltd. (1990)
- 4. Swarnalakshmi, S., Saroja, T. and Ezhilarasi, R. M. A Simple Approach to Group Theory in Chemistry, 1<sup>st</sup> Ed., University Press (2008)
- 5. J E Huheey, EA Keiter, RL Keiter and OK Medhi, Inorganic Chemistry Principles of structure and reactivity, 4th Edition, Pearson Education Inc., 2006
- 6. G L Meissler and D ATarr, Inorganic Chemistry, 3rd Edition, Pearson Education Inc., 2008
- 7. D. Bannerjea, Co-ordination Chemistry, TATA Mcgraw Hill, 1993.
- 8. F. A. Cotton, G. Wilkinson.; C. A. Murillo; M. Bochmann, Advanced Inorganic Chemistry, 6thed.; Wiley Inter-science: New York, 1988.

#### Reference Books

- 1. P Gütlich, E Bill, A X Trautwein, Mossbauer Spectroscopy and Transition Metal Chemistry: Fundamentals and Applications, 1<sup>st</sup> edition, Springer-Verlag Berlin Heidelberg, 2011.
- 2. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel, J. Alexander, John Wiley, 1994, 3rd edn.
- 3. K. F. Purcell, J. C. Kotz, Inorganic Chemistry; Saunders: Philadelphia, 1976.
- 4. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1977.

- 1. Ability to classify molecules into point groups
- 2. To specify the appropriate irreducible representations for theoretical applications
- 3. Identify the structure of coordination complexes using spectroscopic tools such as IR and NMR
- 4. Predict the structure of coordination complexes using spectroscopic tools such as ESR and Mossbauer
- 5. To gain knowledge about the basic principles of Photo Electron Spectroscopy

CO /	PO	PO	PO	PO	PO	PO	PS	PS	PS
PO	1	2	3	4	5	6	0 1	02	03
CO 1	M	M				M	M	M	
CO 2	M	M	M		L		M	M	
CO3	M	M	M	M	Н	M	M	M	M
CO 4	M	M	L	Н	Н	M	M	M	M
CO 5	M	M	-	Н	M	M	M	M	M

#### Physical Chemistry-II

Semester II 25MCHC09 Hours of Instruction/Week: 4
No. of Credits:4

#### **Objectives**

- 1. To impart knowledge on essential concepts of quantum chemistry
- 2. To understand the applications of Schrodinger wave equation
- 3. To determine the kinetics of chemical reactions
- 4. To learn the essentials of adsorption and kinetics of photochemical reactions
- 5. To comprehend on the essential methods of molecular weight determination

#### **Unit 1 Quantum Chemistry**

Success of quantum theory and failure of classical mechanics- formulation of quantum mechanics- the wave nature of sub-atomic particles-wave particle dualism- Heisenberg's uncertainty principle-concept of operators- sums and products of operators- commutator- linear and non-linear operators- Hermitian and Hamiltonian operators- deriving operators for energy and angular momentum from known operators- Eigen values and Eigen functions- postulates of quantum mechanics- physical interpretation of wave function- orthogonality and normalization theorem- Schrodinger wave equation- time dependent and time independent

Unit 2 Applications of Schrodinger Wave Equation and Approximate Methods

Applications of Schrodinger wave equation to – particle in a one dimensional box- particle in a three dimensional cubic and rectangular box-degeneracy, one dimensional harmonic oscillator- classical treatment of simple linear harmonic oscillator- Hermite polynomial and normalized solution and energy values, rigid rotator-rigid rotator as a model for a rotating diatomic molecule- solutions, hydrogen and hydrogen like atoms- approximate methods- need for approximation methods-perturbation theory (I order only)- application to H-like atoms- variation methods- application to helium atom- molecular orbital theory – Huckel theory of conjugated systems, bond order and charge density calculations, applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene-introduction to extended Huckel theory

#### Unit 3 Kinetics and mechanism of chemical reactions

Temperature dependence of reaction rates, Arrhenius equation (self-study), reactions approaching equilibrium, consecutive reactions- steady state approximation, opposing and parallel reaction, simple collision theory of reaction rates- steric factor, absolute reactions theory of bimolecular elementary gas phase reactions – transmission coefficient – treatment of molecular reactions – thermodynamic formulation of ARRT chain reactions, general characteristics study of kinetics of H<sub>2</sub>-Cl<sub>2</sub> reaction- H<sub>2</sub> – Br<sub>2</sub> reaction

#### **Unit 4 Surface reactions**

Adsorption – types of adsorption, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its application- kinetics of catalytic reactions, acid base catalysis, enzyme catalysis- kinetics of photochemical reactions- comparative study of thermal and photochemical mechanisms in hydrogen halogen reactions- rate constants, relaxation, top-flow, NMR, ESR and photolysis techniques- kinetics of ion-ion reactions in solution effect of dielectric constant and ionic strength on the rate, primary and secondary kinetic salt effect- micelles: surface

10h

14h

10h

active agents and their classification, micellization, hydrophobic interaction, critical miceller concentration (cmc), factors affecting cmc of surfactants, thermodynamics of micellization, phase separation and mass action models, reverse micelles, solubilization

#### Unit 5 Macromolecules

Polymers - molecular mass and its distribution, determination of molecular mass by osmometry, viscosity, light scattering and size exclusion chromatography methods, Glass transition temperature, the Flory-Huggins theory of polymer solutions, living radical polymerization, polymer nanocomposite- kinetics of polymerization – free radical, cationic, anionic polymerizations – polycondensation

**Total hours: 60** 

#### **Textbooks**

- 1. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7th Ed., Oxford University Press, (2002)
- 2. Prasad, R. K. Quantum chemistry, New Age International (2001)
- 3. McQuarrie, Donald A. Quantum chemistry, University Science Books (2008)
- 4. Gurtu, J. N. and Gurthu, A. Advanced Physical Chemistry, Pragathi Prakashan, Meerut(2006)

#### Reference books

- 1. Hori a Metiu, Physical Chemistry-Kinetics, Taylor & Francis, New York, (2006)
- 2. Honnay, N.S., Solid State Chemistry (2002)
- 3. Lewars, E. G., Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer (2016)
- 4. Szabo, Attila, and Neil S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Courier Corporation(2012)
- 5. Gurtu, J. N. and Khera, H. C., Physical Chemistry, Pragati Prakashan(2010)

#### **Course Outcomes**

After the completion of the course students will be able to

- 1. Explain the operators in quantum chemistry
- 2. Derive Schrodinger wave equation for one dimensional and three dimensional box
- 3. Describe order and kinetics of chemical reaction
- 4. Derive the adsorption isotherms and kinetics of photochemical reactions
- 5. Elucidate the methods for molecular weight determination

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	M	M	M			M	M	M	M
CO 2	M	M	Н	M	M	M	M	M	M
CO 3	M	M	M	M	M	M	M	M	M
CO 4	M	M				M	M	M	M
CO 5	M	M	M		Н	Н	Н	M	H

#### Spectroscopy-I

Semester II 25MCHC10 Hours of Instruction/Week: 3

No. of Credits: 3

#### **Objectives**

- 1. To gain knowledge on qualitative understanding of IR and Raman spectroscopy and applications
- 2. To gain knowledge of instrumentation and theory of mass spectroscopy
- 3. To learn the applications of flame emission and atomic absorption spectroscopy

#### **Unit 1 IR Spectroscopy**

Basic principles of IR spectroscopy – sample handling, characteristic vibrational frequencies of alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, calculation of vibrational frequencies of bond, detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds), finger print region, effect of hydrogen bonding and solvent effect on vibrational frequencies, distinction between inter and intramolecular hydrogen bonding, fundamental vibration, overtones, combination bands and Fermi resonance, study of progress of reactions, applications of infrared spectroscopy- identification of functional groups in organic molecules, <u>FT-IR spectrometer</u> – instrumentation (self-study)

#### **Unit 2 Raman Spectroscopy**

Principles of Raman spectroscopy- classical theory, polarizability ellipsoids, quantum theory, rotational Raman spectra of linear and symmetric top molecules, vibrational Raman spectra, rotational-vibrational Raman spectra, selection rules, mutual exclusion principle, Stokes and anti Stokes lines, O, P, Q, R and S branches, characteristics of Raman lines, applications Raman spectroscopy, comparison of IR and Raman techniques (Self-study)

#### Unit 3 Mass Spectroscopy -I

Introduction – basic theory, instrumentation-ion production – electron ionization method (EI), chemical ionization method (CI), Fast Atom Bombardment technique (FAB), electron spray ionization, ion abundance, MALDI-TOF spectrometry, factors affecting fragmentation, base peak, molecular ion peak, meta stable peak, parent ion, daughter ion, doubly charged ions, nitrogen rule, ring rule, isotopic peak, isotopic clusters, inductively coupled plasma mass spectroscopy (ICP-MS)-principle and instrumentation

#### Unit 4 Mass Spectroscopy -II

General fragmentation mode in organic molecules- types of cleavage- homolytic, heterolytic, allylic and benzylic,  $\alpha$  and  $\beta$ , ortho effect, McLafferty rearrangement, Retro Diels-Alder reaction, mass spectral fragmentation of organic compounds- aliphatic hydrocarbons- alkanes, cyclo alkanes, alkanes, aromatic hydrocarbon-benzene, toluene, aryl and alkyl halides, alcohols, phenols, ethers, aldehydes, ketones, carboxylic acids, esters anhydrides, amines and nitro compounds

## Unit 5 Atomic Absorption Spectroscopy (AAS), Flame Emission Spectroscopy (FES) and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES)

Atomic absorption spectroscopy – basic principles- instrumentation – flame characteristics – flames and burners- types of interferences- background absorption, spectral line interference, vaporization

10h

7h

10h

interference, ionization interference, applications of atomic absorption spectroscopy, flame emission spectroscopy — basic principles- instrumentation, applications of flame emission spectroscopy difference between AAS and FES (self-study), inductively coupled plasma optical emission spectroscopy (ICP-OES)- basic principle and instrumentation

Total hours: 45

#### Reference Books

- 1. Willard, Merritt, Dean, Settle, Instrumental Methods of Analysis, CBS Publishers & Distributors, New Delhi
- 2. Colin, N. Banwell and Elaine M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill Publishing Company, New Delhi
- 3. Yadav, L.D.S. Organic Spectroscopy, Anamaya Publishers, New Delhi
- 4. Barrow, G.M. Introduction to Molecular Spectroscopy, Mc Graw Hill (2001)
- 5. Kalsi, P.S. Spectroscopy of Organic Compounds, New Age Publishers (2002)
- 6. Sharma, B.K. Spectroscopy, Goel Publishing House, Merut (2000)
- 7. Jagmohan, Organic Spectroscopy: Principles and Applications, Narosa Publishing House, New Delhi (2001)

- 1. Apply the knowledge of interpreting IR data to identify functional group
- 2. Knowledge on the principles of Raman spectroscopy
- 3. Knowledge on instrumentation of Mass spectroscopy
- 4. Knowledge on the mass fragmentation pattern of organic compounds
- 5. Knowledge on identification of elements using AAS, FES and ICP-OES

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	M	M	M	Н	Н	Н	M	M	M
CO 2	M	M		Н	M	Н	M	M	Н
CO 3	M	M	L	H	Н	Н	M	M	Н
CO 4	M	M	L	Н	Н	Н	M	M	Н
CO 5	M	M	Н	Н	M	Н	M	M	Н

#### Physical Chemistry Practical-I

#### SEMESTER II **25MCHC11**

Hours of Instruction/Week: 4

No. of Credits: 2

#### **Objectives**

- 1. To gain practical skill in colorimetric experiments
- 2. To gain knowledge on adsorption isotherm experiments
- 3. To acquaint with potentiometric titrations and practical applications of EMF

#### Unit 1 Colorimetry and Surface Chemistry

1. Estimation of Iron & Nickel

2. Verification of Freundlich and Langmuir adsorption Isotherm of acetic acid on activated charcoal

30h

3. To study the adsorption of methyl red / methylene blue on charcoal

#### **Unit II Potentiometry**

1. Estimation of HCl using NaOH

2. Estimation of CH<sub>3</sub>COOH using NaOH

3. Estimation of acid mixture (HCl + CH<sub>3</sub>COOH) using NaOH

30h

4. Estimation of FeSO<sub>4</sub> using KMnO<sub>4</sub>

5. Estimation of FeSO<sub>4</sub> using K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>

6. Estimation of KCl using AgNO<sub>3</sub>

7. Estimation of Fe<sup>+2</sup> ions by potentiometric titration

8. Determination of the Zinc Ferrocyanide complex by potentiometric titrations

9. Determination of standard potentials (Cu, Zn, Ag)

10. Titration of 0.1 M solutions of oxalic acid, malonic acid and tartaric acid against 0.1 M NaOH solution (Class

11. Determination of solubility of a sparingly soluble salt (BaSO<sub>4</sub>)

12. Determination of dissociation constant of a weak acid (acetic acid)

**Total hours: 60** 

#### Reference Books

1. Peter Mathews, G. Experimental Physical Chemistry, Oxford Science Publications (2000)

2. Daniel, G. et al., Experimental Physical Chemistry, International Students Edition, McGraw Hill Hogakusha Ltd. (2001)

3. Khosla, D.D. and Carg, V.C. Senior Practical Chemistry, R.Chand & Co., New Delhi (2001)

4. Jones, A.M. and Richard, F.E. Practical Physical Chemistry

#### **Course Outcomes**

- 1. Gaining practical skill in colorimetric experiments
- 2. Know to analyze and interpret experimental data
- 3. Ability to carry out potentiometric titrations

4. Understanding the practical applications of EMF

5. Knowledge on the determination of standard electrode potential of (Cu, Ag &Zn) electrodes

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	M	M	Н	M	M	L	M	M	Н
CO 2	M	M	Н	M	M	M	M	M	H
CO 3	L	M	M	H	H	L	M	M	H
CO 4	M	M	Н	M	M	L	M	M	H
CO 5	M	M	M	M	Н	M	M	M	Н

#### Inorganic Chemistry Practical-I

Semester II 25MCHC12

Hours of Instruction/Week: 4

No. of Credits: 2

#### **Objectives**

- 1. To formulate suitable method for inorganic complex preparation
- 2. To estimate select inorganic metal ions by complexometry method
- 3. To determine the amount of ions present in a binary mixture accurately

### Unit 1 Preparation of Selected Inorganic Complexes

- 1. Tetrammine cupric sulphate
- 2. Potassium chloro chromate
- 3. Potassium tris oxalate aluminate
- 4. Hexammine Ni(II)chloride
- 5. Potassium diaquo bis oxalato cuprate II
- 6. Tris thiourea copper (I) sulphate dehydrate
- 7. Trinitro triammine cobalt III
- 8. Dichloro bis (ethylene diamine) cobalt III chloride

#### **Unit 2 Complexometric Titrations**

- 1. Estimation of zinc, nickel and magnesium
- 2. Estimation of mixture of metal ions-pH control, masking and demasking agents
- 3. Determination of manganese in the presence of iron

20h

15h

4. Determination of nickel in the presence of iron

## Unit 3 Quantitative (Two components) Analysis: Gravimetry and Titrimetry (Any three)

Separation and estimation of mixtures by volumetric (v) and gravimetric (G) methods - Any three

- 1. Estimation of Copper (v) and Nickel (G)
- 2. Estimation of Copper (v) and Calcium (G)

25h

- 3. Estimation of Calcium (v) and Barium (G)
- 4. Estimation of Copper (v) and Zinc (G)
- 5. Estimation of Calcium (v) and Copper (G)

Total hours: 60

#### Reference Books

- 1. Inorganic semi micro qualitative analysis V.V. Ramanujam, The National Publishing Co., Ltd., Madras, 1976
- 2. Inorganic Qualitative analysis by Vogel
- 3. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis; 6th ed., ELBS, 1989
- 4. Standard methods of analysis by Scott
- 5: King Inorganic synthesis
- 6. H.M. Bard, Modern Polarographic Methods in analytical Chemistry
- 7. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954
- 8. Advanced Practical Chemistry by Jagadamba sing, R.K. P Singh, Jaya Singh, L.D.S Yadav, I.R Siddiqui and Jaya Srivastava
- 9. Advanced Inorganic Analysis by Agarwal and Keemtila
- 10. J. D. Woollins, Inorganic Experiments, VCH: Weinheim, 1995
- 11. G. Pass, and H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965

- 1. Formulate suitable methods for the preparation of desired inorganic complexes
- 2. Develop practical skills in complexometric titrations
- 3. Gain knowledge on buffer solutions
- 4. To determine the amount of ions present in a binary mixture accurately
- 5. To understand the estimation of mixtures by volumetric, gravimetric methods

CO/PO	PO 1	PO 2.	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	M	M	Н	M	H	M	Н	H	Н
CO 2	M	M	H	M	H	M	H	M	H
CO 3	M	M	H	L	H	H	H	M	H
CO 4	M	M	M	L	M	Н	H	H	H
CO 5	M	M	L	H	H	H	H	M	H

10h

9h

9h

7h

#### Organic Chemistry-III

Semester III 25MCHC13

Hours of Instruction/week: 3
No. of Credits: 3

#### **Objectives**

- 1. To get acquainted with nucleophilic and electrophilic substitution reactions
- 2. To familiarize the concepts of addition and elimination reactions
- 3. To introduce key reactions for applications in organic synthesis and organic transformations

Unit 1 Aliphatic and Aromatic Nucleophilic Substitution Reaction

Aliphatic Nucleophilic Substitution - Mechanism of  $S_N1$  and  $S_N2$ ,  $S_Ni$  reactions, evidences–Factors influencing  $S_N1$  and  $S_N2$  reactions, reactivity and orientation effects, effect of substrate, structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ambident nucleophiles regionselectivity, neighboring group participation by  $\sigma$  and  $\pi$  bonds- Aromatic Nucleophilic Substitution - mechanism of uni molecular and bimolecular aromatic nucleophilic substitution ( $S_NAr$ ), reactivity – effect of substrate structure, attacking nucleophile and leaving group, benzyne mechanism

Unit 2 Aliphatic and Aromatic Electrophilic Substitution Reaction

Aliphatic electrophilic substitution - bimolecular mechanisms- S<sub>E</sub>2, S<sub>E</sub>1 and S<sub>E</sub>i mechanism, substitution accompanied by double bond shifts, effect of substrates leaving group and the solvent polarity on the reactivity, aromatic electrophilic substitution - mechanism of reactions, orientation and reactivity- orientation of substitution in monosubstituted and disubstituted benzene, orientation in other ring systems, ortho-para ratio, quantitative treatment of aromatic substitution reaction- Hammett and Taft equation isomer proportions

#### **Unit 3 Addition Reactions**

Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms, regio and chemo selectivity orientation and stereochemistry, addition to cyclopropane- hydroboration Michael reaction, addition of oxygen (O<sub>2</sub>) across double bonds- selenium dioxides, mercuric acetate, lead tetraacetate, permanganate, manganese dioxide, osmium tetroxide, ozonolysis, Sharpless asymmetric epoxidation, mechanisms of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, amides and nitriles- Stobbe reaction, Wittig reaction (self-study)

#### **Unit 4 Elimination reaction**

Elimination reactions involving  $E_1$ ,  $E_2$ ,  $E_{2C}$  and  $E_{2CB}$  mechanisms and orientation-regioselectivity-Saytzeff and Hoffman rules (self-study), Factors affecting  $E_1$ ,  $E_2$  and  $E_{2C}$  mechanisms-substrate, base, solvent, effect on factors affecting elimination and substitution, stereochemistry of  $E_2$  elimination-syn and anti eliminations, elimination reaction in protecting group chemistry, pyrolytic eliminations, Chugaev reaction cleavage of quaternary ammonium hydroxides, conversion of vicinal dihalides to olefins

**Unit 5 Strategies in Organic Synthesis** 

Strategies in Organic Synthesis- introduction of synthons and synthetic equivalents, disconnection approach, functional group inter conversion of halides, nitriles, azides, amines, and esters -the importance of order of events in organic synthesis, nucleophilic and electrophilic synthons umpolung reactions typical examples one group C-X and two group C-X disconnections - two group disconnections - 1,2-difunctionalised compounds - 1,3-difunctionalized compound and - unsaturated carbonyl compounds, oxidations -chromium trioxide-pyridine, Swern oxidation and Corey-Kim oxidation, Pyridinium chlorochromate (PCC), Pyridinium dichromate (PDC), reductions- Wolff-Kishner, Clemmenson, Rosenmund; reduction with Trialkyl and triphenyltin hydrides, McFadyen-Steven's reduction

**Total hours: 45** 

#### Reference Books

- 1. Skyes, P. Guide Book to Mechanism in Organic Chemistry, Pearson Education (2001)
- 2. Jerry March, Advanced Organic Chemistry-Reaction Mechanisms and Structure, 4th Ed., John Wiley & Sons (1999)
- 3. Bansal, R. K. Organic Reaction Mechanism, 11th Ed., Tata McGraw-Hill, Noida (2006)
- 4. Skyes, P. Guide Book to Mechanism in Organic Chemistry, (2001)
- 5. Pine, S.H., Henrickson, J.B., Gram, D.J. and Hammon, G.S. Organic Chemistry, 3rd Ed., McGraw-Hill Kogakusha Ltd. (2000)
- 6. Gupta, R.R., Kumar, M. and Gupta, V. Heterocyclic Chemistry, Vol I-III Springer Verlag
- 7. Joule, J.A., Mills K. and Smith, G.F. Heterocyclic Chemistry, Chapman and Hall

#### **Course Outcomes**

The students will acquire knowledge of

- 1. Assess the mechanism and reactivity of nucleophilic substitution reactions
- 2. Evaluate the mechanism and reactivity of electrophilic substitution reactions
- 3. Able to predict the stereochemistry and mechanism of addition reactions
- 4. Able to predict the stereochemistry and mechanism of elimination reactions
- 5. Expertise in identifying the transformations, the reagents and planning organic synthesis

CO PO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	Н	M	M		L	M	M	H	
CO <sub>2</sub>	H	M	L				M	M	
CO3	H	Н	L				H	H	
CO4	L	M	L				M	H	
CO5	M	M	L		M	Н	M	Н	L

#### Inorganic Chemistry-III

Semester III 25MCHC14

Hours of Instruction/week: 3
No. of Credits: 3

#### **Objectives:**

- 1. To recognize the fundamental concepts and structural aspects of organometallic compounds.
- 2. To learn the magnetic properties and Photochemistry of complexes
- 3. To learn the structure and bonding in inorganic chains, rings, and cages
- 4. To understand the key role of metal ions in the living systems
- 5. To understand the concepts of nuclear chemistry

#### **Unit 1 Organometallic Compounds**

Ionic compounds, σ-bonded and non -classically bonded organo metallic compounds, nature of carbon- metal bond, EAN rule 18 electron rule- exceptions to the 18 electron rule, ligand hapticity-monohapto, dihapto, trihapto, tetrahapto, pentahapto, hexahapto, heptahapto, octahapto ligands, reactions in organometallic chemistry- oxidative addition, reductive elimination, insertion, elimination and migration

Organometallic compounds of lithium and boron-preparation, properties, structure and uses, organometallic compounds of aluminium- organo-aluminium compounds- structure and bonding, metal carbonyl complexes – synthesis, structure, nature of M-CO bonding, metal carbonyl anions - metal carbonyl halides, binding mode of CO and IR spectra of metal carbonyls, metal nitrosyls - dinitrogen complexes – dioxygen complexes, olefin complexes- Zeise salt- synthesis and structure of cyclopentadienyl complexes- ferrocene- preparation, properties, structure and uses, applications of organometallics in organic synthesis

#### **Unit 2 Magnetochemistry of Transition Metal Complexes**

Magnetic Properties – dia, para, ferro and antiferro magnetism, Curie point applicable to ferro and antiferromagnetism, Neel point applicable to anti ferro magnetism, Quenching of orbital angular momentum, magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent para-magnetism - spin cross over phenomena

Self-study – Colour and complex formation of inner transition elements, colour absorption spectra of Lanthanides and Actinides

#### Unit 3 Inorganic chains, rings, and clusters

**Inorganic Chains-** Isopoly and hetero poly acids of molybdenum and chromium —preparation and structure only, silicones — preparation and structure only

**Inorganic** Rings- phosphazenes – hexachlorocyclo tri phosphazine, polyphosphonitrilic chloride - preparation and structure only

Metal clusters - Dinuclear clusters - trinuclear clusters - tetranuclear clusters - hexanuclear clusters - structural prediction of organometallic clusters

#### **Unit 4 Bioinorganic Chemistry**

Metals and Non-metals in biological systems - Essential and trace elements - Role of different metal ions in biological systems, Storage and transport mechanism - Sodium-Potassium pump - Ferritin - Hemosiderin - Transferrin - blue copper proteins - Catecholase, Photosynthesis - Chlorophyll and Photosystem (PS-I and PS-II) - structure- function relationship, Phorphyrin system - structure and functions of hemoglobin and myoglobin, hemocyanin - hemerythrin- dioxygen binding, transport and

10h

10h

9h

utilization - synthetic oxygen carriers - vitamin B<sub>12</sub>, non-hemeiron- sulphur proteins- rubredoxin & ferridoxins - cytochrome a, b, c - cytochrome P450,

Binding of metal ions and complexes to biomolecules, types of binding - nucleic acid structures - fundamental interactions with nucleic acids - binding interactions of metal complexes with DNA

**Unit 5 Nuclear Chemistry** 

Nucleus: Bathe's notation – types of nuclear reactions, decay of radionuclei- rate of decay - determination of half-life period - secular equilibrium and decay series, relation between t<sub>1/2</sub> and decay constant, average life, carbon dating, rock dating –principle, determination of age of earth and minerals by various dating techniques- modes of decay: alpha, beta, gamma and orbital electron capture - nuclear isomerism - internal conversions - Q value - nuclear cross section - threshold energy and excitation functions, particle acceleration and counting techniques- linear accelerator - cyclotron and synchrotron - betatron - G. M. counter - proportional and scintillation counters.

Self-Study - Radioisotopes in analysis - agriculture - industry and medicine, radioisotopes in predicting mechanism of chemical reactions (Esterification, Friedal Crafts reaction) - uses of radioisotopes in analytical chemistry - isotopic dilution analysis

Total hours: 45

#### **Recommended Text:**

- 1. F. A. Cotton and G. W. Wilkinson, Advanced Inorganic Chemistry, 5th edn, John Wiley & Sons, 1988.
- 2. K. F. Purcell and J. C. Kotz, Inorganic Chemistry; Saunders: Philadelphia, 1976.
- 3. B. D Gupta and A.J Elias, Basic Organometallic Chemistry, 2nd edn., Universities Press, 2013.
- 4. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 4th edn., Pearson, 2012.
- 5. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 3rd ed. New York, NY: John Wiley, 2000.
- 6. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry, University Science Books, 1994.
- 7. J E Huheey, EA Keiter, RL Keiter and OK Medhi, Inorganic Chemistry Principles of structure and reactivity, 4th Edition, Pearson Education Inc., 2006
- 8. Dr Asim K Dass, Bioinorganic Chemistry 2007, Books and Allied (P) Limited.
- 9. Bioinorganic chemistry: Inorganic Elements in the chemistry of life, 2<sup>nd</sup> edition, Wolfgang Kaim, Brigitte schwederski, Axel klein.
- 10. Arnikar, H.J. Essential of Nuclear Chemistry, 4th Ed., New Age International (P) Ltd, New Delhi (1995)
- 11. Freindlander, G., Kennedy, J.W., Macias, E.S. and Miller, J.M. Nuclear and Radiochemistry, 3<sup>rd</sup> Ed., John Wiley and Sons, New York (1981)
- 12. Concepts and Models of Inorganic Chemistry, B. Douglas, D. Mc Daniel, J. Alexander, John Wiley, 1994, 3rd edn.

#### **Reference Books:**

- 1. Gurdeep Raj. (2014). Advanced Inorganic Chemistry. 12th Edition. Geol Publishing House.
- 2. R.D. Madan. (2011). Advanced Inorganic Chemistry.3<sup>rd</sup> Edition. S. Chand & company, New Delhi.
- 3. R. Gopalan. V. Ramalingam, (2001) Concise Coordination Chemistry, 3<sup>rd</sup>edition, Vikas Publishing House Pvt. Ltd.
- 4. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry; University Science Books.

- 1. Knowledge on Structure and bonding in Organo Metallic Compounds
- 2. Familiarization of magnetic properties and photochemistry of complexes
- 3. Understanding the chemistry of cage, chain complexes
- 4. Students will be able to explain the biological redox systems
- 5. To get clear idea about the basics of nuclear chemistry and its application in various fields

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PS O 1	PSO 2	PSO 3
CO 1	M	L			Н	M	M		
CO 2	M	M	L		H	M	M	M	
CO 3	M	M	L		Н		M	M	M
CO 4	M	M	M	M	Н	M	M	M	M
CO 5	M	M	M	M	Н	M	Н	M	M

#### Physical Chemistry-III

Semester III 25MCHC15

Hours of Instruction/Week: 3 No. of Credits: 3

#### **Objectives**

- 1. To acquire knowledge on various concepts of activity coefficients
- 2. To obtain familiarity on electrostatic stabilization methods
- 3. To learn various electrode kinetic reactions
- 4. To get exposure on different electrochemical energy systems
- 5. To get acquainted with electrochemical methods

#### **Unit 1 Ionics**

Activities-activity coefficients and standard states, mean activity coefficients – Debye-Huckel theory and its verification-conductance of strong and weak electrolytes- Debye-Huckel Onsager treatment-evidence for ionic atmosphere ion association, factors influencing ion-association, effect of ion association on conductivity and activity coefficient of electrolytes in solution

#### Unit 2 Thermodynamics of Electric Double Layer

Thermodynamics of the double layer-electrocapillary phenomena-models for double layers - Helmholtz, Gouy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models-semiconductor interfaces- structure of double layer at the semiconductor-solution interface, effect of light at semiconductor-solution interface-dye sensitized solar cells-zeta potential and potential at zero charge -double layer effects on electrode reaction rates-introduction and principles, double-layer effects with and without specific adsorption of electrolyte, diffuse double-layer effects on mass transport

#### **Unit 3 Electrode Kinetics**

Derivation of the fundamental equation of electrode kinetics—Butler Volmer equation, Tafel equation, Over voltage – theory and applications of over voltage-hydrogen and oxygen overvoltage -kinetic derivation of Nernst equation, exchange current density and polarizability of interfaces-types of over potentials-origin and minimization mechanism of electro organic reactions, hydrogen evolution and oxygen reduction reactions-Transition state theory and Gibbs free energy of activation, bulk electrolysis-Quadratic activation –driving force relation – Marcus theory-outer and inner sphere reactions-Underpotential deposition of metals and applications in catalysis-Corrosion – Introduction, factors influencing corrosion, dry and wet corrosion-Electrochemical theory of corrosion – corrosion due to dissimilar metal cells and concentration cells – corrosion prevention- cathodic protection use of inhibitors – anodic and cathodic inhibitors

#### **Unit 4 Electrochemical Energy systems**

Conversion and storage of electrochemical energy—Fuel cells - H<sub>2</sub>-O<sub>2</sub>, hydrocarbon-Solid-Oxide fuel cells (SOFC) and solid polymer electrolyte fuel cells-Metal-air batteries, Na-ion batteries, Al-ion batteries-Mechanism of charge storage intercalation/deintercalation-conversion and alloying-capacitors- mechanism of energy storage, charging at constant current and constant voltage - Electrocatalysis- Influence of various parameters on water splitting, Hydrogen evolution reaction (HER) and Oxygen evolution reaction (OER)

10h

8h

9h

#### Reference Books

- 1. Dudley, H., Williams and Ian Fleming, Spectroscopic Methods in Organic Chemistry, 6<sup>th</sup> Ed., Tata McGraw Hill (2011)
- 2. Parish, R.V. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, 1<sup>st</sup> Ed., Ellis Horwood Series in Inorganic Chemistry (2001)
- 3. Kalsi, P.S. Spectroscopy of Organic Compounds, New Age Publishers (2007)
- 4. Sharma, B.K. Spectroscopy, Goel Publishing House, Krishna Prakashan Media P. Ltd., Meerut (2015)
- 5. Jag Mohan, Organic Spectroscopy- Principles and Applications, 1<sup>st</sup> Ed., Narosa Publishing House, New Delhi (2001)
- 6. Russell, S. Drago, Physical Methods in Chemistry, 1st Ed., Saunders Golden Sunburst Series (1977)
- 7. Gordon M. Barrow, Introduction to Molecular Spectroscopy, Mc Graw Hill (2001)
- 8. Abraham, R.J., Fischer, J. and Loftus, P. Introduction to NMR Spectroscopy, Wiley (2000)
- 9. Silverstein, R.M. and Bassler, G.C. Systematic Identification of Organic Compounds, John Wiley (2000)
- 10. Akitt, J.W. NMR and Chemistry: An Introduction to Modern NMR Spectroscopy, 4th Ed., CRC Press (2000)
- 11. Donald L. Pavia, Introduction to Spectroscopy, 5th Ed., Cengage Learning India Private Limited (2015)

- 1. Knowledge on theoretical principles of UV and ability to interpret UV
- 2. Knowledge on theoretical principles H<sup>1</sup> NMR and ability to interpret H<sup>1</sup> NMR
- 3. Knowledge on theoretical principles <sup>13</sup>C NMR and ability to interpret <sup>13</sup>C NMR
- 4. Knowledge on the principles ESR spectroscopy and its applications
- 5. Understanding the principles and applications of X-ray and Neutron diffraction techniques

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	Н	Н	Н	M	M	Н	Н	M	M
CO 2	Н	Н	Н	M	M	Н	Н	M	M
CO 3	Н	Н	Н	M	M	Н	Н	M	M
CO 4	Н	Н	Н	M	M	Н	H	M	Н
CO 5	Н	Н	Н	M	M	M	Н	M	M

#### **Computational Chemistry**

Semester III **25MCHC17** 

Hours of Instruction/Week: 3 No. of Credits: 3

#### **Objectives**

- 1. To understand the theory of computational chemistry
- 2. To gain knowledge on application of molecular properties in the study of reaction mechanism
- 3. Familiarize with software used in computational analysis

Unit 1 Introduction to Computational Chemistry

Introduction to computational chemistry (molecular modeling) - principle and application of methods (tools) of computational chemistry - a brief description of molecular mechanics, ab initio method, semi empirical methods, density functional theory - Hohenberg-Kohn theorem, Kohn-shan equilibrium and molecular dynamics

**Unit 2 Energy Optimization** 

Concept of potential energy surfaces, Born-oppenhiemer approximation, stationary points, normal mode of vibrations, symmetry, geometry optimization

**Unit 3 Molecular Mechanics** 

Introduction to molecular mechanics-force field - developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and non-bonded interaction term, parameterizing a force field and calculation using force field

Unit 4 Semi Empirical methods

Introduction to semi empirical (SE) methods-Hartre Fock SCF, Roothan concept basis functions Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equation- bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system

Unit 5 Software for Computational Chemistry

Software for structure of molecules - ISIS, Chem draw, Chem Sketch, Molecular modeling software in chemistry- Hyperchem, GAMESS, MOLCHEM, MOPAC- energy minimization, viewing 3D molecules application of molecular properties - partial charge, electrostatic potentials, molecular orbital, geometry of molecule, chemical bonds and stereochemistry in the study of reaction mechanisms, acidity and basicity of molecules

Total hours: 45

#### Reference Books

- 1. Errol Lewars, Computational Chemistry Introduction to Theory and Applications of Molecular Mechanics, 2<sup>nd</sup> Ed., Kluwer publications (2011)
- 2. Christopher, J. Cramer, Essentials of Computational Chemistry Theories and Models, 2<sup>nd</sup> Ed., Wiley publishers (2004)
- 3. Frank Jensen, Introduction to Computational Chemistry, 2<sup>nd</sup> Ed., Wiley publishers (2007)

#### **Course Outcomes**

- 1. Knowledge on methods used in computational chemistry
- 2. Ability to Interpret potential energy surface diagrams
- 3. Able to apply molecular mechanics to molecular properties

9h

9h

9h

9h

- 4. Ability to apply semi empirical methods for computing molecular properties
- 5. Familiarization with molecular modeling software

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	Н	M	L	Н	Н	Н	L	L	Н
CO 2	Н	M	L	H	H	Н	L	L	
CO 3	Н	M	L	H	Н	Н	L	L	
CO 4	H	M	L	H	L	H	L	L	Н
CO 5	Н	M	L	Н	Н	Н	L	L	Н

#### Inorganic Chemistry Practical-II

Semester III 25MCHC18

Hours of Instruction/Week: 6

No. of Credits: 3

#### **Objectives**

- 1. To carry out qualitative inorganic semi micro analysis of mixture of salts
- 2. To get trained in qualitative analysis of less common metal ions
- 3. To gain knowledge on quantitative estimation of alloys

**Unit 1 Qualitative Analysis** 

Analysis of mixtures containing two common and two less common cations. Ions of the common metals: Pb, Cu, Mn, Cr, Al, Ni, Co, Zn, Ba, Sr, Ca, Mg
Ions of less common metals: W, Se, Te, Mo, Bi, Sb, Ce, Th, Zr, Ti, V, Li

65h

Unit 2 Quantitative Analysis

1. Analysis of alloys brass - complexometry (class work only)

25h

2. Available chlorine in bleaching powder (class work only)

**Total hours: 90** 

#### **Course Outcomes**

- 1. Ability to identify common elements in a given complex salt mixture by semi-micro inorganic qualitative methods
- 2. Ability to identify less common elements in a given complex qualitatively
- 3. Ability to estimate metals and alloys by quantitative methods
- 4. Quantitatively estimate available chlorine in compounds
- 5. Apply color theory for the quantitative analysis of elements

#### **Reference Books**

- 1. Mendham, J. and Sivasankar, B. Vogel's Quantitative Chemical Analysis, 6th Ed., Pearson (2009)
- 2. Svehala, G. and Sivasankar, B. Vogel's Qualitative Inorganic Analysis, Pearson, India (2012)

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	Н	M	Н	Н	M	M	Н	M	M
CO 2	Н	M	Н	Н	M	M	H	M	M
CO 3	Н	М	Н	Н	M	M	H	M	M
CO 4	Н	M	Н	Н	M	M	Н	M	M
CO 5 .	Н	M	Н	Н	M	M	Н	M	M

#### Physical Chemistry Practical - II

## Semester III 25MCHC19

#### Hours of Instruction/Week: 4

No. of Credits: 2

#### **Objectives**

- 1. To acquire skills in experiments on physical chemistry
- 2. To get acquainted with method of determination of conductivity
- 3. To measure rates of reactions

#### Unit 1

- 1. Chemical Kinetics I-First order reaction
  - i) Rate constant of the hydrolysis of ethyl acetate catalysed by N/2 HCl
  - ii) Comparison of strength of two acids at room temperatures
  - iii) Determination of temperature coefficient and Arrhenius parameter
- 2. Chemical Kinetics II- Second order reaction
  - i) Saponification of ethyl acetate by NaOH
  - ii) Determination of rate constant for the kinetics of the reaction between potassium persulphate and potassium iodide
- 3. Phase rule studies

30h

- i) Two component systems Simple Eutectic formation (Naphthalene, Biphenyl, m-dinitro benzene, p- nitro toluene, Benzoic acid, Cinnamic acid)
- ii) Ternary system- Acetic Acid, Chloroform, Water- Class Work only
- 4. Determination of the Molecular Weight of Polystyrene from Viscosity Measurements

#### Unit 2

#### Conductometric titrations:

- 1. Estimation of HCl using NaOH
- 2. Estimation of CH<sub>3</sub>COOH using NaOH
- 3. Estimation of Na<sub>2</sub>CO<sub>3</sub> using HCl
- 4. Estimation of KCl using AgNO<sub>3</sub>
- 5. Estimation of acid mixture (HCl+ CH<sub>3</sub>COOH) using NaOH

- 6. Estimation of barium chloride using magnesium sulphate
- 7. Verification of Debye Huckel Onsager equation
- 8. Verification of Ostwalds dilution law
- 9. Solubility of a sparingly soluble salt
- 10. Saponification of Ethyl acetate by NaOH
- 11. Critical Micelle concentration of sodium dodecyl sulphate

Total hours: 60

#### **Reference Books**

- 1. Peter Mathews, G. Experimental Physical Chemistry, Oxford Science Publications (2000)
- 2. Daniel, G. et.al., Experimental Physical Chemistry, International Students Edition, McGraw Hill Hogakusha Ltd. (2001)
- 3. Khosla, D.D. and Carg, V.C. Senior Practical Chemistry, R. Chand & Co., New Delhi (2001)
- 4. Jones, A.M. and Richard, F.E. Practical Physical Chemistry
- 5. Gurtu, J. N., Gurtu, A. (2008). Advanced Physical Chemistry Experiments. India: Pragati Prakashan.

- 1. Knowledge on the determination of rate law from experimental data
- 2. Understanding the practical applications of reaction kinetics
- 3. Gaining practical skill in application of phase rule to two component systems
- 4. Ability to carry out conductometric titrations
- 5. Apply the principle of conductometric titrations

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	Н	M	Н	M	M	M	H	M	M
CO 2	H	M	Н	M	M	M	H	M	M
CO 3	Н	M	Н	M	M	M	H	M	M
CO 4	H	M	H	M	M	M	H	M	M
CO 5	H	M	Н	M	M	M	H	M	M

5h

6h

7h

6h

6h

#### **Environmental Chemistry (Self Study)**

Semester III 25MCHC20

Hours of Instruction/Week: 2
No. of Credits: 2

#### **Objectives**

- 1. To become aware of various kinds of pollution and the methods of eradicating the pollution
- 2. To know about the water quality standards
- 3. To familiarize with waste management methods
- 4. To learnt about the Renewable energy sources
- 5. To sensitization on sustainable ecosystem

#### Unit 1 Chemistry and the Environment/Environmental Pollution

Components of environment – factors affecting environment - environmental pollution – pollutants, classification of pollutants - toxic effects of pollutants - types of pollution: air, water, soil, thermal, radioactive and noise pollutions –prevention and control of pollutions - environmental issue (SDG-13: Climate action)

Unit 2 Water Quality Analysis and Control

Water – sources, molecular structure and physical properties – hydrogen Bonding – water as a solvent – characteristics of water – total dissolved solids (TDS), dissolved oxygen (DO), biological oxygen demand (BOD), chemical oxygen demand (COD), total organic carbon (TOC), fluoride and chloride, analysis of carbon monoxide (CO) by gas chromatography, nitrogen monoxide (NO) by chemiluminescence and sulphur dioxide (SO<sub>2</sub>) by spectrophotometer - comparative account on physical and chemical properties of water and deuterated water (SDG-6: Clean water and Sanitization)

Unit 3 Industrial Pollution and its Management

Pollution due to cement, drug, thermal power plants, nuclear power plants, metallurgy, polymers, plastics, leather and textile industry - waste water treatment - pre and primary treatment - biological treatment - chemical process - solid waste - solid waste management - municipal solid waste- world scenario and Indian Scenario - disposal of wastes - treatment methods- bio-mining - incinerators-composition of soil - micro and macro nutrients - pollution due to fungicides, herbicides and insecticides - ecological and health effects of soil contamination - control of soil pollution (SDG-13: Climate action & SDG- 9: Industry innovation and infrastructure)

Unit 4 Sustainable development and Practices

Sustainability- concept, needs and challenges-sustainable development goals (SDG)- protocols, target, indicators and intervention areas, concept of carbon credit, carbon foot print, climatic changes, zero waste and 3-R concept- sustainable habitat- green buildings, Ggreen materials, energy efficiency and sustainable transport, sustainable Energy and sustainable urbanization- case studies (minimum 2) about sustainable development and ecosystem (SDG-10: Sustainable cities and communities)

Unit 5 New Energy Sources for the New Century

Renewable energy sources - waste bio-mass energy - tidal energy - ocean thermal conversion energy - geothermal energy - wind energy - solar energy-fuel from sunlight - energy from splitting of water - hydrogen from sunlight - hydrogen fuel cells - batteries-photovoltaic cells and its applications-

nuclear energy - nuclear fission and fusion- production of electricity by nuclear reactor and the hazards of radioactivity - living with nuclear power (SDG-7: Affordable and clean energy)

Total hours: 30

#### Reference Books

- Gopala Rao, M. and Marshall Sittig, Outlines of Chemical Technology For the 21<sup>st</sup> Century, 3<sup>rd</sup> Ed., Affiliated East-West Press (1997)
- Eugene W. Rice, Standard Methods for the Examination of Water and Wastewater, 22<sup>nd</sup> Ed., American Public Health Association, Washington (1998)
- 3. Metcalf and Eddy, Wastewater Engineering: Treatment, Disposal and Reuse, 3<sup>rd</sup> Ed., McGraw Hill Inc. New York (1991)
- 4. Prabhakar, V. K. Energy resources and the Environment, Anmol Publications Pvt. Ltd, Delhi, India (2001)
- 5. Ravikrishnan, A., Environmental Sciences and Sustainability, Sri Krishna Hitech Publishing Company Pvt. Ltd. (2024).
- 6. Des W. Connell, Basic Concepts of Environmental Chemistry, 2<sup>nd</sup> Ed., CRC Press, Taylor & Frances Group (2016)
- 7. Sharma, B.K. Industrial Chemistry: Including Chemical Engineering, 16<sup>th</sup> Ed., Goel Publishing House, Meerut (2011)
- 8. Kaur, H. Environmental Chemistry, 12th Ed., Pragathi-Prakasan, (2018)
- 9. Eric Litchtouse, Jan Schwarzbauer, Didierobert, Environmental Chemistry, Springer (2009)
- 10. James E. Girarg, Principles of Environmental Chemistry, 3<sup>rd</sup> Ed., Jones & Bartlett Learning, (2013)
- 11. DE, A.K. Environmental Chemistry, 6th Ed., New Age International Pvt. Ltd. Publishers, (2006)
- 12. Balram Pani, I.K. Text Book of Environmental Chemistry, International Publishing House, (2007)
- 13. Sharma, B.K. Environmental Chemistry, 11th Ed., Krishna Prabash media (P) Ltd. (2007)

- 1. Knowledge on pollution and its mitigation/eradication
- 2. Knowledge on water quality standards
- 3. Knowledge of methods for waste management
- 4. Knowledge on environmental aspects soil chemistry
- 5. Sensitization on renewable energy sources

CO/PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PSO 1	PSO 2	PSO 3
CO 1	M	M				Н	Н		Н
CO 2	M	M	L	M	Н	Н	Н	M	Н
CO 3	M	M	L		Н	Н	Н	M	Н
CO 4	M	M		M	Н	H	Н		H
CO 5	M	M		Н	Н	Н	Н	Н	H