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. Inculcate comprehensive domain knowledge relating to essential and advanced learning areas pertaining to chemistry.
3. Ability to demonstrate experimental techniques and methods
4. Capability of handling sophisticated equipment and instruments for identification of materials/chemical analysis and separation
5. Apply appropriate techniques and skills required for identifying chemistry- related problems and issues
6. Comprehensive communication of the concepts, constructs and techniques of the subject of Chemistry
7. Analyze and interpret data using appropriate methodologies to find evidence-based solutions
8. Become a skilful chemist, by acquiring knowledge about ethical standards, rules and regulations pertaining to scientific project
9. Apply domain knowledge analytical and computational skill to solve societal and environmental problems
10. Think critically and innovate new ideas for eco friendly chemistry
11. Suitability to be employable in chemical industry and R & D organizations

Programme Specific Outcomes

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

Scheme of Instruction and Examination
(For students admitted from 2023 – 2024 onwards)

Part	*Subject Code*	*Name of Paper/Component*	*Hours of Instructions / week*		*Scheme of Examination*				
			T	**P**	**Duration of exam**	**CIA**	**CE**	**Total**	**Credit**
First Semester									
I	23MCHC01	Organic Chemistry -I	5		3	40	60	100	5
	23MCHC02	Inorganic Chemistry -I	5		3	40	60	100	5
	23MCHC03	Physical Chemistry -I	5		3	40	60	100	5
	23MCHC04	Chemistry of Biomolecules (Open Book test)	3		3	100	-	100	3
	23MCHC05	Organic Chemistry Practical -I		5	6	40	60	100	3
	23MCHC06	Organic Chemistry Practical - II		5	6	40	60	100	3
II		CSS / Adult Education / Community Engagement and Social Responsibility	2	-	-	-	-	-	
Second Semester									
I	23MCHC07	Organic Chemistry -II	5		3	40	60	100	5
	23MCHC08	Inorganic Chemistry -II	5		3	40	60	100	5
	23MCHC09	Physical Chemistry -II	5		3	40	60	100	5
	23MCHC10	Physical Chemistry Practical -I		5	6	40	60	100	3
	23MCHC11	Inorganic Chemistry Practical-I		3	6	40	60	100	3
		Interdisciplinary Course	4	-	3	40	60	100	4
	23MCHC12	Mini Project	1	-	-	100	-	100	2
II	23MXCSS1/ 23MXAED1/ 23MXCSR1	CSS / Adult Education / Community Engagement and Social Responsibility	2	-	-	-	-	100	2
		Professional Certification Course							2
Internship during summer vacation (1 month)									
Third Semester									
I	23MCHC13	Spectroscopy- I	4		3	40	60	100	4
	23MCHC14	Spectroscopy- II	4		3	40	60	100	4
	23MCHC15	Research Methodology	3		3	40	60	100	4
	23MCHC16	Phytochemical Methods and Medicinal Chemistry	4		3	40	60	100	4
	23MCHC17	Inorganic Chemistry Practical -II		5	6	40	60	100	3
	23MCHC18	Physical Chemistry Practical - II		4	6	40	60	100	3
	23MCHC19	Computational Chemistry	3		3	40	60	100	5
	23MCHC20	Environmental Chemistry (Self Study)	1		3	40	60	100	4

		Multidisciplinary Course	2		3	100	-	100	2
II	23MCHC21	Internship				100	-	100	2
Fourth Semester									
I	23MCHC22	Research Project	30		8	100	100	200	8
								Total credits	**98**

Note: Minimum 98 + 2 credits required to earn the degree

Other courses to be completed by the students
MOOCS Course: 2 to 4 credits

Courses offered by the department

Interdisciplinary Course	23MCHI01 Nanomaterials and their Applications
Multidisciplinary Course	23MCHM01 Green Aspects in Life
Professional Certification Course	23MCHPC1 Analytical and Phytochemical Techniques

Organic Chemistry-I

Semester I **Hours of Instruction/Week: 5**
23MCHC01 **No. of Credits: 5**

Objectives

1. To recall the concepts of field effects
2. To impart advanced knowledge of stereoisomerism and related phenomena
3. To familiarize with reaction intermediates and determination of reaction mechanism

Unit 1 Concepts Used In Organic Reaction Mechanism, Aromaticity and Tautomerism

Field effects- inductive, inductomeric, electromeric effects and resonance, hyperconjugation, Aromaticity in benzenoids and non benzenoid systems. Tautomerism –keto –enol, amido –imido and nitro –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- calixaranes **15h**

Unit 2 Stereochemistry

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) circular dichroism and optical rotatory dispersion, axial haloketone rule and octant rule and their application to simple decalin systems, Prochirality–enantiotropic and diasteriotropic groups, Chirality due to helical shape, Conformational analysis of acyclic compounds, conformations of cyclohexanes and decalin

Asymmetric synthesis-Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions,determination of enantiometric and diasteromeric excess, enantio-discrimination, Resolution – optical and kinetic **15h**

Unit 3 Reactive Intermediates and Reaction Mechanism

Classical and non-classical carbocations, carbanions, radical- anions, radical-cations, carbenes, arynes and nitrenes-General methods of generation (**Self study**), detection and reactivity of these intermediates, singlet oxygen, its generation and reactions

Determination of reaction mechanism, kinetically and thermodynamically controlled reactions, Energy profile diagrams, detection of reaction intermediates, isotope effects and kinetic effects, Hard and soft acids and bases **15h**

Unit 4 Aliphatic and Aromatic Nucleophilic Substitution Reaction

Mechanism of S_{N1} and S_{N2} S_{Ni} reactions –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 regioselectivity, Neighbouring group participation by σ and π bonds **15h**

Mechanism of uni molecular and bimolecular aromatic nucleophilic Substitution, Reactivity – effect of substrate structure, attacking nucleophile and leaving group

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), Sandmeyer reaction, Hunsdiecker reaction, Reactions of Synthetic Importance (**Self study**) - Arndt-Eistert Homologation, Bischler-Napeiralski **15h**

reaction, Mannich reaction, Oppenaeur oxidation, Willgerodt reaction, Sommelet reaction, Darzen condensation , Elbs Persulphate oxidation, Periodic acid oxidation

Total hours: 75

Textbooks

1. 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)
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. Skyes, P. Guide Book to Mechanism in Organic Chemistry, Pearson Education (2001)
6. Pine, S.H., Henrickson, J.B., Gram, D.J. and Hammon, G.S. Organic Chemistry, 3rd Ed., McGraw-Hill Kogakusha Ltd., (2000)
7. Bansal, R. K. Organic Reaction Mechanism, 11th Ed., Tata McGraw-Hill, Noida (2006)
8. 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 field effects, fullerenes and selected supramolecules
2. Assign R/S, E/Z nomenclature to suitable organic molecules
3. Assess the different methods of determination of reaction mechanism
4. Describe and formulate the mechanism of nucleophilic substitution reactions
5. Acquire knowledge of the concepts of organic reaction mechanisms to reaction of synthetic importance

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M			L	L		L		M	M	M	H	
CO 2	L	L	L				L					M	M	
CO 3	H	H	L							H	H	H	H	
CO 4	L	M	L									M	H	
CO 5	L	M	L		M	L				M	H	M	H	L

Inorganic Chemistry-I

Semester I **Hours of Instruction/Week: 5**
23MCHC02 **No. of Credits: 5**

Objectives

1. To learn concepts of co-ordination chemistry
2. To familiarize with concepts of solid state chemistry
3. To gain knowledge about reagents used in inorganic chemistry

Unit I 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 d'electrons 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 **15h**

Self Study - Spectro chemical series and its importance in CFT, Spinels

Unit II Coordination Chemistry II

Jahn-Teller theorem-tetragonal distortion from octahedral symmetry, Conditions for distortion-Jahn Teller stabilization energy-limitations of CFT, Molecular orbital (MO) theory for octahedral complexes, Types of pi-bonds- effect of pi-bonding on crystal field splitting-evidences for pi-bonding-Nepheleuxetic series, electronic spectra of complexes interpretation including charge transfer spectra-Splitting of free ion terms in octahedral field – correlation diagram – Orgel diagrams for d1 to d9 ions, Uses of Orgel diagrams-Applications, Principles of Tanabe-Sugano diagrams **15h**

Self Study - Quantum numbers of multi-electron atoms – Russell-Sanders coupling – L-S coupling and micro states – Ground state terms for d1 – d10 ions

Unit III Organic and Inorganic Reagents in Inorganic analysis

Organic reagents, common characteristics of organic reagents - Advantages of organic reagents over inorganic reagents, disadvantages of organic reagents- important organic reagents- oxine (C_9H_7ON), dimethyl glyoxime (DMG), alpha-nitroso beta-naphthol, cupferron, aluminon, rubeanic acid, rhodamine-b, benzidine, cupron, magneson, alizarin, nitron and salicylaldoxime, Self Study - Inorganic precipitating reagents **15h**

Unit IV Organo Metallic 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 organo metallic chemistry-oxidative addition, reductive elimination, insertion, elimination and migration

Organo metallic compounds of lithium and boron-preparation, properties, structure and uses, organo metallic 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 cyCO penta dienyl complexes- ferrocene-preparation, properties, structure and uses **15h**

Applications of organometallics in organic synthesis, C-C bond coupling reactions (Heck, Sangoshira, Suzuki)

Unit V Solid State

Crystalline and amorphous solids-polymorphism-isomorphism-Mitcherlich's law of isomorphism-isopolymorphism-COse packing of spheres, packing efficiency, hexagonal COse packed (hcp) and cubic COse packed (ccp) structures, coordination number, Interstitial sites in COsely packed arrangement of atoms- trigonal sites, tetrahedral and octahedral sites, radius ratio rule and its effect on the shape of ionic crystals, Coordination number of cubic lattice—Structure of ionic crystals of AB type – Caesium chloride,Zinc Blende , Wurtzite , AB_2 type-Rutile, Fluorite

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 **15h**

Self Study- Solid state reactions – classification – thermal decomposition reactions – reaction between two solids – Improving reactivity of solids, super conductivity -1, 2, 3 super conductors, BCS (cooper pair) theory, Meissner effect

Textbooks **Total hours: 75**

1. Malik, W.U., Tuli G.D. and Madan, R.D. Selected Topics in Inorganic Chemistry, 17th Ed., S. Chand Company Ltd, (2010)
2. Gurdeep Raj, Advanced Inorganic Chemistry, Volume I & II, 6th Ed., Krishna Prakashan Media (P) Ltd., (2018)
3. Puri, B.R., Sharma, L.R. and Kalia, K.C. Principles of Inorganic Chemistry, 33rd Ed., Milestone Publishers, New Delhi (2017)
4. Sathya Prakash, Tuli, Basu and Madan, Advanced Inorganic Chemistry, 19th Ed., Volume I & II, S. Chand Publishers, (2016)
5. Soni, P.L. and Mohan Katyal, Textbook of Inorganic Chemistry, Sultan Chand & Sons (2006)
6. Anthony R. West, Basic Solid State Chemistry, 2nd Ed., John Wiley & Sons, (1999)
7. Haiduc, I. and Zuckerman, J. J. Basic Organometallic Chemistry, Walter de Gruyter, Berlin, (1985)

Course Outcomes

1. Ability to apply models/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. Understand significance of Organic and Inorganic Reagents in Inorganic analysis
4. Knowledge on Structure and bonding in Organo Metallic Compounds
5. Ability to analyze crystal systems and identify class of defects in crystals

CO / PO	PO 1	PO 2	PO 3.	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	L			M	M						M		
CO 2	M	M	L			M	M					M	M	
CO 3	M	M	L				M					M	M	M
CO 4	M	M	M			M	M					M	M	M
CO 5	M	M	M			M	M					M	M	L

Physical Chemistry-I

Semester I
23MCHC03

Hours of Instruction/Week: 5
No. of Credits: 5

Objectives

1. To widen knowledge on the concepts of thermodynamics and properties of real gases
2. To enable students to get insight to the concepts of non equilibrium thermodynamics
3. To acquire knowledge on electrochemical cell reactions and corrosion phenomena
4. To learn the various applications of electrochemical phenomena

Unit I Thermodynamics

A brief resume of thermodynamics (confined form of I and II 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

III law – Need for III law, Nernst Heat theorem, Statements of III law-Thermodynamics quantities at absolute Zero, Calculation of absolute entropies-apparent exception to III 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 **20h**

Unit II 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, Bose-Einstein and Fermi-Dirac statistics

Partition function - 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 Numerical Problems (Self study) **15h**

Unit III 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, irreversible thermodynamics for biological systems (Self study), coupled reactions **15h**

Unit IV Electrochemistry I

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, structure of the double layer at the interface–derivation of the fundamental equation of electrode kinetics–Butler Volmer equation, decomposition voltage and over voltage, Polarography – theory, Ilkovic equation, half wave potential and its significance. **15h**

Unit V Electrochemistry II

Electrochemical cell reactions – Nernst equation – Fuel cells - H_2- O_2, hydrocarbon, air fuel cells, Storage batteries – primary and secondary – lead acid battery, nickel – cadmium cell, Electrochemical manufacture of soda ash by electrochemical method and aluminium by electrolytic method (Self

study), 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 **10h**

Textbooks **Total hours: 75**

1. Gurdeep Raj, Advanced Physical Chemistry, 42nd Ed., Goel Publishing House, (2018)
2. John M. Bockris and Amulya K.N. Reddy, Modern Electrochemistry, Volume I & II, 2nd Ed. (2008)
3. Gupta and Sharma, K. Advanced Physical Chemistry, Nath & Co. Educational Publishers, (2011)
4. Gurtu, J.N. and Gurthu, 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

1. Understanding of the concepts of thermodynamics and properties of real gases
2. Able to distinguish the various thermodynamic statistics and partition functions
3. Able to apply the concepts of non equilibrium thermodynamics to biological reactions
4. Ability to describe the electrochemical phenomena
5. Able to distinguish different fuel cells and to familiarize with corrosion protection methods

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M				M						M	M	M
CO 2	M	M				M	M					M	M	M
CO 3	M	M	M		M							M	M	M
CO 4	M	M	M				M					M	M	M
CO 5	M	M	M	M	H	M	H	M	H	H	H	M	M	M

Chemistry of Biomolecules
(Open Book)

Semester I
23MCHC04

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

Objectives

1. To understand the versatile knowledge about the synthesis, biological importance of various natural products
2. To understand the key role of various elements in the living systems
3. To acquire basic knowledge about the heterocyclic chemistry

Unit I Proteins, Nucleic acids and Enzymes

Protein - amino acids in proteins - non protein amino acids -synthesis of amino acids and polypeptides - primary and secondary structure of a protein - the N terminal and C- terminal residue analysis
Nucleic acids - structure and synthesis of nucleosides - structure and synthesis of nucleotides - structure of RNA and DNA and their biological importance **9h**
Enzymes - Enzyme –substrate complex –theories proposed- active center, enzyme specificity. Allosteric Enzymes and Co-enzymes

Unit II Vitamins and Carbohydrates

Types, structure discussion, properties and biological importance of Vitamin A, Vitamin B complex: B_1, B_{12}, Folic acid, Vitamins C, D and E
Carbohydrates: Synthesis and biological importance of glycosides, amino sugars, sucrose, maltose, cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar, chitosan, and chrysin. **8h**

Unit III Metals in Biology

Metals and Non-metals in biological systems - Essential and trace elements - Role of different metal ions in biological process - Porphyrins, corrin and chlorin as Biological ligands, structural models. Vitamin B_{12}-Reactions of the alkyl cobalamins, One-electron Reduction and Oxidation
Ionophores - Sodium-Potassium transfer across the membrane – Calcium ATPase pump Ferritin – Hemosiderin- Transferrin- Copper protein - structure and functions of type-I, typeII and type-III **10h**
Photosynthesis: Chlorophyll - Photosystem-I (PS-I) & II (PS-II) - Structure-function relationship

Unit IV Heme and Non-Heme Proteins

Oxygen transport and storage: Structure and functions of Hemoglobin, Myoglobin, Hemerythrin and Hemocyanin, Bohr Effect, synthetic models. Importance of 2,3- diphosphoglycerate, CO and CN poisoning, hematin formation **10h**
Non-heme iron-sulphur proteins - Ferridoxins - Rubredoxins – Cytochrome. a,b,c, cytochrome P450, Cytochrome C oxidase

Unit V Heterocyclic Compounds

Synthesis, reactions, reactivity and aromaticity of indole, isoindole, oxazole, imidazole, thiazole, carbazoles, uric acid and xanthines **8h**
Oxygen Heterocyclic Compounds: Classification, color reactions of various classes of flavonoids – chemistry and synthesis of flavones (luteolin), isoflavones (daidzein), flavonols (kaempferol) and anthocyanidins (cyanidin)

Total hours: 45

Reference Books

1. Finar, I.L. Organic Chemistry, Volume I & II
2. Bansal, R. K. Heterocyclic Chemistry, 3rd Ed., Wiley Eastern Ltd., New Delhi (1999)
3. Dr. Asim K. Dass, Bioinorganic Chemistry, Books and Allied (P) Ltd. (2007)
4. Wolfgang Kaim, Brigitte Schwederski, Axel Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of life, 2nd Ed., John Wiley & Sons (2013)
5. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, 3rd Ed.
6. Gurdeep R.Chatwal, Organic Chemistry of Natural Products, Volume II
7. Wermuth, C. G. Medicinal Chemistry for the 21st Century, Blackwell Scientific Publications, (1992)
8. Huheey, J. E. Inorganic Chemistry, 4th Ed., Harper & Row Publishers, Singapore (2006)
9. Cotton, F.A. and Wilkinson, G. Advanced Inorganic Chemistry, 6th Ed., Wiley Inter Science Publication, John Wiley & Sons, New York, USA (1999)
10. Lippard, S. J. and Berg, J.M. Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi (1997)
11. Rohatgi Mukherjee, K. K. Fundamentals of Photochemistry (Revised edition), Wiley Eastern Ltd. (1996)
12. Lehninger, A.L., Nelson, D.L. and Coxworth, M.M. Principles of Biochemistry, New York (1993)
13. Satyanaryan, U. Biochemistry, 2nd Ed., Books and Allied (P) Ltd., Kolkata (2002)
14. Das, A.K. A Textbook of Medicinal Aspects of Bioinorganic Chemistry, CBS Publishers and Distributors, New Delhi (1991)

Course Outcomes

1. To analyze the structure and functions of the natural products such as proteins, nucleic acid and enzymes
2. Appreciate the significance in chemistry of vitamins and carbohydrates
3. To understand the key function of the role of metals and non-metals in biological systems
4. To acquire knowledge about heme and non-heme Proteins
5. Understand the concepts of synthesis and reactivity of heterocyclic compounds and flavonoids

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	L			L	L	M		L			M	H	L
CO 2	M	L			M	L	L					M	M	
CO 3	M	L			H	L						M	M	
CO 4	M	L			M	L			L			M	M	
CO 5	H	M			M	M	M			L		H	H	L

Organic Chemistry Practical-I

Semester I **Hours of Instruction/Week: 5**
23MCHC05 **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 I 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, Sugar, Anilides Aldehyde, ketones, simple phenol, phenolic compounds, esters, primary, secondary and tertiary amines, nitro compound

- ❖ 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: 75

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)

Course Outcomes

1. Skill in carrying out different laboratory techniques for Purification, Crystallization, and Distillation
2. formulate strategies for the binary mixture separation
3. identification of organic compounds
4. plan for synthetic procedures in derivatization of organic compounds
5. Identification of organic compounds plan for synthetic procedures in derivatization of organic compounds

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M	H	L		M		M	M	M	H	H	H	H
CO 2	M	M	H	L		M		M			H	H	M	H
CO 3	M	M	H	L	L	L		M		M	H	H	M	H
CO 4	M	M	M	L	M	L	M	M			H	H	H	H
CO 5	M	M	L		L	L		M	H		H	H	M	H

Organic Chemistry Practical-II

Semester I
23MCHC06

Hours of Instruction/Week: 5
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

1. Estimation of phenol, aniline, Glucose. Ascorbic acid, ethyl methyl ketone, lactose from milk
2. Determination of saponification value, iodine value of oil samples.
3. Experiments involving column chromatography TLC and paper chromatography for separation and identification of organic compounds.
4. Extraction of Caffeine from tea leaves –Isolation of casein from milk

40 h

Unit II Organic Preparations

Two stage preparation of organic compounds involving synthetic methods like oxidation, acylation, nitration, sulphonation, bromination, esterification, hydrolysis and condensation (six preparations.)

35 h

Total hours: 75

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)

Course Outcomes

1. Ability to prepare organic compounds
2. Skills in estimation of organic compounds
3. Skills in extraction of selected natural products
4. Knowhow of chromatographic techniques
5. Familiarization on oil analysis

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M	H	L		M		M	M	M	H	H	H	H
CO 2	M	M	H	L		M		M			H	H	M	H
CO 3	M	M	H	L	L	L		M		M	H	H	M	H
CO 4	M	M	M	L	M	L	M	M			H	H	H	H
CO 5	M	M	L		L	L		M	H		H	H	M	H

Organic Chemistry-II

Semester II **Hours of Instruction/Week: 5**
23MCHC07 **No. of Credits: 5**

Objectives

1. To enable students to get knowledge of concerted organic reactions and their mechanisms
2. To enable students to get knowledge of photochemistry of carbonyl compounds and unsaturated systems
3. To familiarize the concepts of addition and elimination reactions
4. To get acquainted with electrophilic substitution reactions
5. To introduce key reactions for applications in organic synthesis and organic transformations

Unit I Pericyclic Reactions

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**) **15h**

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 II Photochemistry of Carbonyl Compounds and unsaturated Systems

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),**

Photochemistry of carbonyl compounds, n –π and π-π^* transition (Self study), Norrish, type I and Norrish type II cleavages, Paterno-Buchi reaction, photo reduction, photo chemistry of enones, hydrogen abstraction, rearrangement of α,β unsaturated ketone and cyclohexadienones

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, Photo chemistry of vision **15h**

Unit III Addition and Elimination Reactions

Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms, regio and chemoselectivity orientation and stereochemistry, addition to cyclopropane. Hydroboration **(Self study)**Michael reaction, addition of oxygen (o_2) across double bonds, Sharpless asymmetric epoxidation, mechanisms of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids esters and nitriles. Stobbe reaction, Wittig reaction (Self study)

Elimination reactions involving E_1, E_2, E_1CB, and E_{2C} mechanisms and orientation, orientation of the double bond, Saytzeff and Hoffman rules (**Self study**), pyrolytic eliminations, Chugaev reaction cleavage of quaternary ammonium hydroxides, conversion of vicinal dihalides to olefins **15h**

Unit IV Aliphatic and Aromatic Electrophilic Substitution Reaction

Bimolecular mechanisms- SE_2 and SEi, SE_1 mechanism, substitution accompanied by double bond shifts, Effect of substrates leaving group and the solvent polarity on the reactivity

Mechanism of electrophilic aromatic substitution 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, isomer proportions, energy profile diagrams

Vilsmeir-Haack reaction, Reimer Tiemann reaction, Pechmann and Houben Hoesch reaction, Gattermann-Koch reaction, Diazonium coupling, Scholl reaction and Bradsher reaction **(Self study)** **15h**

Unit V Name Reactions and Strategies in Organic Synthesis

Name Reactions: Robinson annulations, Suzuki Coupling, Wittig reaction, Stark enamine synthesis and Shapiro reaction

Strategies in Organic Synthesis: An introduction of synthons and synthetic equivalents, disconnection approach, functional group interconversion of halides, nitriles, azides, amines, and esters -the importance of order of events in organic synthesis, nucleophilic and electrophilic synthons umpolong 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 and reductions **15h**

Reference Books **Total hours: 75**

1. Depuy and Chapman, Photochemistry, (2000)
2. DePuy, C.H. and Chapman, O.L. Molecular Reactions and Photochemistry, Prentice-Hall, New Delhi (1987)
3. Jerry March, Advanced Organic Chemistry-Reaction Mechanisms and Structure, 4th Ed., John Wiley & Sons (1999)
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. Molecular orbital symmetry and be able to evaluate concerted reactions *via* FMO and PMO approach, electrocyclic reactions, cycloadditions and sigmatropic rearrangements
2. Photochemical reactions of alkenes, carbonyl and aromatic compounds
   Identify the mechanism of various photochemical reactions
3. Able to predict the stereochemistry and mechanism of addition and elimination reactions
4. Assess the mechanism and reactivity of electrophilic substitution reactions
5. Expertise in identifying the transformations, the reagents and planning organic synthesis

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1		H			M		M					M	M	
CO 2			H	M	M		M			L	L	M	M	
CO 3	M	M			M	M	M			H		H	M	
CO 4	M	M			M	M	M			H		H	M	
CO 5	M	M			M	M	M			H		H	M	

Inorganic Chemistry-II

Semester II
23MCHC08

Hours of Instruction/Week: 5
No. of Credits: 5

Objectives

1. To understand the concept of group theory and its applications
2. To learn the general characteristics of f-block elements and analyse the magnetic properties of their complexes
3. To understand the advanced concepts of nuclear chemistry, types of nuclear reactions and applications

Unit I 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, **Self study** – Optical activity and dipole moment on the basis of point group symmetry **15h**

Unit II 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, **Self study** – Isomorphism and direct product representation **15h**

Unit III Stability of Complexes

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_N and S_E S_N^1 and S_N^2 mechanism. Hydrolysis reaction- Aquation and Base hydrolysis, S_N^{1CB} mechanism Anation reactions, Ligand substitution reaction in square planar complexes- trans effect, 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 **15h**

Unit IV Magnetochemistry of Transition Metal Complexes and Lanthanides & Actinides

Magnetic Properties – Dia, Para, ferro and antiferro magnetism, Curie point applicable to ferro and anti ferro magnetism, Neel point applicable to anti ferro magnetism. Quenching of orbital angular momentum. Colour and complex formation of inner transition elements.Lanthanides and Actinides **Self study** – Colour absorption spectra of Lanthanides and actinides. Comparison between Lanthanides and Actinides **15h**

Unit V Inorganic Chains, Rings and Nuclear Reactions

Inorganic Chains- Isopoly and hetero poly acids of molybdenum and chromium –preparation and structure only, Silicones – Preparation and structure only

Inorganic Rings- Phosphazenes – hexa chloro cyclo tri phosphazine, polyphosphonitrilic chloride - Preparation and structure only

Nuclear reactions: Bathe's notation – types of nuclear reactions – elastic and inelastic scattering – Cross section – Q value – Transuraniens – Photonuclear reaction – Radioactive capture – Evaporation and spallation breeder reactor - 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, dating methods **15h**

Reference Books **Total hours: 75**

1. Ramakrishnan, V. and Gopinathan, M.S. Group Theory in Chemistry, 2nd Ed., Vishal Publications (2013)
2. Gurdeep Raj, Ajay Bhagi and Vinod Jain, Group Theory and Symmetry in Chemistry, 3rd Ed., Krishna Prakashan Media (P) Ltd., Meerut (2010)
3. Raman, K.V. Group Theory and Its Applications to Chemistry, 4th 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, 1st Ed., University Press (2008)
5. Sathya Prakash, Tuli, Basu and Madan, Advanced Inorganic Chemistry, Volume I & II, 19th Ed., S. Chand Publishers (2016)
6. Soni, P.L. and Mohan Katyal, Text Book of Inorganic Chemistry, 20th Ed., Sultan Chand and Sons (2006)
7. Arnikar, H.J. Essential of Nuclear Chemistry, 4th Ed., New Age International (P) Ltd, New Delhi (1995)
8. Freindlander, G., Kennedy, J.W., Macias, E.S. and Miller, J.M. Nuclear and Radiochemistry, 3rd Ed., John Wiley and Sons, New York (1981)

Course Outcomes

Students will be able to

1. Ability to classify molecules into point groups
2. Knowledge of applications of group theory
3. Understanding the chemistry of cage, chain complexes
4. Familiarization of general characteristics of f-block elements and magnetic properties of their complexes
5. Knowledge on nuclear reactions and applications

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M				M						M	M	
CO 2	M	M	M		L	M	M					M	M	
CO 3	M	M	M			M	M					M	M	
CO 4	M	M	L		L	M	L					M	M	
CO 5	M	M			M	M	M					M	M	

Physical Chemistry-II

Semester II **Hours of Instruction/Week: 5**
23MCHC09 **No. of Credits: 5**

Objectives

1. To widen the knowledge in kinetics and mechanism of chemical reactions
2. To understand the chemistry and kinetics of fast reactions
3. To get acquainted with quantum mechanical approach of atoms and molecules

Unit I 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 uni molecular reactions – Ter molecular reactions –Thermodynamic formulation of ARRT chain Reactions, general characteristics study of kinetics of H_2 Cl_2 reaction. H_2 – Br_2 reaction, Kinetics of polymerization decomposition of N_2O_5, H_2O_2, reaction (explosion limits) **15h**

Unit II Fast 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, Kinetics of catalytic reactions, acid base catalysis, enzyme catalysis **15h**

Unit III Surface Chemistry

Adsorption – Types of adsorption (Self Study), Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, B.E. T adsorption isotherm and its application

Heat of adsorption, Estimation of surface areas of solids from solution adsorption studies Chemisorption –kinetics and thermodynamics, Surface reactions and mechanisms

Unit IV Quantum Chemistry I **15h**

Success of quantum theory and failure of classical mechanics-experimental foundation of quantum mechanics- The black body radiation, photoelectric effect, Compton effect and atomic spectra (Self study), Formulation of quantum mechanics-the wave nature of sub-atomic particles-wave particle dualism-Heisenberg's uncertainty principle- Schrodinger wave equation

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

Unit V Quantum Chemistry II

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 **15h**

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 **15h**

Total hours: 75

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

1. Understanding of kinetics and mechanistic aspects of chemical reactions
2. Knowledge on kinetic aspects of fast reactions
3. Ability to distinguish the various adsorption isotherms
4. Knowledge on steps involved in studying a system quantum mechanically
5. Ability to apply HMO treatment of simple and conjugated π electron systems

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M	M			M	M				M	M	M	M
CO 2	M	M	H	M		M	M				M	M	M	M
CO 3	M	M	M	M	M	M	M		L	M	M	M	M	M
CO 4	M	M				M	M				M	M	M	M
CO 5	M	M	M			M	M		L		L	M	M	M

Physical Chemistry Practical-I

SEMESTER II **Hours of Instruction/Week: 5**

23MCHC10 **No. of Credits: 3**

Objectives

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

Unit I **15 h**

1. **Colorimetry**
   Estimation of Iron & Nickel
2. **Surface Chemistry**
   Verification of Freundlich and Langmuir adsorption Isotherm of oxalic acid on activated charcoal

Unit II Potentiometry

1. Potentiometric titrations
   a) Acid – base titrations
      i) HCl-NaOH-HCl
      ii) CH_3COOH-NaOH-CH_3COOH
      iii) HCl – NaOH - (HCl + CH_3COOH
   b) Redox titrations
      i) $FeSO_4$-$KMnO_4$-$FeSO_4$
      ii) $FeSO_4$-$K_2Cr_2O_7$-$FeSO_4$
   c) Precipitation titrations **60 h**
      KCl-$AgNO_3$-KCl
2. Applications of EMF
   a) Determination of standard potentials (Cu, Zn, Ag)
   b) Determination of solubility of a sparingly soluble salt
   c) Determination of dissociation constant of a weak acid using Quinhydrone electrode

Total hours: 75

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. Ability to carry out potentiometric titrations
2. Knowledge on the determination of standard electrode potential of (Cu, Ag &Zn) electrodes
3. Understanding the practical applications of EMF
4. Gaining practical skill in colorimetric experiments
5. Knowhow to analyze and interpret experimental data using adsorption isotherm models

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M	H	L	M	L					M	M	M	L
CO 2	M	M	H	L	L	M					M	M	M	L
CO 3	L	M	M	M	M	L					M	M	M	L
CO 4	M	M	H	L	L	L					M	M	M	L
CO 5	M	M	M	L	M	M					M	M	M	L

Inorganic Chemistry Practical-I

Semester II **Hours of Instruction/Week: 3**
23MCHC11 **No. of Credits: 3**

Objectives

1. To formulate suitable method for inorganic complex preparation
2. To estimate selected inorganic metal ions by complexometry method
3. To gain skill in the preparation of selected inorganic complexes

Unit I Preparation of Selected Inorganic Complexes **25h**

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

Unit II Complexometric Titrations **20h**

1. Estimation of Fe^{3+}
2. Estimation of Cu^{2+}
3. Estimation of Ca^{2+}
4. Estimation of Mg^{2+}
5. Estimation of Ni^{2+}
6. Estimation of Zn^{2+}

Total hours: 45

Reference Books

1. Ramanujam, V.V. Inorganic Semi Micro Qualitative Analysis, The National Publishing Co. Ltd., Madras, (1976)
2. Vogel, Inorganic Qualitative analysis
3. Vogel, Inorganic Quantitative analysis
4. Scott, Standard Methods of Analysis
5. King, Inorganic Synthesis
6. Bard, H.M. Modern Polarographic -Methods in Analytical Chemistry
7. Palmer, W.G. Experimental Inorganic Chemistry
8. Jagadamba Sing, Singh, R.K.P., Jaya Singh, Yadav, L.D.S., Siddiqui, I.R and Jaya Srivastava, Advanced Practical Chemistry
9. Agarwal and Keemtila, Advanced Inorganic Analysis

Course Outcomes

1. Ability to prepare an inorganic complex
2. Formulate suitable methods for the preparation of desired inorganic complexes
3. Understanding the principles of EDTA titrations
4. Knowledge on buffer solutions
5. Develop practical skills in complexometric titrations

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M	H	M							M	M	M	L
CO 2	M	M	H	M	M						M	M	M	
CO 3	M	M	H	M	M						M	M	M	H
CO 4	M	M	M	M	M						M	M	M	H
CO 5	M	M	H			M					M	M	M	H

Spectroscopy-I

Semester III **Hours of Instruction/week: 4**
23MCHC13 **No. of Credits: 4**

Objectives

1. To gain knowledge on aspects of UV, NMR, ESR spectroscopy
2. To acquaint with the qualitative aspects of UV,NMR and ESR techniques
3. To acquaint with X-ray and Neutron diffraction techniques and their applications

Unit I UV Visible Spectroscopy

Electronic transitions (185-800nm), Beer-Lambert's law, effect of solvent on electronic transitions, UV absorption of carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, polyynes, UV spectra of aromatics and heterocyclic compounds, Woodward –Fieser rules for conjugated dienes, α,β-unsaturated carbonyl compounds and benzene derivatives , Steric effect in biphenyls, Instrumentation of UV of double beam spectrometer (Self Study) **12h**

Unit II NMR Spectroscopy I

General introduction and definition, chemical shift, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols , carboxylic acids, amines, amides and mercapto)-factors affecting chemical shift, chemical shift equivalence spin-spin coupling– shielding mechanism-coupling constant-variation of coupling constant with dihedral angle-Karplus Conroy curve, spin-spin interaction between 2,3,4,and 5 nuclei (I order spectra), Double Resonance, -hindered rotation, simplification of complex spectra-chemical exchange, effect of deuteration, contact shift reagents, solvent effects, nuclear Overhauser effect (NOE), Resonance of other nuclei – Phosphorous and Fluorine NMR, Significance of NMR in Magnetic Resonance Imaging, FT technique and its advantages over conventional NMR (Self Study) **12h**

Unit III NMR Spectroscopy II

C^{13}NMR spectroscopy-general considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon), coupling constants.Two dimensional NMR spectroscopy – overview of COSY, NOESY, DEPT techniques- (Self Study) **12h**

Unit IV ESR Spectroscopy

Principles of ESR spectroscopy-Factors affecting the intensity, position- multiplet structure of the spectra- hyperfine splitting of some systems-zero field splitting, Krammer's degeneracy, g-value, factors affecting g-value and its significance, Application of ESR in Food analysis

ESR spectra of simple systems (Self Study) **12h**

Unit V X-RAY Diffraction and Neutron Diffraction

Principles of molecular structure-crystal structure-Bragg's equation-determination of crystal structure-Rotating crystal method,Powder Method, Neutron diffraction- principles and application to molecular structure determination-Advantages over X-ray diffraction studies (Self Study) **12h**

Total hours: 60

Reference Books

1. Dudley, H., Williams and Ian Fleming, Spectroscopic Methods in Organic Chemistry, 6th Ed., Tata McGraw Hill (2011)
2. Parish, R.V. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, 1st 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, 1st 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)

Course Outcomes

1. Knowledge on the principles of UV and ability to interpret UV
2. Knowledge on the principles H^1 NMR and ability to interpret H^1 NMR
3. Knowledge on the principles ^{13}C NMR and ability to interpret ^{13}C NMR
4. Knowledge on the principles ESR spectroscopy and apply the technique for food analysis
5. Understanding the principles and applications of X-ray and Neutron diffraction

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	H	M	M		M		H				M	M	M	M
CO 2	H	M			M		H				M	M	M	M
CO 3	H	M	L		M		H				M	M	M	M
CO 4	H	M	L		M		H		M		M	M	M	M
CO 5	H	M	H		M	L	H		M		M	M	M	M

Spectroscopy-II

Semester III
23MCHC14

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

Objectives

1. To gain knowledge on qualitative applications of Raman, IR, Mass and Mossbauer spectral techniques in structure elucidation
2. To know the applications of flame emission and atomic absorption spectroscopy
3. To solve problems in spectroscopy

Unit I 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. FT IR spectrometer –Instrumentation (Self Study) **12h**

Unit II Raman Spectroscopy

Principles of Raman spectroscopy- Classical and quantum theories, rotational, vibrational, rotational – vibrational Raman spectra, selection rules, mutual exclusion principle, Stokes and anti Stokes lines, Characteristics of Raman lines, Applications Raman spectroscopy, Comparison of IR and Raman techniques **(Self Study)**

Unit III Mass Spectroscopy **12h**

Introduction –ion production –EI, CI, FD, FAB, ion abundance, Mass spectral fragmentation of organic compounds, factors affecting fragmentation, base peak, molecular ion peak, meta stable peak, parent ion, daughter ion, doubly charged ions, Mclafferty rearrangement, nitrogen rule, ring rule, isotopic peak, isotopic clusters

Examples of mass spectral fragmentation of organic compounds **(Self Study)** **12h**

Unit IV Mossbauer Spectroscopy

Basic principles, spectral parameters and spectral display, Application of the technique to the study of bonding and structure of Fe^{2+} and Fe^{3+} compounds – Chemical shift, Quadrupole effects, Effect of magnetic field, nature of M-L bond, coordination number and structure **12h**

Unit 5. Atomic Absorption Spectroscopy (AAS) and Flame Emission Spectroscopy (FES)

Atomic Absorption Spectroscopy – Basic principles- instrumentation – flame characteristics – Flames and burners- types of interferences- background absorption, spectral .line interference, vaporization 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) **12h**

Total hours: 60

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)

Course Outcomes

1. Apply IR to identify functional group by IR
2. Knowledge on the principles Raman
3. Knowledge on instrumentation of Mass spectroscopy
4. Knowledge on the principles Mossbauer spectroscopy
5. Knowledge on identification of elements using flame emission and atomic absorption spectroscopy

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M	M		M		M				M	M	M	
CO 2	M	M			M						M	M	M	
CO 3	M	M	L		M						M	M	M	
CO 4	M	M	L		M						M	M	M	
CO 5	M	M	H		M	L			M		M	M	M	

Research Methodology

Semester III
23MCHC15

Hours of Instruction/Week: 3
No. of Credits: 4

Objectives

1. To develop skills in formulating various research designs
2. To learn the application of technology in research
3. To gain knowledge on statistical tools and analysis

Unit I 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 exPOratory research-Importance of research in Science (Self study)

Unit II Components of Research Design **9h**

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 III Techniques of Analysis **9h**

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 **9h**

Unit IV 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) **9h**

Unit V 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) **9h**

Total hours: 45

Reference Books

1. Gurumani, N. An introduction to Biostatistics, 2nd Ed., MJP publishers (2004)
2. Kothari, C.R. Research Methodology: Methods and Techniques, 2nd 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)

Course Outcomes

1. Familiarization of various research concepts
2. Knowledge on formulating research designs
3. Ability to apply statistical analysis to research
4. Skills in the application of technology in research
5. Ability to write a good research report

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PS O 1	PS O 2	PS O 3
CO 1		M			M		H					M		M
CO 2	M	M			M		H		M					
CO 3	M	M	L		M	M	H	M	M	M	M	M	M	M
CO 4	M				M	M	H		M					
CO 5	M				M		H	M					M	

Phytochemical Methods and Medicinal Chemistry

Semester III
23MCHC16

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

Objectives

1. To enable post graduate students in Chemistry to gain knowledge in phytochemical techniques and medicinal chemistry
2. To enable them to be familiar with techniques of extraction, separation and purification and simple identification strategies of drugs/natural products
3. To acquaint with drug action and structure-activity relationship

Unit I

Extraction, separation and purification and identification strategies of drugs/natural products

Extraction Techniques – General principles of solvent extraction –continuous extraction (soxhlet extraction) – extract fractionation, principles and technique of simple distillation – fractional distillation- steam distillation-reduced pressure distillation-rotary evaporation

Separation Techniques – Simple crystallization- experimental aspects – solvents for crystallization, Chromatographic techniques- experimental details and applications of column chromatography(CC), thin layer chromatography(TLC), paper chromatography(PC), gas liquid chromatography(GLC), Special methods– alkaloid extraction and pigment extraction

Purification Techniques – Theory of melting and freezing – melting point and vapour pressure – effect of impurities on melting point – mixed melting point- determination of melting point and boiling point, Principle and technique – sublimation, recryztalisation, freeze drying and pistol drying

Identification Techniques – Preliminary methods of identification of extracts – Phyto chemical aspects-colour tests – TLC and fluorescent characteristics, proximate methods

Unit II Drug action **12h**

Physiochemical properties and biological action – influence of route of administration. Biotransformation – absorption from stomach – absorption from intestines – sites of loss – metabolism and excretion, harmful drugs and their side effects

The receptor concept-protein receptor-drug receptor interactions, binding modes of alcohols and phenols, aromatic rings, amines, amides, ketones and aldehydes, thiols, ethers and heterocycles

Chemical aspects of the Drug – shape of the drug – Positional isomers, Stereoisomerism- chirality-enantiomers, diastereoisomers, Geometrical isomers-Easson-Stedman theory, Conformationally flexible to conformationally rigid molecule (Illustration with examples), Mechanistic implication of enantiomers

Forces involved in Drug – Receptor complex–covalent bonds, electrostatic (ionic) interactions, ion-dipole-dipole interactions, hydrogen bonds, charge transfer complexes, hydrophobic interactions, and dispersion forces (Vander waals)

Unit III Structure-Activity relationship **12h**

Structural modifications to Increase Potency-Homologation, chain branching, Ring chain transformation, extension of the structure, isosters/bioisosters. Quantitative Structure –Activity Relationships in relevance to Drug molecules – Application of Hammett Equation-electronic effects, Taft equation-steric effects, Lipophilicity effects-basis of Hansch equation, correlation between physiochemical parameters and biological activity, Craig Pot

12h

Unit IV Representative Class of Drug Molecules – I

Antibiotics –Mode of action and structural features of Chlorophenicol, Penicillin- semi synthetic Penicillin, Streptomycin-Cephalasporin and Tetracycline

Antifungal antibiotics-Nystatin, Fusicidic acid and Griesofulvin (structural features not required)

Antihistamine and anti malarials- Antihistamines - Mechanism of action, second generation non sedating antihistamines, Antimalarials –classification –Amino quinoline analogues, Pyrimidine analogues, Quinine analogues, Guanidine analogues and their mechanism of action 12h

Unit V Representative Class of Drug Molecules – II

Anti-hypertensives – COnidine, Losartan, Methyldopa – mechanism of action, Hypotensive agents – Diazoxide, Sodium nitroprussside – mechanism of action, Anti-arythamic agents- Quinidine, Lorcainide- mechanism of action, Antitubercular drugs –Ethambutol hydrochloride, Isoniazid, and Rifampicin, Mechanism of action

Cardiovascular Drugs-classification, Mechanism of action of cardiac glysocides- Digoxin, Digitoxin

History of pandemic precursor viruses - Corona, Ebola, SARS –possible synthetic and herbal remedies 12h

Total hours: 60

Reference Books

1. Harborne, J.B. Phytochemical Methods-A Guide to Modern Techniques of Plant Analysis, 3rd Ed., Springer Publication (2008)
2. Ahluwalia, V.K. and Madhu Chopra, Medicinal Chemistry, 2nd Ed., Ane Books Pvt. Ltd. (2018)
3. Ashutosh Kar, Medicinal Chemistry, 5th Ed., New Age International Publishers (2010)
4. Graham L. Patrick, An Introduction to Medicinal Chemistry, 4th Indian Ed., Oxford publishers (2009)
5. Krishnaswamy, N.R. Chemistry of Natural Products- An Unified Approach, 2nd Ed., Unified Press (2010)
6. Krishnaswamy, N.R. Chemistry of Natural Products-A Laboratory Handbook, 1st Ed., University Press India Pvt. Ltd. (2003)

Course Outcomes

1. Familiarization of phytochemical techniques -extraction, separation and purification
2. Understanding on principles of drug action
3. Correlate drug action with structure
4. Understanding the mechanism of action of antibiotics
5. Understanding of mechanism of action of cardiovascular drugs and anti malarials

CO / PO	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	H	M		H		L			L					M
CO 2	H	M						M	L		M			M
CO 3	H	M						M	L		M			M
CO 4	H	M							L		M			M
CO 5	H	M							L		M			M

Inorganic Chemistry Practical- II

Semester III
23MCHC17

Hours of Instruction/Week: 5
No. of Credits: 3

Objectives

1. To carry out quantitative inorganic analysis of mixture of salts
2. To get trained in qualitative analysis of less common metal ions
3. To acquaint with methods of estimation in quantitative analysis

Unit I 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 **55h**
Ions of less common metals: W, Se, Te, Mo, Bi, Sb, Ce, Th, Zr, Ti, V, Li

Unit II Quantitative Analysis

1. Analysis of alloys brass – complexometry (class work only)
2. Available chlorine in bleaching powder (class work only) **20h**

Course Outcomes **Total hours: 75**

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 colorimetry 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	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	H	M	H	H	M	M	M	M		M	M	H	M	M
CO 2	H	M	H	H	M	M	M	M		M	M	H	M	M
CO 3	H	M	H	H	M	M	M	M		M	M	H	M	M
CO 4	H	M	H	H	M	M	M	M		M	M	H	M	M
CO 5	H	M	H	H	M	M	M	M		M	M	H	M	M

Physical Chemistry Practical - II

Semester III
23MCHC18

Hours of Instruction/Week: 4
No. of Credits: 3

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

UnitI

1. Chemical Kinetics I-First order reaction
   i) Rate constant of the hydrolysis of methyl 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
   i) Two component systems – Simple Eutectic formation
   ii) Determination of CST of Phenol – water system. Effect of electrolyte KCl or Succinic acid on CST of Phenol – water system

30h

Unit II

Conductivity Studies

i) Conductometric titrations
   a) HCl-NaOH-HCl
   b) CH_3COOH-NaOH-CH_3COOH
   c) Na_2CO_3-HCl-Na_2CO_3
   d) KCl-$AgNO_3$-KCl
ii) Application:
   a) Verification of DHO equation
   b) Verification of Ostwalds dilution law
   c) Solubility of a sparingly soluble salt

30h

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. 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	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	H	M	H	M	M	M	M	H	M	M	M	H	M	M
CO 2	H	M	H	M	M	M	M	H	M	M	M	H	M	M
CO 3	H	M	H	M	M	M	M	H	M	M	M	H	M	M
CO 4	H	M	H	M	M	M	M	H	M	M	M	H	M	M
CO 5	H	M	H	M	M	M	M	H	M	M	M	H	M	M

Computational Chemistry

Semester III **Hours of Instruction/Week: 3**
23MCHC19 **No. of Credits: 5**

Objectives

1. To understand the theory behind computational chemistry
2. To get the knowledge about application of molecular properties in the study of reaction mechanism
3. Familiarize with software used in chemistry

Unit I

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 and molecular dynamics **9h**

Unit II

Concept of potential energy surfaces, Born-oppenhiemer approximation, stationary points, normal mode of vibrations, symmetry, geometry optimization **9h**

Unit III 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 **9h**

Unit IV Semi Empirical methods

Introduction to semi empirical (SE) methods-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 **9h**

Unit V Drawing chemical structures

ISIS & Chem draw, Molecular modeling software in chemistry-Hyperchem, GAMES, 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 and acidity, basicity of the molecules **9h**

Total hours: 45

Reference Books

1. Errol Lewars, Computational Chemistry Introduction to Theory and Applications of Molecular Mechanics, 2nd Ed., Kluwer publications (2011)
2. Christopher, J. Cramer, Essentials of Computational Chemistry Theories and Models, 2nd Ed., Wiley publishers (2004)
3. Frank Jensen, Introduction to Computational Chemistry, 2nd 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
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	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	H	M	L		L		M	M	M	L	M	L	L	
CO 2	H	M	L		L		M	M	M	L	M	L	L	
CO 3	H	M	L		L		M	M	M	L	M	L	L	
CO 4	H	M	L		L		M	M	M	L	M	L	L	
CO 5	H	M	L		L		M	M	M	L	M	L	L	

Environmental Chemistry (Self Study)

Semester III **Hours of Instruction/Week: 1**

23MCHC20 **No. of Credits: 4**

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

Unit I 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 **3h**

Unit II Water Quality Analysis and Control

Sources of water – molecular structure and physical properties – hydrogen Bonding – water as a solvent – quality characteristics of water - TDS,DO,BOD,COD,TOC,fluoride and chloride, analysis of CO by gas chromatography, NO by chemiluminescence and SO_2 by spectrophotometer - comparative account on physical and chemical properties of H_2O and D_2O. **3h**

Unit III 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

Unit IV Soil Chemistry

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 **3h**

Unit V 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 - 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 **3h**

Total hours: 15

Reference Books

1. Gopala Rao, M. and Marshall Sittig, Outlines of Chemical Technology - For the 21st Century, 3rd Ed., Affiliated East-West Press (1997)
2. Eugene W. Rice, Standard Methods for the Examination of Water and Wastewater, 22nd Ed., American Public Health Association, Washington (1998)
3. Metcalf and Eddy, Wastewater Engineering: Treatment, Disposal and Reuse, 3rd Ed., McGraw Hill Inc. New York (1991)
4. Prabhakar, V. K. Energy resources and the Environment, Anmol Publications Pvt. Ltd, Delhi, India (2001)
5. Des W. Connell, Basic Concepts of Environmental Chemistry, 2nd Ed., CRC Press, Taylor & Franics Group (2016)

6. Sharma, B.K. Industrial Chemistry: Including Chemical - Engineering, 16th Ed., Goel Publishing House, Meerut (2011)
7. Kaur, H. Environmental Chemistry, 12th Ed., Pragathi-Prakasan, (2018)
8. Eric Litchtouse, Jan Schwarzbauer, Didierobert, Environmental Chemistry, Springer (2009)
9. James E. Girarg, Principles of Environmental Chemistry, 3rd Ed., Jones & Bartlett Learning, (2013)
10. DE, A.K. Environmental Chemistry, 6th Ed., New Age International Pvt. Ltd. Publishers, (2006)
11. Balram Pani, I.K. Text Book of Environmental Chemistry, International Publishing House, (2007)
12. Sharma, B.K. Environmental Chemistry, 11th Ed., Krishna Prabash media (P) Ltd. (2007)

Course Outcomes

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	PO 7	PO 8	PO 9	PO 10	PO 11	PSO 1	PSO 2	PSO 3
CO 1	M	M				M		L	M	M	M	H		M
CO 2	M	M	L			M		L	M	M	M	H		M
CO 3	M	M	L			M		L	M	M	M	H		M
CO 4	M	M				M		L	M	M	M	H		M
CO 5	M	M				M		L	M	M	M	H		M