Department of Chemistry, School of Sciences

M.Sc. Chemistry

Two years Master Degree Programme

(Four Semester) (CBCS)

Semester	Code	Title of the Course	Semester End Exam	IA	Total	L	P	Credits
First Semester	MSCH101CCT	Coordination Chemistry	70	30	100	4	0	4
	MSCH102CCT	General Organic Chemistry	70	30	100	4	0	4
	MSCH103CCT	Physical Chemistry-1	70	30	100	4	0	4
	MSCH101DST MSCH102DST **Optional**	**Elective** 1.Green Chemistry 2. Organic Spectroscopy	70	30	100	4	0	4
	P-101	Coordination Chemistry	35	15	50	0	4	2
	P-102	Organic ChemistryPractical –I	35	15	50	0	4	2
	P-103	Physical Chemistry Practical–I	35	15	50	0	4	2
		Communicative English-1	35	15	50	2		2
		TOTAL	**420**	**180**	**600**	**18**	**12**	**24**
Second Semester	MSCH201CCT	Reaction mechanism in Coordination Compounds	70	30	100	4	0	4
	MSCH202CCT	Reaction mechanism and Reagents	70	30	100	4	0	4
	MSCH203CCT	Physical Chemistry-II	70	30	100	4	0	4
	Optional MSCH201DST MSCH203DST	**Elective** **1**.Introduction to Medicinal Chemistry **2**. Material Chemistry	70	30	100	4	0	4
	P-201	Preparation and gravimetric analysis of complex compounds	35	15	50	0	4	2
	P-202	Organic Chemistry Practical –II	35	15	50	0	4	2
	P-203	Physical Chemistry Practical-II	35	15	50	0	4	2
		Fundamental of Information Technology	35	15	50	2		2
		TOTAL	**420**	**180**	**600**	**18**	**12**	**24**

Semester	Code	Title of the Course	Semester End Exam	IA	Total	L	P	Credits
Third Semester	CHEM-301	Organometallic compounds	70	30	100	4	0	4
	CHEM-302	Name Reactions & Synthetic organic chemistry	70	30	100	4	0	4
	CHEM-303	Physical Chemistry-III	70	30	100	4	0	4
	CHEM-304 **Generic**	Bio-analytical and Forensic Chemistry	70	30	100	4	0	4
	P-301	Analytical method for qualitative and quantitative analysis	35	15	50	0	4	2
	P-302	Organic Chemistry Practical –III	35	15	50	0	4	2
	P-303	Physical Chemistry Practical-III	35	15	50		4	2
		Communicative English-II	35	15	50	2	-	2
		TOTAL	**420**	**180**	**600**	**18**	**12**	**24**
Fourth Semester		Inorganic polymers, Nuclear Chemistry and Bio-inorganic Chemistry	70	30	100	4	0	4
		Heterocyclic compounds and Natural products	70	30	100	4	0	4
		Physical Chemistry-IV	70	30	100	4		4
	Generic	Food Chemistry	70	30	100	4		4
		PROJECT	150 (Dissertation)	50 Viva	200	0	0	8 (Project)
		TOTAL	**430**	**170**	**600**	**16**	**0**	**24**
		GRAND TOTAL Credits				70		96

*Note: Student should opter 2 non-CGPA courses of 2 credits each across 4 semesters

TOTAL CREDITS = 24+24+24+24= 96

(**L** = Lecture, **P** = Practical, **IA**= Internal Assessment, **IAE**= Internal Assessment Examination,
SS / SL = Student Seminar / Seminar lecture presented by students, **SA**= Student Attendance, **SEE** = Semester End Examination)

4 Credits of Theory = 4 Hrs Teaching /week ;2 Credits of Practical = 4 Hrs/r week

M.Sc. Chemistry

M. Sc. I Semester

Paper Title: ***Coordination Chemistry***

Paper Code- MSCH101CCT **Credits: 4**

Objective:

This paper comprising of 4 units: i) quantitative treatment of crystal field theory (CFT); ii) Jahn-Teller effect and distortion in octahedral complexes; iii) molecular orbital theory (MOT) of octahedral complexes; and iv) electronic absorption spectra and magnetic properties of transition metal complexes.

Outcomes:

After studying this paper, students would be able to know about the following in details:

i) central idea of crystal field theory, crystal field splitting in different complexes and also calculation of crystal field splitting energy (CFSE) for different complexes; ii) Distortion in different complexes with reference to Jahn- Teller effect and calculation of Jahn-Teller stabilization energy for tetragonally distorted octahedral complexes of cupric ion (d^9 ion); iii) MOT theory in octahedral complexes and illing of MOs with electrons for strong and weak field ligands for d^n electrons (n =1 to 10) ion; and iv) Orgel diagram for d^1 to d^9 system in octahedral and tetrahedral complexes. Calculation of 10 DqRacahparameter. Knowledge of Nephelauxetic effect, and quenching of orbital magnetic moment. Effect on magnetic moment of complexes, Effect on magnetic moment by M-M bond, super exchange and spin-spin cross over in the complexes optically active chelates.

Unit-I: Quantitative treatment of Crystal field theory (CFT)

Introduction and characteristics feature of CFT, Crystal field splitting in octahedral, tetrahedral and square planar complexes. Distribution of d^n electrons (n= 0 to 10) in t_{2g} and e_g orbitals in octahedral, tetrahedral and square planar complexes. Calculation of crystal field stabilisation energy (CFSE) values of d^n systems (n= 0 to 10) for octahedral, tetrahedral and square planar complexes with respect to weak and strong field ligands. Relation between Δ_s, Δ_o and 10 Dq.

Unit-II: Jahn-Teller effect and distortion in octahedral complexes

Distorted octahedral complexes, types of distortion in octahedral complexes with suitable examples, Types of distortion in octahedral complexes. Jahn-Teller effect. Distortion shown by specific octahedral complexes. Conditions for no, slight and large distortion. Splitting of

t_{2g} and e_g orbitals in tetragonally elongated and compressed octahedral complexes of cupric ion.; lowering of molecular symmetry. Calculation of Jahn-Teller stabilization energy for tetragonally distorted octahedral complexes of cupric ion (d^9 ion). Interpretation of the electronic absorption spectrum of $[Cu(OH)_6]^{2+}$ on the basis of jahn – Teller effect.

Unit-III: Molecular orbital theory (MOT) of octahedral complexes

Introduction, Central idea of MOT, Formation of Sigma molecular orbitals (MOs) in octahedral complexes, Order of energy level of different MOs. Filling of MOs with electrons for strong and weak field ligands for d^n electrons (n =1 to 10) ion; $[Ti(H_2O)_6]^{3+}$ $[Co(NH_3)_6]^{3+}$, $[CoF_6]^3$Sigma (σ) and pi (π) bonding in octahedral complexes for $[FeF_6]^{3-}$.

Unit-IV: Electronic absorption spectra and magnetic properties of transition metal complexes

Ground state term, symbol, splitting of ligands. Rules for electron transition. Orgel diagram for d^1 to d^9 system in octahedral and tetrahedral complexes. Calculation of 10 DqRacahparameter. Nephelauxetic effect and nature of bond in complexes. Charge transfer of redox spectra with special reference to M-L and L-M, CT spectra, anomalous magnetic moment of complexes, Quenching of orbital magnetic moment. Effect on magnetic moment of complexes, Effect on magnetic moment by M-M bond, super exchange and spin-spin cross over in the complexes optically active chelates.

Reference Books:

1. New Concise Inorganic Chemistry by J.D. Lee Edition III Compton Printing Ltd London.

2. Principles of Inorganic Chemistry by HR Puri, R. Sharma & S.P. Jauhar, Vishal Publications Jalandhar.

3. Modern Aspects of Inorgaic Chemistry by H.J. Emelens and Sharpe A.G., The English Language Book Society and Rouledge& Kegan Paul.

4. Inorganic Chemistry, Principles of Structure and Reactivity by James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Edition IV, Pearson Education Press.

M.Sc. Chemistry

M. Sc. I Semester

Paper Title: *Volumetric Analysis*

Paper Code: 150 CCP **Credits: 2**

Objective

This paper consists of i) titrimetric analysis which includes the study of calibration and use of apparatus and preparation of various solution of different concentration (M/N), acid-base titration and oxidation- reduction titrimetric.

Outcomes

After studying this paper, students would be able to know:

1. How are apparatus handled and calibrated.
2. How are solutions prepared of different concentration.
3. How are carbonate, hydroxide and bicarbonate estimated when present together in a mixture, and also estimation of free alkali in different samples of soaps and detergents.
4. How are iron (II) are estimated using either $KMnO_4$ or $K_2Cr_2O_7$ solution and also estimation of oxalic acid and sodium oxalate in a given mixture.

A: Titrimetric Analysis

1. Calibration and use of apparatus.
2. Preparation of solutions of different concentration (Molarity/Normality of titrants

B: Acid- base Titrations

1. Estimation of carbonate and hydroxide present together in mixture.
2. Estimation of carbonate and bicarbonate present together in a mixture.
3. Estimation of free alkali present in different soaps/detergents

C: Oxidation-Reduction Titrimetry

1. Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.
2. Estimation of oxalic acid and sodium oxalate in a given mixture.
3. Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

M.Sc. Chemistry

M. Sc. I Semester

Paper Tile: *Organic Chemistry-I*

Paper Code- **Credits: 4**

Course Objective

1. Understand bonding, hybridization, resonance, and physical properties of organic molecules.
2. Learn reaction mechanisms, intermediates, and their stability.
3. Develop knowledge of stereochemistry and optical activity.
4. Explore the chemistry, synthesis, and reactivity of organic functional groups.

Course Outcome

1. Explain bonding concepts, resonance, and physical properties.
2. Analyze reaction mechanisms and stability of intermediates.
3. Interpret stereochemical representations and optical activity.
4. Identify synthesis and reactivity patterns of functional groups.

Unit-I: Bonding and Physical Properties of Organic Molecules

Nomenclature of simple organic compounds (acyclic, cyclic). Concept of hybridization, resonance, orbital pictures of bonding (sp^3, sp^2, sp, C-C, C-N & C-O system).Inductive effect, bond polarization, and polarizability, steric inhibition of resonance. Hückel's rules for aromaticity & antiaromaticity, homoaromaticity. Physical properties of bond distance, bond angles, mp/bp& dipole moment in terms of structure and bonding. Concept of acids and bases: effect of structure, substituent and solvent on acidity and basicity.

Unit-II: Basic Reaction Mechanism and Intermediates

Mechanism classifications - ionic, radical and pericyclic; heterolytic bond cleavage and heterogenic bond formation, homolytic bond cleavage and homogenic bond formation; representation of mechanistic steps using arrow formalism. Reactive intermediates: carbocation, carbanions, carbon radicals, carbenes-structure using orbital picture, electrophilic/nucleophilic behavior, stability, generation and fate (elementary idea).

Unit-III: Optical Activity and Stereochemistry

Representation of molecules in saw-horse, Fischer, flying-wedge and Newman formulae and their inter translations, symmetry element and molecular chirality. Configuration: stereogenic unit i) stereocenters: systems involving 1, 2, 3 centers, stereogenicity, chirotopicity, pseudoasymmetric (D/L and R/S) descriptor, threo/ erythro / meso and syn/anti nomenclature. Stereo axis: chiral axis in allenes& biphenyls, R/S descriptor: cis/trans, syn/anti, E/Z descriptors (at C=C and C=N bonds). Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), racemic compounds.

Unit- IV: Chemistry of Organic Functional Groups

Alkanes, olefins, alkynes, halides, alcohols, phenols, ketones, aldehydes, carboxylic acids, ethers, derivatives of carboxylic acids, amines, nitro and cyano compounds; synthesis and basic reactivity with mechanisms.

Reference Books:

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, PearsonEducation.
2. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
3. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
4. I. L. Finar, Organic Chemistry, Vol-1, 6th edition, Pearson Education.
5. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley.

M.Sc. Chemistry

M. Sc. I Semester

Organic Chemistry Practical–I

Paper Code- P-102 **Credits: 2**

Course Objective

1. Develop skills in separation and purification of organic compounds.
2. Apply purification techniques like crystallization, distillation, and chromatography.
3. Identify functional groups through chemical reactions.
4. Use chemical and spectral methods for compound identification

Course Outcome

1. Perform separation and purification of organic compounds.
2. Utilize various purification techniques effectively.
3. Conduct solubility tests for classification.
4. Identify functional groups through characteristic reactions.
5. Analyze unknown compounds using spectral and chemical methods.

List of Experiments:

1. Separation and purification of organic compounds, melting point and boiling point of some common Organic compounds.
2. Purification Techniques: Crystallization, Decolourization, fractional crystallization, Sublimation, Simple distillation, Fractional distillation, Vacuum distillation and Steam distillation, Isolation and purification of products by chromatographic techniques: TLC &Column Chromatography, Solubility tests for organic compounds
3. Characteristic reactions of functional groups. Identification of unknowns - chemical andspectral methods.

Reference Books:

1. Organic Chemistry Lab manual,

2. Practical Organic Chemistry-G. Mann & B.C Saunders, ELBS Edition and Longman Group Limited, 2002.

M.Sc. Chemistry

M. Sc. I Semester

Paper Title: *Physical Chemistry–I*

Paper Code: **Credits: 4**

Course Objectives:

This course aims at to accustom the students the basic concepts of thermodynamics, Equilibrium and Non-Equilibrium Thermodynamics along with the non-ideal systems. To study the partial molar property, fugacity and its significance and statistical thermodynamics.

Course Outcomes:

After completion of this course successfully, the students will be able to

1. Get basic idea about fundamental laws of thermodynamics
2. Learn applications of equilibrium thermodynamics
3. Be introduced about the non-equilibrium thermodynamics
4. be introduced about the fundamentals of statistical thermodynamics
5. Learn the application of the concept of partition function

Unit-I: Basic Thermodynamics

Brief description of the laws of thermodynamics, Concepts of Entropy and Residual Entropy, Free energy and its Temperature dependence, Thermodynamic Equilibria and Free Energy Functions, Physical Equilibria Involving Phase Transitions, Thermodynamic Maxwell Relations.

Unit-II: Equilibrium Thermodynamics

Chemical potential and Entropies, Partial molar quantities: Partial molar free energy, Partial molar volume and Partial molar heat content and their significances. Determinations of the partial molar quantities. Thermodynamic Functions of Mixing, Non-ideal systems: Excess functions for non-ideal solutions.

Unit-III: Non-Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, Basic Postulates and Methodology, Onsager's Theory, Phenomenological Laws and Equations, Transformations of the generalized fluxes and forces, Microscopic Reversibility and Onsager's Reciprocal Relations, Entropy Production and entropy flow, Theorem of Minimum Entropy Production, Chemical Reactions, Coupled Reactions and Electro-kinetic Phenomena.

Unit-IV: Statistical Thermodynamics

Concept of distribution, Thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition function - Translational, Rotational, Vibrational and Electronic partition functions, calculation of thermodynamic properties in terms of partition function. Applications of partition functions. Heat capacity behaviour of solids - Chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics - distribution law and application to helium

Reference Books:

1. Thermodynamics for Chemists by S. Glasstone.
2. Atkin's Physical Chemistry by Peter Atkins and Julio de paula.
3. An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R. Mishra, Vikas Publishing House Pvt. Ltd. Quantum Chemistry by Ira N. Levine.
4. Statistical Thermodynamics (Hardback) By (author) M.C. Gupta, Publisher: New Age International.
5. Thermodynamics, J. Rajaram and J.C. Kuriacose, Educational Publishers.
6. Thermodynamics, R. C. Srivastava, Subit K. Saha, Abhay K. Jain, Prentice Hall of India, Pvt. Ltd.
7. Physical Chemistry, T. Engel and P. Reid, Pearson Education and Dorling Kindersley (India) 2006.
8. Physical Chemistry, Statistical Mechanics, HoriaMetiu, Taylor & Francis, 2006 (530.13 MET 276461)

M.Sc. Chemistry

M. Sc. I Semester

Paper Title: *Physical Chemistry Practical–I*

Paper Code- **Credits: 2**

Course Objectives:

To train the students about determination of heat of reaction, partial molar volume, solubility of compound, construction of phase diagram.

Course Outcomes:

After completion of this course successfully, the students will be able to

1. Understand how to determine heat of reaction
2. Determination of partial molar volume
3. Determination solubility of compound
4. Construction of phase diagram.

List of Experiments:

1. Determine the heats of reaction for the reactions: (i) $CO_3^{2-} + H_2O \rightarrow HCO_3^- + OH^-$ (ii) $HC_2O_4^- + H_2O \rightarrow H_2C_2O_4 + OH$
2. Determination of partial molar volume of solute (e.g.,KCL) and solvent in a binary mixture
3. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.
4. Find out the dimerization constant of benzoic acid in benzene by titration method
5. Construct the phase diagram of water-ethanol-benzene system

6. Find out the molar mass of succinic acid by partition method
7. To determine the surface tension of a liquid by stalagmometer (drop number method)

Reference Books:

1. Vogel's Textbook of Quantitative Analysis, revised. J. Bassett. R. C. Denney, G. H. Jeffery and J. Mendham, ELBS .
2. Practical Physical Chemistry, A. M. James and F, E. Prichard. Longman
3. Findley's Practical Physical Chemistry, B. P. Levitt. Longman.
4. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
5. Experimental Physical Chemistry – F. Daniels et al.

M.Sc. Chemistry

M. Sc. I Semester

Elective Optional 1: *Paper Title: Green Chemistry*

Paper Code- **Credits: 4**

Course Objectives

This course introduces the principles and practices of green chemistry, responding to growing environmental concerns. It promotes sustainable and environmentally friendly chemical processes. Students will learn the basic concepts, goals, and principles of green chemistry, along with its limitations. Students will learn various techniques and their significance in laboratories and industries. The students will understand the applications of renewable raw materials and green processes in sustainable chemical processes. The students will develop critical thinking and problem-solving skills to address environmental and sustainability challenges.

Course Outcomes

Upon completing this course, students will be able to understand the need for green chemistry and its principles to address environmental and sustainability challenges. The students will develop critical thinking and problem-solving skills to implement green chemistry in solving real world challenges. The students will learn the significance and applications of renewable resources and green chemistry methodologies such as microwave-assisted synthesis for cost effective and eco-friendly transformations.

Unit-I: Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry.Definition, Concepts and basic principles of green chemistry.Goals of Green Chemistry.Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit-II: Principles of Green Chemistry and Microwave Assisted Organic Synthesis

Twelve principles of Green Chemistry with their explanations and examples. Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions _ Functional group transformations – condensations reactions – oxidations – reductions reactions.

Unit-III: Green Catalysis and Future trends in Green Chemistry

Introduction to solid acid catalysts and their significance in industrial applications; phase-transfer catalysis, Oxidation reagents and catalysts; Biocatalysis: basic principles, enzyme catalysed reactions, Photocatalysis: Introduction and significance with examples. Renewable Raw Materials: Carbohydrates, Ethanol, Lactic acid.

Unit-IV: Applications of Green Chemistry

Applications of phase transfer catalysis. Applications: environmental, solvents, time and energy benefits. Green synthesis of ibuprofen, design and use of CO2-surfactants for precision cleaning in industries. Green chemistry process for polyester regeneration.

Reference Books:

1. P.T.Anastas and J.C.Warner, *Green Chemistry:Theory and Practice,* Oxford University, a. Press,1998.
2. *Green separation processes, methods and application*, Fonso, National Scientific Book Agency, Delhi-110053.
3. Sauer, N. N. (2000). *Green Chemistry: Frontiers in Benign Chemical Syntheses and Processes* Ed. Anastas P. T., and Williamson T. C., (US Environmental Protection Agency). Oxford University Press: New York, NY.
4. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
5. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

M.Sc. Chemistry

M. Sc. Ist Semester

Elective Optional 2: *Paper Title: Organic Spectroscopy*

Paper Code- **Credits: 4**

Course Objectives

This course aims to provide students with a comprehensive understanding of various spectroscopic techniques, including Electronic and Infrared Spectroscopy, NMR Spectroscopy, 13C-NMR Spectroscopy, and Mass Spectrometry. Students will learn the fundamental principles, instrumentation, and applications of these techniques in structural elucidation of organic compounds.

Course Outcomes

On the completion of this course, students will be able to apply the principles of Electronic and Infrared Spectroscopy to analyse and identify functional groups and structures in organic compounds. The students will be able to interpret NMR spectra including chemical shifts, coupling constants, spin systems and nuclear Overhauser effects for structural elucidation. The students will identify and apply 13C-NMR Spectroscopy using chemical shift effects, proton coupling, and techniques like off-resonance decoupling to determine the structure of organic compounds. The students will understand the principles of mass spectra of various organic compounds, including ion formation, fragmentation modes, and characteristic patterns for different functional groups. The students will have the knowledge and skills to elucidate the structure of unknown organic compounds by integrating data from electronic, IR, NMR and mass spectra demonstrating proficiency in spectral interpretation.

Unit-I: Electronic and Infrared Spectroscopy:

Theory of electronic and IR spectroscopy (revision of the basic concepts/solving problems). Application of electronic and IR spectroscopy in structural elucidation of organic compounds (various functional classes to be considered).

Unit-II: NMR Spectroscopy

Principles of NMR, instrumentation, chemical shift- (revision of the basic concepts); Interpretation of PMR spectra. a) Coupling constants and AB, A_2B_2/A_2X_2, AMX and ABX spin systems.

1. Double resonance and decoupling.

2. Nuclear Overhauser Effect and its applications.
3. NMR Shift reagents

Unit-III: ^{13}C –NMR Spectroscopy

Introduction, 13C- chemical shifts effects (α-, ß-, γ-, δ-substituent effects, π-conjugation, heavy atom effect and ring size effects), proton coupled and proton decoupled ^{13}Cspectra. Off-resonance decoupling, APT & DEPT techniques.

Unit-IV: Mass Spectrometry

Even and odd electron ions and fragmentation modes a) McLafferty rearrangement and retro-Diels-Alder fragmentation. b) Mass spectra of compounds like alcohols, amines, ethers carbonyl compounds, hydrocarbons, halogen compounds, nitro compounds and cyanides.

Reference Books:

1. P.S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., 1995, 2nd Ed.
2. J. R. Dyer, Applications of Absorption Spectroscopy of Organic compounds, Prentice Hall of India, 1987.
3. R.M. Silverstein, F. X. Webster, Spectrometric Identification of Organic compounds, John Wiley & Sons Inc., 2011, 7th Ed. (reprint).
4. V.M. Parikh, Absorption Spectroscopy of Organic Molecules, Addison Wesley Longman Publishing Co., 1974.
5. D.H Williams & I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata Mcgraw Hill Education, 2011, 6th Ed.
6. William Kemp, Organic Spectroscopy, Palgrave Macmillan, 1991, 3rd Ed.
7. William Kemp, NMR in Chemistry: A Multinuclear Introduction, Macmillan, 1986.
8. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R.

M.Sc. Chemistry

M. Sc. IInd Semester

Paper Title: ***Reaction mechanism in Coordination Compounds***

Paper Code: MSCH201CCT **Credits: 4**

Course Objective:

This paper comprising of 4 units: i) Basic concepts of inorganic reaction mechanism ii) Ligand substitution reactions in octahedral complexes iii Ligand substitution reactions in square planar complexes and iv) Electron transfer (or Oxidation -Reduction) reaction

Course Outcomes:

After studying this paper, students would be able to know about the following in details:

i) basic terminology applicable to inorganic reaction mechanism, labile and inert octahedral complexes theory, factors affecting the lability of complex, transition state (activated complexes and calculation of crystal field activation energy(CFAE), ii) mechanism of nucleophilic substitution reaction in octahedral complexes and factors affecting the mechanism, Anation reactions, substitution reactions without breaking metal-ligand bond, iii) mechanism of nucleophilic substitution reaction in square planar complexes and factors affecting the mechanism, trans- effect and its application, and also Chatt and Orgel pi-bonding theory and iv) study of electron transfer reaction with mechanism of one-electron transfer reactions-outer sphere and inner sphere mechanisms (ligand bridged process), factors affecting the rates of direct electron transfer reactions and two-electron transfer reactions-complimentary and non-complimentary reactions.

Unit-I: Basic concepts of Inorganic Reaction Mechanism

Substrate, attacking reagents-electrophilic and nucleophilic, types of substitution reactions-nucleophilic or ligand substitution (SN) and electrophilic or Metal substitution (SE) reactions. Labile and inert octahedral complexes, interpretation of lability and inertness of transition metal complexes - Valence Bond and Crystal Field theories, factors affecting the lability of complex, transition state or activated complexes. Calculation of crystal field activation energy (CFAE).

Unit-II: Ligand substitution reactions in Octahedral Complexes

Mechanism of unimolecular and bimolecular nucleophilicsubstituitionreaction (S_N1 and S_N2) in octahedral complexes , acid hydrolysis, mechanisms of acid hydrolysis, factors affecting

the mechanism, base hydrolysis and its mechanism. in octahedral complexes. Anation reactions, substitution reactions without breaking metal-ligand bond.

Unit III: Ligand substitution reactions in square planar complexes

S_N1 and S_N2 mechanism in Pt(II) complexes, factors affecting the rate of substitution reactions in square planar complexes, trans-effect, theories of trans-effect-Grinberg's electrostatic polarization theory and Chatt and Orgel pi-bonding theory, application of trans-effect.

Unit-IV: Electron Transfer (or Oxidation -Reduction) Reaction

Introduction, types of electron transfer reactions in complex compounds, mechanism of one-electron transfer reactions-outer sphere and inner sphere mechanisms (ligand bridged process), factors affecting the rates of direct electron transfer reactions, two-electron transfer reactions-complimentary and non-complimentary reactions.

Reference Books:

1. Advance Inorganic Chemistry, Cotton and Willkinson.
2. New Conise Inorganic Chemistry, Fifth Edition, J.D. Lee.
3. Principles and Structure and Reactivity, James, E. Huheey.
4. Modern Coordination Chemistry, Lewis and Wilkins.

M.Sc. Chemistry

M. Sc. IInd Semester

Paper Title: *Inorganic Chemistry –II LAB*

Paper code: 201 CCP **Credits: 2**

Course Objective

This paper consists of i) preparation of complexes of different metals such as tetraamminecopper (II) sulphate, Cis and trans $K[Cr(C_2O_4)_2.(H_2O)_2]$, tetraamminecarbonatocobalt (III) ion and potassium tris(oxalate) ferrate(III); and ii) Gravimmetric analysis which includes estimation of nickel (II) using Dimethylglyoxime (DMG), estimation of copper as CuSCN, estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$ and estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminiumoxinate).

Course Outcome

After studying this paper, students would be able to know the procedure of the following experiments in details:

Lab Experiment

1. How are complexes of Cu like tetraamminecopper (II) sulphate, Cr like and trans $K[Cr(C_2O_4)_2.(H_2O)_2]$, Co like tetraamminecarbonatocobalt (III) ion and and Fe like potassium tris(oxalate)ferrate(III) prepared .

1. How is gravimmetric analysis done and how are estimation of

    i) nickel (II) using dimethylglyoxime (DMG); ii) copper as CuSCN; iii) iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$ and Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminiumoxinate).

M.Sc. Chemistry

M. Sc. IInd Semester (Organic Chemistry)

Paper Title: ***Reaction mechanism and Reagents (Theory)***

Paper Code: L-T-P: 4-0-0 **Credits: 4**

Course Objectives:

The student will gain a deep understanding of the fundamental principles of organic name reaction and their mechanism, electrophile, nucleophile and free radicals, name of reagents, and its application for the oxidation and reduction of reaction, different name rearrangement reaction.

Course Outcomes:

After completion of the course student will be able to understand:

1. about principles and application of different basic and organic name reaction and their reaction mechanism.
2. about electrophile, nucleophile, and free radical.
3. about reagent and their application in different name reaction and for oxidation and reduction reaction.
4. about different rearrangement reaction (Beckmann and Hoff-Mann Rearrangement, etc.)

Unit-I: Addition to carbon- carbon multiple bond

Types of addition reaction, Electrophilic, nucleophilic and free radical addition reaction. Mechanism and stereochemical aspects of all types of addition reaction. Michael addition, Sharpness asymmetric epoxidation.

Unit-II: Addition to carbon- hetero multiple bond

Addition of Grignard reagents to carbonyl compounds, carboxylic acid, ester and nitriles. Addition of organo-zinc and lithium to carbonyl and unsaturated carbonyl compounds (Wittig reaction and reformats Ky reaction). Mechanism of some condensation reaction involving enolate formation like Aldol, Perkins, Knoevenagel, Claisen, benzoin and stobbe reaction).

Unit-III: Rearrangements

General knowledge of some mechanistic terminology such as nature of migration, migratory aptitude and memory effect. Beckmann and Hoff-Mann Rearrangement, Pinacol-pinacolone and Fries Rearrangement.

Unit-IV: Reagents used for oxidation and reduction reactions

Oxidation: PCC, PDC, Collins's reagents, chromyl chloride (Étard reaction), SeO_2, $KMnO_4$, HIO_4 and Osmium tetra oxide. Tollen's reagent, Feeling solution and Benedict solution.

Reduction: $LiAlH_4$, $NaBH_4$, HI Dibal-H, Rosenmund reduction, Clemmensen reduction, Wolfkishner reduction.

Reference Books:

1. T. W. Greens, P. G. M. Wuts. Protective groups in Organic synthesis, 3rd /4 th Ed. John Wiley & Sons, INC
2. Organic chemistry- Clayden, Greeves, Warren and Wothers
3. Advance organic chemistry by Jerry March
4. Advance organic chemistry by Carey and Sundberg,
5. Advance organic chemistry by Francis A. carey
6. Designing Organic Synthesis, S. Warren, Wiley.
7. Organic Synthesis- Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlage VCH

M.Sc. Chemistry

M. Sc. IInd Semester (Organic Chemistry)

Paper Title: *Reaction mechanism and Reagents (Lab)*

Paper Code: L-T-P: 4-0-2 **Credits: 2**

Course Objective:
This course is designed basically to learn the presence of extra element in an organic compound, functional group, qualitative analysis of organic compounds, Identification f compounds using IR spectroscopy.

Course Outcome:
After completion of the syllabus, students would be able to
Identification of extra elements (N, S, both N & amp; S, Halogen) present in organic compounds followed by the preparation of Lassigne solution.
Identification of functional groups present in organic compounds.
Qualitative analysis of organic compounds.
Preparation of acetanilide using aniline.
Identification of organic compounds using IR spectroscopy.

Experiment No 1: Preparation of Lassaige solution and detection of extra elements present in organic compounds.
Experiment No 2: Identification of functional groups present in organic compounds.
Experiment No 3: Qualitative analysis of organic compounds.
Experiment No 4: Preparation of acetanilide using aniline.
Experiment No 5: Identification of Compounds using IR spectroscopy.

M.Sc. Chemistry

M. Sc. IInd Semester

Paper Title: *Physical Chemistry–II*

Paper Code: **Credits: 4**

Course Objectives:

To equip students with various concepts of electrochemistry, electro analytical techniques and Theories and basic concepts of Chemical kinetics - mechanism of acid, base and enzyme Catalysis reaction.

Course Outcomes:

After completion of this course successfully, the students will be able to

1. Understand different aspects of Electrochemistry
2. Get the fundamentals of electrochemistry and electrochemical cells
3. Impart knowledge on the fundamentals of chemical kinetics
4. Study the kinetics of different types of reactions and methodologies
5. Understanding rate laws based on Chemical Kinetics

Unit– I: Electrochemistry – I

Reversible cells – Chemical cells and concentration cells – Types of reversible electrodes – Electrode potentials. Reactions in reversible cells – Nernst equation – thermodynamic and kinetic derivation – Concentration cells with and without transference. Liquid junction potential and its determination.

Potentiometric titrations – Determination of pH, Solubility product from EMF measurements.

Theory of electrolytic conductance – Debye - Huckel Onsager equation and its verification – Wein effect. Conductometric titrations, Determination of solubility of a sparingly soluble salt.

Unit-II: Electro Chemistry – II

Concept of activity and activity coefficient of an electrolyte. The mean ionic activity coefficient. Calculation of mean ionic activity coefficients. Debye Huckel theory of solutions. Debye Huckel Limiting law and its verification.

Electrode polarization – Decomposition potential and over voltage. Influence of C.D. on over voltage. Influence of P^H on over voltage, influence of temperature on over voltage – Theories of over – voltage. Hydrogen over – voltage.

The Deposition and corrosion of metals: Physical nature of electrodeposited metals – 1) Current density 2) Concentration of electrolyte 3) Temperature 4) Colloidal matter 5) Electrolyte 6) Basis metal. Throwing power separation of metals by electrolysis. Electrochemical passivity. Theories of passivity. Corrosion of metals. Hydrogen evolution type.

Unit-III: Chemical Kinetics – I

Theories of reaction rates – Collision theory, steric factor. Theory of Absolute Reaction Rates – Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reaction rates.

Unimolecular reactions – Lindeman's theory – Brief explanation of HKRR and Slater's treatments. Termolecular reactions. Complex reactions – Rate expressions for opposing, parallel and consecutive reaction (all first order type).

Chain reactions: General Characteristics, Steady State treatment $H_2 – I_2$, H2 – Br_2, H2 – Cl_2 reactions. Comparison of hydrogen halogen reactions. Rate expressions for chain reactions

Unit-IV: Chemical Kinetics – II

Homogeneous catalysis. Mechanism of catalysis. Equilibrium treatment. Steady state treatment. Acid base catalysis: Mechanism of acid base catalysis. Catalysis by enzymes. Influence of P^H. MicholisMenton law. Influence of temperature. Examples. Decomposition of acetaldelyde catalysed by Iodine. Catalysed decomposition of hydrogen peroxide.

Free radicals in chemical reactions. Hydrogen oxygen reaction. Upper and lower explosion limits. Heterogeneous reactions. Bimolecular reactions. Adsorption. Langmuir adsorption isotherm. Electronic theories of chemisorption and heterogeneous catalysis.

Introduction to enzyme catalysis. Michales – Menton Kinetics – Effect of pH and effect of temperature on the rates of enzyme reactions.

Reference Books:

1. Atkin's Physical Chemistry by Peter Atkins and Julio de paula.
2. Introduction to Electrochemistry by S. Glasstone
3. Chemical Kinetics by K.J. Laidler.
4. Text Book of Physical Chemistry by Levine.

M.Sc. Chemistry

M. Sc. IInd Semester

Paper Title: *Physical Chemistry Practical–II*

Paper Code: **Credits: 2**

Course Objectives:

To train the students about determination of order of the reaction and energy of activation, solubility product of sparingly soluble salt and strength of acids by conductrometrically, determination of strengths of halides and valency of mercurous ions potentiometrically

Course Outcomes:

After completion of this course successfully, the students will be able to

1. Understand how to determine order of the reaction and energy of activation
2. Determination of solubility product of sparingly soluble salt
3. Determination of strength of acids by conductrometrically
4. Determination of strengths of halides and valency of mercurous ions potentionmetrically

Experiments

1. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
2. Determination of solubility and solubility product of sparingly soluble (e.g., PbSO4, BaSO4) conductometrically.
3. Determination of the strength of strong and weak acids in a given mixture conductometrically.
4. Determination of strengths of halides in a mixture potentionmetrically
5. Determination of the valency of mercurous ions potentiometerically.
6. Determination of the strength of strong and weak acids in a given mixture using a potentiometer / pH meter.
7. Determination of pKa of dibasic acid (Oxalic acid)
8. Determination of hydrolysis constant of aniline hydrochloride

9. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reaction.
10. To investigate the auto-catalytic reaction between potassium permanganate and oxalic acid.
11. Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media
12. . Determination of energy of activation of acid catalyzed hydrolysis of an ester.

Reference Books:

1. Findlay's Practical Physical Chemistry by J.A. Kitchnar
2. . Text-book of Quantitative Inorganic Analysis including elementary Instrumental Analysis- A.I.Vogel, Revised by J.Bassott, R.C.Banney
3. Experimental Physical Chemistry – F.Daniels&J.Williams
4. Experimental Physical Chemistry – R.C.Das&B.Behra
5. Systematic experimental Physical Chemistry by- Rajbhoj and Chondhekar.
6. Experimental physical Chemistry- V.D. Athawale and P. Mathur
7. Advanced practical physical Chemistry- J. B. Yadav
8. Advanced physical Chemistry Experiments- Gurtu and Gurtu

M.Sc. Chemistry

M. Sc. IInd Semester

Elective: Optional 1/Paper Title: *Introduction to Medicinal Chemistry*

Paper Code: **Credits: 4**

Course Objectives

This course provides a comprehensive introduction to medicinal chemistry, focusing on the discovery, design, and development of drugs. Students will learn about natural sources of drugs, their origin, synthetic approaches, and procedures involved in drug development and approval. Students will learn the principles of drug design and consequences of drug-receptor interactions. Students will understand the role of medicinal chemists in designing and synthesizing new drug molecules. Students will learn the synthesis, mechanism of action, and structure-activity relationship (SAR) of various drug classes (local anaesthetics, analgesics, antiepileptics, and cardiovascular agents).

Course Outcomes

By the end of this course, the students will be able to **o**utline the strategy for discovery of drugs from different sources and its application in pharmacological research and practice. They will be able to describe modern techniques in drug discovery and development. They can summarize the history and steps involved in the production of natural products and describe neurotransmitters in relation to the interaction of agonist and antagonists with the receptor. The student will recognize different methods and techniques during different phases of drug discovery and development. The students will identify the safest use of the different classes of drugs in nervous and cardiovascular system disorders.

Unit-I: Introduction to Drugs

Requirement of an ideal drug, Sources of drugs, Important terms used in chemistry of drugs, Classification and nomenclature of drugs.

Unit-II: Drug Design

Analogues and pro-drugs, Concept of lead compounds, features governing drug design – The method of variation, drug design through disjunction, conjunction, tailoring of drugs, Cimetidine – a rational approach to drug design.

Unit-III: Drug Development and Drug Action

Screening of natural products, isolation and purification, structure determination, Structure-activity relationship, QSAR, Synthetic analogues, Natural Products as leads for new pharmaceuticals, Receptor theories, Oxaminiquine – a case study.Mechanism of drug action.

Unit-IV: Study of The Following Class of Major Drugs:

Local anaesthetics, Analgesics: Narcotic and non-steroidal anti-inflammatory, narcotic antagonists (Mechanism of Action and Synthesis of Ibuprofen), Antiepileptic drugs

Cardiovascular agents: Cardiovascular diseases, Antianginal agents and vasodilators, Antihypertensive agents.

Reference Books:

1. R. F. Doerge, Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Edited by, J. B. 65Lippincott Company, Philadelphia, USA, 8th Ed.
2. M. E. Wolff, Burger's Medicinal Chemistry, Part I and II, John Wiley, 4th Ed.
3. W. O. Foye, Principles of Medicinal Chemistry, K. M. Varghese and Co., Bombay, 3rd Ed.
4. Lednicer&Mitscher, Organic Chemistry of Drug Synthesis Vols I and II, John Wiley.
5. Graham Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, Oxford, 1998.
6. D. J. Abraham, Burgers Medicinal Chemistry and Drug Discovery, Vol. I, John Wiley and Sons, New Jersey, 2003, 6^{th} Ed.

M.Sc. Chemistry

M. Sc. IInd Semester

Elective Optional 2/ Paper Title: *Material chemistry*

Paper Code: **Credits: 4**

Course Outcomes:

1. Understand the fundamentals, scope, and significance of material chemistry.
2. Explore material structures, bonding, defects, and their impact on properties.
3. Learn various synthesis and processing techniques for materials.
4. Familiarize with advanced material characterization methods.
5. Classify different material types and their structure-property relationships.
6. Examine applications and emerging trends in materials science.

Course Outcomes:

1. Explain material chemistry principles and their technological relevance.
2. Analyze bonding, structure, and properties of materials.
3. Demonstrate knowledge of material synthesis and processing methods.
4. Utilize characterization techniques for material analysis.
5. Differentiate and evaluate various classes of materials.
6. Identify applications in electronics, biomedical, energy, and environment.
7. Recognize emerging trends like 2D materials and AI in materials science.

Unit-I: Introduction, Structure and Properties Of Materials

Definition and scope of Material chemistry, Historical background, importance ofmaterial chemistry in modern technology, interdisciplinary nature of materials science, types of bonding in materials, crystal structures and defects, X-ray diffraction, transmission electron microscopy, Physical properties- density, thermal expansion, thermal conductivity, electrical properties; mechanical properties- strength, ductility, toughness, hardness; thermal properties, electrical properties, magnetic properties, optical properties.

Unit-II: Synthesis and Processing Of Materials

synthesis of materials by sol-gel method, hydrothermal method, precipitation method, electron beam evaporation method, physical vapor deposition method, chemical vapor deposition method, thin film deposition techniques method, solid state reaction, mechanical processing, ion implantation.

Unit-III: Characterisation and Classes Of Materials

X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), Auger electron microscopy (AEM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray photoelectron spectroscopy, metals, ceramics, polymers, composites, semiconductors, nanomaterials

Unit-IV: Applications and Emerging Trends of Materials Science

Graphene and other 2D materials, topological insulators, skyrmions and other novel magnetic materials, artificial intelligence in materials science, electronic application, biomedical application, energy application, environmental applications, optical applications.

M.Sc. Chemistry

M. Sc. IIIrd Semester

Paper Title: *Organometallic compounds*

Paper code: CHEM-301 DCT **Credits: 4**

Course Objective

This paper has been introduced to study: i) classification, nomenclature and characteristics of organometallic compound; ii) organometallic compounds of main group elements and transition metals; iii) metal carbonyl; and iv) metal nitrosyl in details.

Course Outcomes

After studying this paper, students would be able to know about the following in details:

i) classification, nomenclature and characteristics of different types of organometallic compounds; ii) general characteristics of organometallic compounds of main group elements, stability of organometallic compounds, sigma and pi bonded organometallic compounds, nature of bonding, organometallic compounds of lanthanides and actinides; iii) classification of carbonyls, general methods of preparations, chemical properties and structure and bonding in metal carbonyls. Effective atomic number (EAN) rule applicable for metal carbonyls and vibrational spectra of metal carbonyls for bonding and structural elucidation; and iv) modes of bonding in nitrosyl as NO^+, structure, bonding and important reactions of transition metal nitrosyl and vibrationnnal spectra for structural elucidation and bonding in metal nitrosyl.

Unit-I: Classification, Nomenclature and characteristics of organometallic compound

Introduction, classification based on Hapticity, classification based on the polarity of M-C bond (position of the metal in the Periodic Table), nomenclature of organometallic compounds, general characteristics of different types of organometallic compounds.

Unit-II: Organometallic compounds of main group elements and transition metals.

General characteristics of organometallic compounds of main group elements, stability of organometallic compounds, preparative routes for meta-carbon bond formation. Cyclopentadienyl complexes of main group elements. Sigma and pi bonded organometallic compounds, nature of bonding, organometallic compounds of lanthanides and actinides,

Unit-III: Metal carbonyl

Introduction, classification of carbonyls, general methods of preparations, general chemical properties. Structure and bonding in metal carbonyls. Effective atomic number (EAN) rule applicable for metal carbonyls. Vibrational spectra of metal carbonyls for bonding and structural elucidation.

Unit-IV: Metal nitrosyl

Introduction, modes of bonding in nitrosyl as NO^+. Structure, bonding and important reactions of transitoion metal nitrosyl. Vibrationnnal spectra for structural elucidation and bonding in metal nitrosyl.

Reference Books:

1. Advance Inorganic Chemistry, Cotton and Willkinson.
2. New Conise Inorganic Chemistry, Fifth Edition, J.D. Lee.
3. Advanced Inorganic Chemistry, Puri & Sharma

M.Sc. Chemistry

M.Sc. Chemistry, IIIrd Semester

Paper Title: ***Analytical Methods for Qualitative and Quantitative Analysis–III Lab***

Paper code: 301 DCP **Credits: 2**

Course Objective

This paper has been introduced to study i) spectrophotometric/colorimetric analysis, ii) chromatographic analysis and iii) qualitative and quantitative analysis.

Course Out comes

After studying this paper, students would be able to know the procedure of the following experiments in details:

1. Principle of spectrophotometric / colorimetric analysis and how is done. This study involves i) estimation of Cu in a brass sample, ii) nitrate in water sample by colorimetric method and iii) Ca and Mg in milk and egg.
2. Principle of chromatographic technique and how are metal cations separated from a mixture using chromatographic technique for example [Separation of Ni (II) and Co (II) and Fe (III) and Al (III)].
3. Separation of iron and estimation of Zinc from a given mixture solution, separation of copper and estimation of Nickel from a given mixture solution and qualitative analysis of a mixture of four metal ions including one of the following rare metals: W, Mo, Se, Te, V, Ce, Th, Zr and U, using qualitative and quantitative analysis.

M.Sc. Chemistry

M.Sc. Chemistry IIIrd Semester

Paper Title: ***Name Reactions & Synthetic organic chemistry (Theory)***

Paper code: L-T-P: 4-0-0 **Credits: 4**

Course Objectives

This paper has been introducing to impart the knowledge of different name reactions with their applications and applications of organometallic in organic synthesis. Moreover, this paper is also helpful in gaining the knowledge of mechanism of electrolytic reactions and cycloaddition and sigma-tropic reactions.

Course Outcomes

After completing this paper, students would be able to:

1. Know about the different name reactions and organometallic compounds and their applications which will be helpful in laboratory as well as in industry.
2. Understand the mechanism of electrolytic, cycloaddition and sigma-tropic reactions applicable in laboratory and industry as well.

Unit-I: Name reactions and their applications

Corey-Bakshi-Shibata, Reformatsky, Simmons-Smith, Corey–Seebach, Chan alkyne, Allan–Robinson,Bergman Mitsunobu, Staudinger,Barton-deoxygenation and decarboxylation, Ciamician–Dennsted, Ciamician–Dennsted, Vilsmeier–Haack, Weinreb amide, and Fischer indolizationreactions, Buchner, Pictet-Spengler, Takai, Rubottom, Darzens, Stobbe, , Weiss–Cook, Regitz, Reissert, Deobner, Sakurai, CoreyFuchs, Nayori,Blanc, Allan–Robinson, Bergman, Parham cyclization,

Unit-II: Applications of organometallics in organic synthesis

Introduction to organometallic compounds, Classifications, Hapticity, 18-electrons and Wade rules, metal clusters, sandwiched compounds, fluxional molecules, catalysis, Structure and bonding in metalalkyls, aryls, allyls, cyclopentadienyl and arene complexes, Oxidative-Addition and Insertion reactions at M-C bond & M-H bond, transmetallation and cyclization reaction, hydroformylation using cobalt octacarbonyl. Hydrogenation by Willkinsons catalyst, Tebbe reagent, Ziese's salt, Wacker process, Pauson-Khand, Nicholas, Buchwald-Hartwig, Ziegler-Natta, Schwartz, coupling reactions: Heck, Suzuki, Stille, Sonogashira, Hiyama,Fukuyama, Negishi, Kumada, Chan-Lam, Castro- Stephan, Petasis, Glaser, Hay and NozakiHiyama-Kishi, Tsuji-Trost allylation

Unit-III: Electrocyclic Reactions

General pericyclic selection rules and their applications, Frontier molecular, orbitals of ethylene, 1,3-butadiene, 1,3,5-herxatriene, 1,3,5,7-octatectraene and allyl systems. Electrocyclic reactions: conrotatory and disrotatory motions of 4nπ, [4n+2]π, and allyl systems. Correlation diagrams for 4π-electrons and 6π-electrons systems, torque selectivity (a special kind of selectivity in pericyclic reactions), and pericyclic reactions of ionic species including Nazarov cyclization reaction.

Unit-IV: Cycloaddition and Sigma-tropic Reactions

General orbital symmetry rules: [2+2] cycloaddition reactions, [2+2+2] cycloaddition reactions, [4+2] cycloaddition reactions, [6+4] cycloaddition reactions, [5+2] cycloaddition reactions, [8+2] cycloaddition reactions, [14+2] cycloaddition reactions, Ene reaction, Studinger reaction, and some other group transfer reactions.

Reference Books:

1. Advanced Organic Chemistry; Jerry March, Fourth edition, Wiley & Sons,(2007). Morriosn Boyed.
2. Photochemistry and pericyclic reactions by jagdamba Singh and Jaya Singh, NewAcademic Science,2009.
3. Organometallic and bioinorganic chemistry by AjayKumar.
4. Organometallic·Chemistry- R.C. Mehrotra & A. Singh, Wiley EasternLtd.(2000)

M.Sc. Chemistry

M.Sc. Chemistry IIIrd Semester Practical

Paper Title: ***Name Reactions & Synthetic organic chemistry (Practical)***

Paper code: L-T-P: 0-0-2 **Credits: 2**

Course Objectives:

Acquire the knowledge of reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry. Understand reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry. Apply the knowledge and understanding of new situations, reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry

Course Outcomes:

At the end of the course, the learners should be able to:

Prepare various organic compounds using various reactions. Develop skills in handling apparatus, measuring the quantities and carryout the reaction, separating the products, purifying them and analyse the products formed. applies the skill in preparing novel organic moieties. Develop interest in the areas of reactions and mechanisms of Substitution, Elimination, Addition, Pericyclic and Organic Photochemistry

Course Contents:

Synthesis of Organic compounds Synthesis, purification and characterization of about 8 organic compounds involves one or two stages. Separation and identification of organic compounds & Column chromatography Separation of two component mixtures by chemical methods and their identification by chemical reactions.

List of some suggested compounds

1. β-Napthyl methyl ether from β-Naphthol
2. m-dinitrobenzene from Nitrobenzene
3. Azo dye from primary amine
4. Aromatic acid from ester
5. Benzanilide from aniline

6. p-nitroaniline from Acetanilide

7. p-Bromo acetanilide from aniline

8. Phthalimide from phthalic acid

9. 1,2,3-Tribromo benzene from aniline

Recommended Books:

1. Practical organic chemistry by Mann & Saunders

2. Text book of practical organic chemistry by Vogel

3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin.

M.Sc. Chemistry

M.Sc. Chemistry IIIrd Semester Practical

Paper Title: *Physical Chemistry-III*

Paper code: L-T-P: 0-0-2 **Credits: 4**

Course Objectives:

To equip students with various concepts and mechanism of acid, base and enzyme Catalysis reaction, concept of micelles, emulsion and reverse micelles, chemistry of macromolecules and adsorption processes on solid surfaces

Course Outcomes:

After completion of this course successfully, the students will be able to

1. provide physical insight into adsorption processes on solid surfaces.
2. Understand enzyme catalysis.
3. Understand various applications of emulsions, reverse micelles.
4. Determine of molecular weight of polymers.
5. Understanding kinetics of polymerization.

Unit-I: Adsorption

Surface tension, Capillary action, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET adsorption isotherm, Surface films (Electro-kinetic phenomenon), Catalytic activity at surfaces. Catalysis on metal surfaces, Metal oxide surfaces. Application of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

Unit-II: Catalysis

General characteristics of catalytic reactions, Acid-base catalysis, Enzyme catalysis, Mechanism and kinetics of enzyme-catalysed reactions, Michaelis-Menten equation, Heterogeneous catalysis, Surface reactions, Autocatalysis and Oscillatory reactions

Unit-III: Micelles

Surface active agents, Classification of Surface-active agents, Co-surfactants, Micellization, Microemulsions, Aggregate structures of surfactants, Critical Micellar Concentration,

Surfactant packing parameter, Factors affecting the CMC of surfactants, Counter ion binding to micelles, Hydrophobic interaction, Thermodynamics of micellization, Mass action models, Solubilization and Phase diagram of ternary microemulsion system.

Unit-IV: Macromolecules

Classification and Chain configuration of macromolecules, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, electrically conducting polymers, Polymerization's reactions, Kinetics of polymerization, Mechanism of polymerization. Theory of Molecular masses of polymers and their physical determinations by Osmometry, Viscometry and Light scattering methods, Sedimentation, Calculation of average dimensions of various chain structures

Reference Books:

1. Physical Chemistry 8th Ed., P. W. Atkins and J. de Paula, Oxford University Press,2006.
2. Physical Chemistry of Surfaces - A. W. Adamson - John Wiley Sons.
3. Catalytic Chemistry, Bruce C. Gates, John Wiley & Sons, Inc. 1992(541.395GAT)
4. Catalysis at Surfaces, I. M. Campbell, Chapman and Hall, New York,1998.
5. Introduction to Colloid and Surface Chemistry 2nd Ed., D. J. Shaw, Butterworths,1970
6. Principles of Physical Chemistry, Puri, Sharma, Pathania, Shoban Lal Nagin Chand & Co., EducationalPublishers.
7. Micelles, Theoretical and Applied Aspects, Y. Moroi, Plenum Press, New York.
8. Introduction to Polymer Science, V. R. Gowarikar, N. V. Vishwanathan and J. Sridhar - Wiley Eastern

M.Sc. Chemistry

M. Sc. IIIrd Semester

Paper Title: *Physical Chemistry Practical– III*

Paper code: **Credits: 2**

Course Objectives:

To train the students about verification of Freindlich Adsorption isotherm, determination of cryospoic constant, weight of unknown nonvolatile solute and CST.

Course Outcomes:

After completion of this course successfully, the students will be able to

1. Verify Freindlich Adsorption isotherm
2. Determination of CST of Phenol water System
3. Distribution coefficients
4. Determination of CMC of surfactants

Lab Experiments

1. Adsorption of acetic acid or Oxalic acid on the surface of charcoal and verification of Freindlich Adsorption isotherm
2. Determination of the concentration of the given acid using the isotherms
3. Determination of cryospoic constant using known solute.
4. Determination of molecular weight of unknown nonvolatile solute
5. Determination of CST of Phenol water System
6. Effect of Neutral Salt on CST
7. Distribution of acetic acid between n-butanol and water.
8. Distribution of iodine between CCl_4 and water.
9. Distribution of benzoic acid between Benzene and water & to prove dimerization of benzoic acid in benzene.
10. Find CMC of a given surfactant and, hence, calculate ΔG_{mix} of the surfactant

Reference Books:

1. Systematic experimental Physical Chemistry by- Rajbhoj and Chondhekar.
2. Experimental Physical Chemistry – R. C. Das & B. Behra
3. Harris, D. C. Quantitative Chemical Analysis 6th Ed. W. H. Freeman & Co (2002).
4. Advanced Practical Physical Chemistry, J.B. Yadav - Goel Publishing House.

5. Advanced Experimental Chemistry, Vol. I - Physical, J.N. Gurtu and R. Kapoor– S. Chand & Co.
6. Selected Experiments in Physical Chemistry, N.G. Mukherjee – J.N. Ghose &Sons.
7. Experiments in Physical Chemistry, J.C. Ghosh - Bharti Bhavan.
8. Senior Practical Physical Chemistry, B.D.Khosla; V.C.Garg, Adarsh Khosla R. Chand &Co

M.Sc. Chemistry

M. Sc. IIIrd Semester

Generic: ***Bioanalytical and Forensic Chemistry***

Paper code: **Credits: 4**

Course Objective:

The objective of the "Bioanalytical and Forensic Chemistry" paper is to provide students with an in-depth understanding of the interdisciplinary applications of chemistry in the fields of biology, medicine, and forensic science. The course aims to:

Introduce students to bioanalytical techniques used for the detection and quantification of biomolecules, clinical chemistry, human-nutrition, food analysis, processing and preservation and forensic Science chemistry, narcotics and toxicology.

Equip students with the knowledge of forensic chemistry principles, especially in the context of criminal investigations.

Provide students with the necessary skills to work with analytical tools for bioanalytical and forensic applications.

Course Outcomes:

Upon completion of this course, students will be able to:

Demonstrate a comprehensive understanding of bioanalytical techniques and their applications in biomedical research.

Apply various instrumental methods (e.g., HPLC, GC-MS, UV-Vis spectroscopy, NMR) for the analysis of biological samples.

Understand the chemical basis of linical chemistry, human-nutrition, food analysis, processing and preservation and forensic Science chemistry, narcotics and toxicology.

Understand the ethical and legal aspects of forensic chemistry in criminal investigations, ensuring proper evidence handling and analysis procedures.

Unit-I: Clinical Chemistry:

1.1. Composition body fluid; detection of abnormal levels of certain constituents leading to diagnosis of diseases; sample collection and preservation of physiological fluids;

1.2. Analysis of physiological fluids- blood, urine and serum; estimation of blood glucose, cholesterol, urea, haemoglobin; urine-urea, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphates.

Unit-II: Human-Nutrition:

Estimation of enzymes, carbohydrates, essential amino acids, proteins and lipid.

Unit-III: Food Analysis, Processing and Preservation:

Analysis of food such as milk, milk products, tea, coffee and beverages (soft drinks, alcoholic drinks),. Flour, starch, honey, jams and edible oils. Analysis of preservatives, coloring matter, micronutrients.

3.2. Food processing and food preservation: Refining milling, canning, concentration, freezing Drying, pasteurisation sterilization irradiation.

Unit-IV: Forensic Science: Chemistry, Narcotics and Toxicology

Forensic Chemistry: Its role in crime; Types of cases received for Analysis; Procedures for sample selection, collection, preservation, identification.

Narcotics: Definition; Narcotic drugs and Psychotropic; substances; Problems of drug abuse; drug addiction. Classification of Narcotic drugs;

Analytical Toxicology; Extraction of poisons from various matrices including visceral samples; Isolation; Purification identification and interpretation of findings. Use of both Classical and Modern Instrumental methods of chemical analysis of poisons.

Reference Books:

1. C. S. James, Analytical Chemistry of Foods, Blackie Academic and Professional Publisher, UK, 1995, 1st Ed.
2. R. L. Nath, Practical Biochemistry in Clinical Medicine, Academic Publishers, 1990, 2nd Ed.
3. V. Malik, Drug and Cosmetics Act, Eastern book company, 2016, 25th Ed.
4. B. S. Kuchekar, A. M. Khadatare, Forensic Pharmacy, NiraliPrakashan publisher, 2007, 7th Ed.
5. S. R. Mikkelsen, E. Corton, BioanalyticalChemistr, John Wiley and Sons, 2016, 2nd Ed.
6. M. B. Jacob, Chemical Analysis of Food and Food Products, CBS publisher, 2013, 3rd Ed.
7. S. Bell, Forensic Chemistry, Pearson Prentice Hall Publishers, 2006, 2 nd Ed.
8. Encyclopaedia of Analytical Chemistry, Volume 3, Academic Press

M.Sc. Chemistry

M. Sc. IVth Semester

Paper Title: ***Inorganic polymers, Nuclear Chemistry and Bio-inorganic Chemistry***

Paper Code: MSCH 401 **Credits: 4**

Course Objectives:

This paper has been introduced to learn about i) inorganic polymers, ii) nuclear chemistry, iii) metalloenzymes and iv) applications of bioinorganic chemistry

Course Outcomes:

After studying this paper, the students would be able to know in details of the followings :

General properties of inorganic polymers, study of silicon, phosphorous based inorganic polymers and coordination polymers and their types, ii) Elemnstary idea about nuclear particles and nuclear forces, different types of nuclear reactions, radioactive tracers and carbon dating, iii) role of enzymes in various biological activities, Role of alkali and alkaline earth metal and Zn, Co, Fe and Cu, Carboxy peptidase, Carbonic anhydrase. , Sodium pump, and calcium pump and iv) metal deficiency diseases, toxic effects of metals, metals used for diagnosis and chemotherapy, Gold compound as anti-rheumatic agent, Cyclic nitrogen fixation.

Unit-I: Inorganic polymers

General properties, glass transition temperature, Silicon based polymers, properties of silicones, Phosphorus based polymers, Phosphorus based chain polymers, Coordination polymers and their types, Two-dimensional coordination polymers, and three-dimensional networks.

Unit-II: Nuclear Chemistry

Nuclear particles, nuclear forces, nuclear fission and fusion, Hydrogen bomb, Radioactivity, Rate of radioactive disintegration, Nature of radiation from radioactive elements, Radioactive tracers, Carbon dating.

Unit-III: Metalloenzymes

Inhibition and poisoning of enzymes, Role of alkali and alkaline earth metal and Zn, Co, Fe and Cu, Carboxy peptidase, Carbonic anhydrase. Ions in biological system, Sodium pump, Calcium pump.

Unit-IV: Application of Bioinorganic Chemistry

Metal deficiency and diseases. Toxic effects of metals, metals used for diagnosis and chemotherapy, gold compound as anti-rheumatic agent, Cyclic nitrogen fixation.

Reference Books:

1. Advance Inorganic Chemistry, Cotton and Willkinson.
2. New Conise Inorganic Chemistry, Fifth Edition, J.D. Lee.
3. Advanced Inorganic Chemistry , Puri & Sharma.

M.Sc. Chemistry

M.Sc. Chemistry IV Semester

Paper Title: ***Heterocyclic compounds and Natural products (Theory)***

Paper Code: L-T-P: 4-0-0 **Credits: 4**

Course Objective:

This paper has been introduced to impart the teaching with regard to the study of heterocyclic compounds having one, two and more heteroatom in their ring. Further, this syllabus also motivates to learn about the alkaloids and terpenoids.

Course Outcomes:

After completing the syllabus, students will gain and be able to

1. Know the rules of nomenclature of heterocyclic compounds with one, two or more hetero-atoms in their structure.
2. Synthesis, chemical reactivates of heterocyclic compounds and also their applications.
3. Detailed study of alkaloids and terpenoids and their medicinal importance.

Unit-I: Heterocyclic compounds with one hetero atom

Introduction, Nomenclature, classification, synthesis, reactivity and importance of pyridine, pyrrole and thiophene.

Unit-II: Heterocyclic compounds with two or more than two hetero atoms

Introduction, Nomenclature, synthesis, reactivity and importance of pyrazole, lmidazole, Oxazole, Thiazole, lsoxazole, lsothiazole, Pyridazine, Pyrimidine, Pyrazine, Benzimidazole, Benzoxazole and Benzthiazole.1,2,3-triazoles, 1,2,4-triazoles, Tetrazoles, 1,2,4-Oxadiazole, 1,3, 4-Oxadiazole,1,2,5 - Oxadiazole, Tetrazines, Synthesis and importance of Purine and Pteridines, Synthesis of Caffeine, Theobrome and Theophylline.

Unit-III: Alkaloids

Introduction, Classification, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Morphine.

Unit-IV: Terpenoids

Introduction, occurrence, isolation, Classification, nomenclature, general methods of structure determination, isoprene rule. Structure determination, synthesis of the following representative molecules: Citral, geraniol, α-Pinene, Camphor.

Reference Book:

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag. Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
2. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science,
3. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
4. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon press.Chemistry of Natural Products: A unified Approach, N.R. Krishnaswamy, Universities Press, Hyderabad.

M.Sc. Chemistry

M. Sc. IVth Semester

Paper Title: Physical Chemistry-IV

Paper Code: **Credits: 4**

Course Objectives:

This course aims at to accustom the students the principles and applications of quantum mechanics in detail with further introduction of different types of operators. Basic concepts of laws of photochemistry

Course Outcomes:

After completion of this course successfully, the students will be able to

1. Understand operator algebra and application of Schrödinger wave equation
2. Basic principles and laws of Quantum Chemistry
3. Understand of the quantum chemistry of free electron and H- atom
4. To Understand the advance aspects of photochemical reactions.
5. Understanding role of photochemistry in environment

Unit-I: Quantum Chemistry – I

A quick review of the following: Black body radiation – Planck's concept of quantization (derivation not required). Photoelectric effect. Hydrogen spectrum. Bohr's theory and its failures – Wave particle duality and uncertainity principle – Significance of these microscopic entities Emergence of Quantum mechanics.

Operators: Operators algebra – Commutation of operators, linear operators. Complex functions. Hamlitian operators. Operators ∇ and ∇^2. Eigen functions and Eigen values. Degeneracy. Linear combination of Eigen functions of an operator, well behaved functions. Normalized and orthogonal functions.

Postulates of Quantum mechanics. Physical interpretation of wave function. Observables and operators. Measuability of properties. Average value of observable. The time dependent and time independent Schrodinger equation.

Unit-II: Quantum Chemistry – II

Particle in a box. One dimensional and three dimensional. Plot of Ψ and Ψ^2 – Discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. Calculations using wave functions of the particle in a box – Normalisation and orthogonality, measurability of energy, position momentum, average values and probabilities. Application of the spectra of conjugated molecules.

Schrodinger equation for the Hydrogen atom – Separation of variables. Quantum numbers n, 1 and m. Hydrogen like wave functions. Complete wave function angular and radial functions. Radial distribution functions. Hydrogen like orbitals and their representation – Polar plots, Contour plots and boundary diagrams.

Unit-III: Photochemistry-I

Introduction, Absorption of light and nature of absorption spectra, electronic transitions, Franck–Condon principle, electronic excitation, photo-dissociation and Pre-dissociation, photo-reduction, photo-oxidation, role of photochemistry in environment (Greenhouse effect, ozone depletion).

Unit-IV: Photochemistry-II

Photophysical phenomenon. Jablonskidigram. Kasha's rule, fluorescence, phosphorescence, delayed fluorescence, differences between phosphorescence and delayed fluorescence. Inter & intra molecular excitation energy transfer (EET) processes. Quenching of fluorescence and kinetics of biomolecluar quenching processes, Stern-Volmer equation, formation of photodimer, (with suitable examples) excimer and exciplex.

Reference Books:

1. G. Friedlander, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry, John Wiley (1981).
2. G. Choppin, J. O. Liljenzin and J. Rydberg, Radiochemistry and nuclear chemistry,Butterworth (1996).
3. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern Ltd. (1995).
4. B. K. Sharma, Nuclear and Radiation Chemistry, Krishna Publication.
5. Photo chemistry- J.G.Calverts&J.N.Pits.
6. Fundamentals of Photochemistry- K.K.Rohatgi, Mukharji.
7. Photochemistry of Solutions – C. A. Parker
8. Physical Chemistry – P. W. Atkins.
9. Physical Chemistry – G. M. Barrow

M.Sc. Chemistry

M. Sc. IVth Semester

Generic/Paper Title: Food Chemistry

Paper Code: **Credits: 4**

Course Objective:

The objective of the "Food Chemistry" paper is to provide students with a comprehensive understanding of the chemical composition of food, the principles of food processing, and the impact of food constituents on human health. The course aims to:

Introduce students to the major components of food and their role in nutrition and health and equip students with the knowledge of food additives including dairy products, beverages, food additives, adulterants, and contaminants and artificial food colorants.

Course Outcomes:

Upon completion of this course, students will be able to:

Demonstrate an understanding of the chemical composition of various food products and the role of different food constituents in human health.

Understand the principles behind food preservation methods and the chemical reactions involved.

Identify common food additives, preservatives, and contaminants and understand their roles, benefits, and potential health risks.

Understand the regulatory frameworks and standards governing food safety, labeling, and quality control.

Unit-I: Dairy Products

Composition of milk and milk products. Analysis of fat content, and minerals in milk and butter, Estimation of added water in milk.

Unit-II: Beverages

Analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in a toddy, estimation of methyl alcohol in alcoholic beverages.

Unit-III: Food Additives, Adulterants, And Contaminants

Food preservatives like benzoates, propionates, sorbates, disulphites. Artificial sweeteners: Aspartame, saccharin, dulcin, sucralose, and sodium cyclamate. Flavors: Vanillin, alkyl esters (fruit flavors), and monosodium glutamate.

Unit-IV: Artificial Food Colorants:

Coal tar dyes and non-permitted colors and metallic salts. Analysis of pesticide residues in

food.

Reference Books:

1. B.K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by AsthoushKar
3. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol.II, INC, New York.
4. Analysis of Foods – H.E. Cox; 13. Chemical Analysis of Foods- H.E. Cox and Pearson.
5. Foods – Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age Internatl (1998).
6. Physical Chemistry – P. Atkins and J. de Paula -7 th Ed. 2002, Oxford University Press
7. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6 th ed. 2001, FAI.
8. Organic Chemistry by I. L. Finar, Vol. 1 & 2

M. Sc. IVth Semester

PROJECT

Credits: 8