St. Aloysius (Autonomous) College, Jabalpur
Department of Chemistry

M.Sc. (CHEMISTRY)
(FOUR SEMESTER COURSE)

M.Sc. I & II Semester syllabus is as per the New NEP (M.P. Higher Education). M.Sc. III & IV semesters have core and elective papers with 4 credits and 2 practical papers of 2 credits each. Choice Choice-Based Credit system has been implemented in PG Chemistry since 2018-19

Distribution of Credits in Each Semester

M.Sc I + II Semester

2 Core paper – 06 Credits each	4*6 = 12 Credits
2 Practical's – 04 Credits each	2*4 = 8 Credits
Internship/ Apprenticeship or Seminar – 02 Credit	1 *2 = 2 Credits
Total Credits	**22 Credits**

M.Sc III Semester

3 Core paper – 04 Credits each	3 *4 = 12 Credits
2 Elective paper – 04 Credits	2 *4 = 8 Credits
2 Practical's – 02 Credits each	2*2 = 4 Credits
Skill Development – 01 Credit	1 *1 = 1 Credits
Tutorial – 01 Credit	1 *1 = 1 Credits
Total Credits	**26 Credits**

M.Sc IV Semester

2 Core paper – 04 Credits each	2 *4 = 8 Credits
2 Elective – 04Credits	2 *4 = 8 Credits
1 Minor Project/Dissertation/Internship	5 Credits
Skill Development – 01 Credit	1 *1 = 1 Credits
Total Credits	**22 Credits**

SEMESTER I

Course Code	Course	Credit	Theory Marks	CCE Marks
CC- 11(T)	Advanced Organic Chemistry	6	60	40
CC- 12(T)	Advanced Inorganic Chemistry	6	60	40
PC- 11	Advanced Organic Chemistry Practicum Core	4	60	40
PC- 12	Advanced Inorganic Chemistry Practicum Core	4	60	40
	Internship/ Apprenticeship or Seminar	2	100	-
Total			**340**	**160**
Grand Total			**500**	

SEMESTER II

Course No.	Course	Credit	Theory Marks	CIA Marks
CC- 21 (T)	Advanced Physical Chemistry	6	60	40
CC- 22 (T)	Research Methodology for Chemists	6	60	40
PC- 21	Advanced Physical Chemistry Practicum	4	60	40
PC- 22	Research Methodology for Chemist Practicum	4	60	40
VAC (CHM/ EESC)	Value Added Courses	2	100	-
Total			**340**	**160**
Grand Total			**500**	

SEMESTER III

Course No.	Course	Credit	Theory Marks	CIA Marks
Course MCH 301	Inorganic Chemistry	4	50	50
Course MCH 302	Physical Chemistry	4	50	50
Course MCH 303	**Spectroscopy III**	4	50	50
Course MCH 304 **I Elective**	**Course MCH 304 A** Medicinal Chemistry **Course MCH 304 B** Chemistry of Natural Products **Course MCH 304 C** Polymer (Any Two from **MCH304 A to C**)	4	50	50
Course MCH 304 **II Elective**		4	50	50
Course MCH 305	Organic Chemistry Practical	2	50	50
Course MCH 306	Physical Chemistry Practical	2	50	50
Total			**350**	**350**
Grand total			**700**	

SEMESTER IV

Course No.	Course	Credit	Theory Marks	CIA Marks
Course MCH 401	Inorganic Chemistry	4	50	50
Course MCH 402	Organic synthesis strategies	4	50	50
Course MCH 403 **Departmental Elective**	**Course MCH 403 A** Environmental Chemistry **Course MCH 403 B** Chemistry of materials (Any One from **MCH403A or 403 B**)	4	50	50
Course MCH 404 **Open Elective**	**Course MCH 404 A** Biochemistry **Course MCH 404B** Bioorganic Chemistry	4	50	50
Course MCH 405	Minor Project/Dissertation/Internship	5	100	
Total			**300**	**200**
Grand Total			**500**	

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory)*	*Marks*	
M.Sc. I SEM	Core	CC- 11 (T)	Advanced Organic Chemistry	Max: 100	Min: 40

COURSE OBJECTIVE:

To develop an understanding of reactivity, structure and bonding, mechanisms, stereochemistry and aliphatic and aromatic substitution reactions of organic compounds

UNIT-1

Indian Knowledge system and its relevance to Aromaticity:

Concept of Aromaticity - Traditional Insight

Chemistry of natural aromatic compounds: Eugenol (from cloves),, Thymol (from ajwain), Curcumin (from turmeric) and Vanillin (frof vanilla).

Contributions of Acharya Prafulla Chandra Ray (The Father of Chemistry) in Organic Chemistry.

Aromaticity:

Concept of aromaticity, Aromaticity in benzenoid and non-benzenoid compounds, Antiaromatic compounds, Nongromatic compounds, Homoaromatic compounds, PMO approach, Annulenes, Metallocenes, Crown ether complexes and cryptates.

Keywords: Aromatic Compounds PMO Approach, Benzenoid and Non Benzenoid Systems, Annuletes and Metallocenes

UNIT -2

Free radical reactions:

Structure, stability and geometry, and properties of Free radicals. Free radical substitution mechanisms, mechanism at an aromatic substrate, neighbouring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, reactivity in the attacking radicals, the effect of solvent on the reactivity.

Name Reactions:

Birch Reduction, Nef reaction, Bouveault-Blanc reaction, Chichibabin, Mannich reaction, Meerwein-Ponndorf- Verley reduction, Oppherneur oxidation, Curtius reaction, Claisen Schmidt reaction, Sharpless-epoxidation, Pechmann reaction. Aldol Condensation, Knoevenagel reaction, Mannich reaction, Benzoin condensation, Perkin reaction, Sandmeyer's and Hunsdiecker reaction.

Keywords: Free Radical Substitution, Stability of Radicals, Organic Reactions

UNIT -3

Reaction Mechanism: Structure and Reactivity

Curtin-Hammett Types of reaction mechanisms, thermodynamic requirements, kinetic and thermodynamic contre Principle. Potential energy diagrams, transition states and intermediates, methods of determining the mechanism, and isotope effects.

Generation, structure, stability and reactivity of carbocations, carbanions, free radical, carbenes and nitrens.

Effect of structure on reactivity-resonance and field effects, quantitative treatment. The Hammett equation and linear free energy relationships, substituent and reaction constants, Taft equation.
Keywords: Reaction Pathways, Thermodynamic and Kinetic Control, Reactive Intermediates, Linear Free Energy Correlations

UNIT-4

Pericyclic Reactions:

Molecular orbital symmetry, Frontier orbitals of ethylené, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reaction. Woodward-Hoffmann correlation diagrams. FMO and PMO approach.
Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.
Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 system. 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.
Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, 3,3-and 5,5-sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements, Ene reaction and Fluxional tautomerism.
Keywords: Orbital Symmetry, Electrocyclic Reactions, Cycloadditions, Sigmatropic Rearrangements, Woodward-Hoffmann Rules

UNIT- 5

Photochemical Reactions:
Photochemistry of alkenes of matic compounds, Paterno-Buchi reaction, di-pi methane arrangement, Photo-Fries rearrangement, Barton reaction, formation polymers and Photothemisuy of vision. of smog, Photodegradation of polymer and photochemistry of vision.
Keywords: Photo reduction, Photo rearrangements, Photocycloadditions, Smog Formation, Photodegradation

Course Learning Outcome

Upon successful completion of this Course, learners will be able to:

- Understand the traditional insight of Aromaticity and contributions of Acharya Prafulla Chandra Ray (Father of Indian Chemistry).
- Explain the concept of aromaticity and differentiate between aromatic, maticity an antiaromatic, nonaromayo and homoaromatic compounds using structural features and roscopic data.
- Apply the PMO approach to interpret aromatic character in systems like annulenes, metallocenes, and crown ether complexes.
- Demonstrate the mechanisms of major condensation reactions such as enolate intermediates.
- Assess the stability and reactivity of Free radicals and describe their behavior in reactions like allylic halogenation, Sandmeyer, and Hunsdiecker transformations.
- Interpret reaction mechanisms through energy diagrams, transition states, and isotope effects; relate structural effects to reactivity using Hammett and Taft correlations.
- Classify pericyclic reactions and predict their stereochemical outcomes based on orbital symmetry principles and the Woodward-Hoffmann rules.
- Describe the mechanisms and applications of photochemical reactions such as Paterno-Büchi, di-methane rearrangement, and photo-Fries rearrangement in organic synthesis.

Suggested Readings:

1. Ray, Prafulla Chandra, A History of Hindu Chemistry, Asian Educational Services, New Delhi.
2. Sivarajan, V.V., Balachandran, I., Ayurvedic Drugs and Their Plant Sources, Oxford and IBH Publishing Co. Pvt. Ltd., New Delhi.
3. March, J. Advanced Organic Chemistry: Reactions, Mechanisms and Structure. John Wiley.

4. Sykes, Peter. A Guidebook to Mechanism in Organic Chemistry. Orient Longman.
5. Mukherji, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. Macmillan.
6. Carey, F.A. and Sundberg, R.J. Advanced Organic Chemistry, Part A and B. Plenum.
7. Kalsi, P.S. Organic Reactions and Their Mechanisms. New Age International.
8. Coxon, J. and Holtom, B. Organic Photochemistry. Cambridge University Press.
9. Dupuoy, C.H. and Chapman, O.L. Molecular Reactions and Photochemistry. Prentice Hall.
10. Kagan, J. Organic Photochemistry. Academic Press.
11. Kundall, R.P. and Gilbert, A. Photochemistry. Thomson Nelson.
12. Clayden J., Greevs N., and Warren S., Organic Chemistry, Oxford Publ.
13. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Parts A and B Plenum.
14. Carruthers, W., Coldham, I., Modern methods of organic synthesis, Ombudge University Press. Education
15. Warren, S., Organic Synthesis: The Disconnection Approach, John Wiley & Sons.
16. Jagdamba Singh, L. D. S. Yadav Organic Chemistry, Pragati Prakashan.

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory)*	*Marks*	
M.Sc. I SEM	Core	CC- 12 (T)	**Advanced Inorganic Chemistry**	Max: 100	Min: 40

COURSE OBJECTIVE:

To develop an understanding of structure and chemical bonding present in inorganic compounds and the basic concept of *Reaction Mechanism of Transition Metal Complexes*.

UNIT- 1

Indian Knowledge System and its relationship with Electronic Spectral Studies of Transition Metal Complexes:

- Ancient Indian texts such as Rasaratna Samuccaya and Rasashastra describing preparation and medicinal use of metal complexes (bhasmas), reflecting an empirical grasp of metal-ligand interactions.
- The colour changes of metal salts and their complexes in dyeing and purification processes, demonstrating practical knowledge related to electronic transitions and ligand field effects.
- The Ayurvedic concept of 'Rasa' metaphorically aligning with the changes in molecular energy states and interactions observed in spectroscopic ground states and electronic transitions.

Electronic Spectral Studies of Transition Metal Complexes:

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), Selection rule for electronic spectroscopy. Intensity of various types of electronic transitions. Calculations of 10Dq, B and β parameters, and charge transfer spectra. Franck-Condon principle and Applications (No. of transitions, and energy orders). Charge transfer (CT) mechanism; Ligand to Metal and Metal to Ligand Charge Transfer Bands. Effect of Solvent Polarity on CT Spectra.

Keywords: Electronic Transitions, Orgel Diagrams, Tanabe-Sugano Diagrams, d-Orbital Transitions, Crystal Field Splitting (10Dq), Charge Transfer, Spectra, Spectral Applications, Solvent Polarity Effects

UNIT- 2

Stereochemistry and Bonding in Main Group Compounds:

Bent rule and energetics of hybridisation, some simple reactions of covalently bonded molecules. Walsh diagram (triatomic and penta-atomic molecules), and dπ-pπ bond.

Metal-Ligand Equilibrium in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by potentiometry and spectrophotometry.

Keywords: Bent Rule, Hybridization Energetics, Walsh Diagram, dn-pr Bonding, Chelate Effect, Stability of Metal Complexes, Potentiometry, Spectrophotometry

UNIT- 3

Organometallic chemistry:

Introduction: 18-electron rule and its limitations, electron counting; Transition Metal hydrides, alkyls,

aryls, carbonyls, nitrosyls, phosphines and related ligands. Wade's rule, metal-metal bond counting. Mechanism of Substitution reactions. Organometallic complexes of π-bound ligands (Alkene, Alkyne, Allyl, Diene, Cyclopentadienyl, Arenes and other Alicyclic Ligands); Mechanism and application of Oxidative Addition and Reductive Elimination reaction, Insertion and β-hydride elimination. Fischer and Schrock carbene.

Application of organometallic complexes in homogeneous catalysis:

Alkene hydrogenation (Wilkon's catalyst, Monsanto, Cativa reaction), Alkene Hydroformylation, Wacker's reaction, Cross-coupling reaction; Heck coupling, Sonagashira reaction, Suzuki Miyara coupling, Hiyama-coupling, Stille coupling). Buchwald-Hartwig amination, Tebbe's reagent, Grubbs catalyst.

Keywords: Organometallic chemistry, Wade's rule, Organometallic complexes, Mechanism of Substitution reactions

UNIT- 4

Metal-Clusters

Higher boranes, carboranes, metallo-boranes, and metallo-carborane compounds with metal-metal multiple bonds, STYX no. cluster types identifications, calculations of bond order and magnetic behaviour.

Metal π-Complexes

Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and tertiary phosphine as ligands.

Keywords: Metal-Clusters, Metal Carbonyls, STYX Number, Magnetic Behaviour, Vibrational Spectra, Bonding and Structure, Transition Metal Nitrosyl, Tertiary Phosphine Ligands

UNIT- 5

Symmetry, Group Theory and its Applications

Introduction of symmetry aspects with operations, Associated operations, Products of symmetry operations, Definition of group, subgroup, Conjugacy relation and classes. Point symmetry groups, Schoenflies symbols, representations of groups by matrices, and Character of representations.

Matrix representation of symmetry operations: Transformation matrices, The Great Group Orthogonality Theorem (GOT) and its importance, Character tables. Derivation of character table for different point groups, Infra-red and Raman active molecular vibrations of different molecules.

Keywords: Group Theory, Symmetry Operations, Transformation Matrices, Group Orthogonality Theorem, Character Tables, Point Groups, Molecular Vibrations

Course Learning Outcomes (CLO)

Upon successful completion of this Course, learners will be able to:

- Relate ancient Indian knowledge of metal complexes (bhasmas) to modern metal-ligand chemistry.
- Understand the connection between traditional colour changes, electronic transitions, and the Ayurvedic concept of 'Rasa'.
- Analyse and interpret the electronic spectra of transition metal complexes using Orgel and Tanabe-Sugano diagrams, understanding d-orbital transitions and selection rules for electronic spectroscopy.
- Apply the concepts of crystal field theory, including calculations of 10 Dq, B, and β parameters, and evaluate the intensity of various types of electronic transitions.

- Understand and explain the bonding and stereochemistry of main group compounds, utilising the Bent rule and Walsh diagrams, and exploring hybridisation energetics and dn-πn bonding.
- Evaluate the stability and formation constants of metal-ligand complexes in solution, including stepwise and overall formation constants, and understand the chelate effect and its thermodynamic origin.
- Identify and classify metal-cluster compounds, including higher boranes, carboranes, and metallo-carboranes, while calculating bond order and understanding the magnetic behaviour and STYX number of these clusters.
- Study and apply the bonding and structural elucidation of metal π-complexes, including metal carbonyls, transition metal nitrosyls, dinitrogen complexes, and tertiary phosphine ligands, with a focus on their vibrational spectra and important reactions.

Suggested Readings:

1. Rasaratrna Samuccaya, Various editions with commentary on Rasashastra and bhasmas.
2. Mukherjee, K.C., Rasashastra: The Ancient Science of Indian Alchemy, Motilal Banarsidass, Delhi.
3. Cotton, F.A., Wilkinson, G.W., Advanced Inorganic Chemistry, John- Wiley and Sons.
4. Huheey J.E., Keiter E.A., Keiter, R.L., Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India.
5. Douglas, B.E., McDaniel D.H, Alexander J.J., Concepts and Models of Inorganic Chemistry, John Wiley.
6. Das, A.K. Das, M., Fundamental concepts of Inorganic Chemistry, CBS publishers and distributors.
7. Miessler G.L., Tarr, D.A., Inorganic Chemistry, Pearson Education.
8. Wilkinson, G., Comprehensive Coordination Chemistry, Pergamon Press.
9. Sharpe, A.G., Modern Aspect of Inorganic Chemistry. Routledge and Kegan Paul PLC
10. Lever, A.B.P., Inorganic Electronic Spectroscopy, Elsevier.
11. Hollas, J.M., Modern Spectroscopy, John Wiley.
12. Chang R., Basic Principles of Spectroscopy, Mc Graw Hill.
13. Gupta, B.D., Basic Organometallic Chemistry: Concepts, Syntheses and Applications Paperback, Universities Press.
14. Bajpai, D.N., Advanced Physical Chemistry, S. Chand and Company Ltd.
15. Cotton F.A., Chemical Applications of Group Theory, John Wiley & Sons.

Suggested equivalent online courses and Web Sources:

1. https://archive.nptel.ac.in/course.html
2. https://ugcmoocs.inflibnet.ac.in/index.php/courses/moocs
3. https://swayam.gov.in/explorer

Assessment and Evaluation		
Maximum Marks: 100 **Internal Assessment (CCE): 40** **External Assessment (UE): 60**		
Internal Assessment		
	Continuous and Cumulative Evaluation (CCE) Methods will be based on the following defined components:	**Marks**
a.	**Class Tests**	
b.	**Presentation/ Assignment/ Quiz/ Group Discussion**	
c.	**Appropriate weightage of attendance in the Class**	
	Total	**40**
External Assessment		
	Theory Paper as per University Examination	
	Total	**60**
	Grand Total	**100**

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Practical)*	*Marks*	
M.Sc. I SEM	Core	PC- 11	**Advanced Organic Chemistry**	Max: 100	Min: 40

Duration: 6 hours

Course Learning Outcomes (CLO)

Upon successful completion of this Course, learners will be able to:

- Describe the theoretical principles and fundamental concepts underlying organic laboratory experiments.
- Apply laboratory skills to perform single-step and three-step synthetic preparations in organic and inorganic chemistry.
- Discuss aromatic substitution and other key organic reactions; predict products and intermediates, and explain reaction types and mechanists.
- Identify and analyze the products obtained through various experimental techniques; demonstrate effective purification and recrystallization strategies.

Practical List:

- **Organic synthesis (Single Step)**

1. Synthesis of 2,4-dinitro-1-chlorobenzene from chlorobenzene,
(Aromatic Electrophilic Substitution)

2. Synthesis of 9,10-anthraquinone by oxidation of anthracene by chromium trioxide.
(Oxidation Reaction)

3. Naphthol by dimethyl Sulphate. (Methylation Reaction) Synthesis of methyl 2-naphthyl ether(2-methoxynaphthalene, nerolin) by methylation of 2-

- **Organic synthesis (Multi Step)**

1. Nitrobenzene → m-dinitrobenzne → m-nitroaniline

2. Acetanilide → p-bromoacetanilide- → p-bromoaniline

3. Phthalimide → anthranilic acid → 2-chlorobenzoic acid (Sandmeyer Reaction)

4. Benzoin → benzyl → benzilic acid

- **Quantitative Analysis**

To determine the percentage of hydroxyl groups in the given organic compound by acetylation

- **Qualitative analysis**

1. Separate and identify the compounds in the given binary organic mixture, and also prepare at least one derivative of each identified compound.
2. Estimation of Hydroxyl Group by the acetylation method.
3. Spectrophotometric estimation of Glucose by Fehling Solution

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Practical)*	*Marks*	
M.Sc. I SEM	Core	PC- 12	**Advanced Inorganic Chemistry**	Max: 100	Min: 40

Duration: 6 hours

Course Learning Outcomes (CLO)

Upon successful completion of this Course, learners will be able to:

- Describe the theoretical principles and concepts related to experiments.
- Apply laboratory skills in Inorganic chemistry synthesis and estimation.
- Identify and analyze the product obtained by different techniques.
- Gain the knowledge of preparing complexes/ inorganic compounds, prediction of products, and their applications.
- Understand basic principles of spectroscopy and demonstrate applications of various spectroscopic techniques.
- Perform experiments, analyse and interpret the experimental results.

Practical List:

1. Synthesis:

Preparation of selected inorganic complexes

(1)$[Ni(acac)_2(H_2O)_2]$

(2)$[Co(acac)_2(H_2O)_2]$

(3)Manganese (III) acetylacetonate complex

(4)$Fe_4[Fe(CN)_6]_3$

(5)$[Ni(dmg)_2]$

(6)$[Ni(NH_3)_6]Cl_2$

2. Chromatography:

Separation and identification of metal cations by paper chromatography.

3. To separate and estimate Mg(II) and Fe(III) by solvent extraction method.

4. Synthesis of potassium *tris*-oxalato ferric hydrate and estimation of percentage oxalate by permanganate

5. Synthesis of *trans*- *bis*-glycinato copper (II) complex and estimation of copper.

6. To separate and estimate Mg(II) and Zn(II) by ion exchange method.

7. To estimate a mixture of two metal ions (Fe^{2+} and Mg^{2+}) by the volumetric and gravimetric method.

8. To determine the molecular composition of ferric salicylate complex by Job's method

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Class	*Course Type*	*Course Code*	*Course Title (Theory)*	*Marks*	
M.Sc. II SEM	Core	CC-21(T)	**Advanced Physical Chemistry**	Max: 100	Min: 40

COURSE OBJECTIVE:

To develop an understanding of quantum mechanics, thermodynamics, electrochemistry, surface chemistry and chemical dynamics.

UNIT- 1

Indian Knowledge System and its relevance to Quantum Mechanics:

Indian Atomism and the Concept of Discreteness-Vaisheshika Darshan. Philosophy of Anu and Paramanu, Comparison with modern atom theory and quantized energy levels.

Quantum Mechanics

Schrödinger equation and the postulates of quantum mechanics.

Discussion of solutions of the Schrödinger equation for the same model systems, viz., Particle in a box, Rigid rotator, Harmonic oscillator.

Approximation Methods

Variational and perturbation Methods: Applications of the variation method and perturbation theory to the Helium atom.

Molecular Orbital

Hückel theory conjugated systems, bond and charge density calculations, Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene

Keywords: Schrödinger equation, Quantum postulates, Particle in a box, Rigid Rotator, Harmonic Oscillator, Approximation methods, Helium atom, Hückel theory, Molecular orbital theory (MOT)

UNIT-2

Classical Thermodynamics:

Partial molar Quantities: Partial molar free energy, partial molar volume and partial molar heat content, Chemical Potential and their significance, Determinations of these quantities. Variation of chemical potential with temperature and pressure.

Concept of fugacity and determination of fugacity. Variation of fugacity with temperature and pressure. Thermodynamics of Non-Ideal Solutions, Activity and Activity Coefficient

Statistical Thermodynamics:

Partition function, calculator of thermodynamic functions in terms of the partition function. Applications for partition function: translational, rotational, vibrational, and electronic partition functions. Entropy of a monoatomic ideal gas. Gibbs-Duhem Equation.

Keywords: Partial molar quantities, Activity and fugacity, Partition function.

UNIT- 3

Chemical Dynamics:

Chemical kinetics, methods of determining rate laws, collision theory of reaction rates, steric factor, Arrhenius equation, and the activated complex theory, kinetic salt effects, steady state kinetics, transition

state theory, kinetics of enzyme reactions, Dynamics of chain reaction (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions), homogenous catalysis.

Complex and Fast Reaction:

Complex Reactions: Opposing reactions, Complex reactions, and Parallel reactions.

Fast reactions: Experimental techniques for fast reactions, viz., flow method, relaxation method, flash photolysis.

Keywords: Rate laws, Arrhenius equation, dynamics of chain reactions, kinetics of fast reactions.

UNIT- 4

Surface Chemistry:

Adsorption: Surface tension, Gibbs adsorption isotherm, estimation of surface area by the BET equation.

Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, thermodynamics of micellization.

Keywords: Adsorption, BET Equation, Surface area, Micelles, Critical Micellar Concentration (CMC)

UNIT- 5

Electrochemistry:

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions. Debye-Huckel-Jerum mode.

Polarography- Principle and Instrumentation, Ilkovic equation, half-wave potential, and its significance.

Voltammetry: General principle and instrumentation, Cyclic Voltammetry, and Linear Scan Voltammetry,

Keywords: Debye-Hückel theory, Electrode interface, Cyclic voltammetry, Linear Scan Voltammetry

Course Learning Outcomes (CLO)

Upon successful completion of this Course, learners will be able to:

- Apply the Schrödinger equation, wave functions, and energy levels to quantum systems and interpret
- Use Hückel Molecular Orbital theory to analyze conjugated systems and calculate bond orders and charge densities. Higher
- Explain the Laws of calculating partial molar properties and understand activity and fugacity in real gases.
- Utilize quantum statistics and partition functions to connect microscopic states with macroscopic thermodynamic properties.
- Analyze reaction kinetics using classical and advanced theories, leading to mechanisms of chain, photochemical, and fast reactions.
- Describe surface phenomena such as adsorption, surface tension, and estimate surface areas using the BET theory.
- Understand surfactants, micellization, critical micelle concentration, and thermodynamics of micellar systems.
- Explain ion interactions in solutions, Debye-Hückel-Onsager theory extensions, and electrified

interface thermodynamics.

- Interpret electrochemical concepts like charge transfer, polarography, and voltammetry.

Suggested Readings:

Books

1. Radhakrishnan, S., Indian Philosophy, Oxford University Press.
2. Chattopadhyaya, D., Indian Philosophy, A popular Introduction, People's Publishing House, New Delhi.
3. Kak, S., The Astronomical Code of the Rigveda, Aditya Prakashan, Delhi.
4. Kuppuram, G., Kumudamani, K. History of Science and Technology in India, Sundeep Prakashan, New Delhi.
5. Atkins, P.W., Physical Chemisty ELBS.
6. Chandra, A.K., Introduction to Quantum Chemistry, Tata McGraw-Hill.
7. Levine, I.N. Quantum Chemistry, Prentice Hall.
8. Laidler, K.J., Chemical Kinetics, McGraw-Hill.
9. Rajaraman, J., Kuriacose, J., Kinetics and Mechanism of Chemical Transformation, Macmillan.
10. Moroi, Y Micelles: Theoretical and Applied Aspects, Plenum Press.
11. Bockris, J.O.M., Reddy, A.K.N., Modern Electrochemistry, Plenum Press.
12 . Prasad R.K., Introduction to Quantum Chemistry, New Age International.
13. Bajpai D.N. Advanced Physical Chemistry, S. Chand and Company Ltd.

Suggested equivalent online courses and Web Sources:

- https://archive.nptel.ac.in/course.html
- https://ugcmoocs.inflibnet.ac.in/index.php/courses/moocs
- https://swayam.gov.in/explorer

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory)*	*Marks*	
M.Sc. II SEM	Core	CC-22(T)	**Research Methodology for Chemists**	Max: 100	Min: 40

COURSE OBJECTIVE:

- Developing students' ability to design and conduct chemical research, collect and analyze data using appropriate tools and techniques
- To train post-graduates capable of undertaking higher-level chemical research

UNIT- 1

Indian Knowledge System and Research in Chemistry:

Experimental Design in Rasashastra-Defined protocols for preparation, testing, and validation of chemical substances, paralleling modern experimental methodology.

Ethics in Research-Principles of Satya (truth) and Dharma (duty) promoted honesty, reproducibility, and integrity in research work.

Introduction and purpose of chemistry research. Classification of research types: basic, applied, and experimental. Qualitative approaches include case studies, interviews, and observational methods; quantitative approaches include surveys, experimental designs, and statistical analysis. Literature survey using scientific databases and digital platforms. Identification of research gaps and formulation of research problems and hypotheses. Structure of research proposals, including title, objectives, methodology, expected outcomes, and timelines. Referencing techniques, citation styles, and bibliography.

Keywords: Research in Chemistry, Research Types, Literature Survey, Hypothesis, Proposal Writing, Referencing, Citations

UNIT- 2

Research Ethics and Scientific Integrity:

Introduction to ethical issues in scientific research. Definition and types of misconduct, such as plagiarism, falsification, and fabrication. Use of similarity detection tools such as Turnitin and DrillBit. Authorship criteria, contributor roles, and conflict of interest. Identification of predatory journals and unethical publishing practices. Publication misconduct, peer review ethics, and strategies for maintaining scientific integrity in chemical research.

Keywords: Ethics in Research, Plagiarism, Falsification, Fabrication, Similarity Tools, Authorship, Predatory Journals, Scientific Integrity

UNIT- 3

Computational Tools for Chemists:

Utilization of standard office software (MS Word, MS Excel, PowerPoint) in documentation, data organization, statistical analysis, graphical representation, and effective presentation of scientific data. Introduction to scientific software tools specific to chemistry: ChemSketch and ChemDraw for drawing molecular structures and reaction schemes, Origin and similar graphing software for advanced data

visualization; software for creating statistical charts such as pie charts, histograms, and bar diagrams. Basics of programming logic with applications in solving chemistry-related numerical problems. Development of simple programs for calculations involving the Van der Waals equation, chemical kinetics (rate constants), radioactive decay (half-life and average life), and solution chemistry (normality, molarity, molality). Programming approaches for evaluating atomic properties like electronegativity and lattice energy.

Keywords: Computational Tools, Chemical Structures, MS Office, ChemDraw, Origin Software, Data Visualization, Programming

UNIT- 4

Laboratory Practices in Chemical Research:

Fundamental laboratory techniques essential for chemical research, including preparation of standard solutions (molarity, normality, molality), serial dilutions, handling of reagents, recrystallization, distillation, solvent extraction, filtration, drying, and melting point determination. Emphasis on laboratory safety protocols, chemical storage, labeling, and waste disposal. Proper use of personal protective equipment (PPE) and adherence to safety guidelines. Calibration and standardization of instruments and reagents to ensure quality control. Troubleshooting common experimental errors, maintenance of laboratory notebooks, and ensuring reproducibility and reliability of experimental results.

Keywords: Solution Preparation, Laboratory Safety, Chemical Handling, Standardization, Quality Control, Reproducibility

UNIT- 5

Green Chemistry and Sustainable Research Practices:

Environmental and societal impacts of chemical research, emphasizing the importance of sustainability and safety. Introduction to green chemistry principles and their alignment with the United Nations Sustainable Development Goals (SDGs) aimed at reducing waste, minimizing hazardous substances, and promoting energy-efficient and environmentally benign chemical processes. Discussion of ethical considerations related to environmental safety and responsible research conduct. Strategies to incorporate green chemistry concepts into research design, experimentation, and industrial applications to promote sustainable innovation in chemistry.

Keywords: Green Chemistry, Sustainability, Environmental Safety, Ethical Research, Waste Minimization, Eco-friendly Processes, Sustainable Development Goals.

Course Learning Outcomes (CLO)

Upon successful completion of this Course, learners will be able to:

- Explain the purpose and types of chemistry research and distinguish among basic, applied, experimental, and computational research approaches.
- Formulate testable hypotheses and identify relevant research gaps through effective use of chemical databases and critical literature review.
- Analyze and interpret scientific articles to extract research objectives, methodologies, results, and conclusions relevant to chemical investigations.
- Design concise and well-structured research proposals with clearly defined titles, objectives, methodologies, timelines, and expected outcomes.
- Describe ethical principles in chemical research, including responsible conduct, authorship norms, plagiarism, fabrication, falsification, and publication integrity.
- Recognize predatory journals and unethical publishing practices and apply tools like Turnitin or

DrillBit to ensure research originality.

- Utilize standard computational tools (MS Word, Excel, PowerPoint) for documentation, data analysis, and scientific presentations.
- Draw chemical structures and reaction schemes using ChemDraw and ChemSketch.
- Develop basic programs to solve chemistry-related problems involving thermodynamics, kinetics, radioactive decay, and solution chemistry.
- Perform essential laboratory techniques such as solution preparation, recrystallization, distillation, and standardization with attention to safety and quality control.
- Demonstrate proper laboratory safety practices, chemical handling procedures, and adherence to waste disposal protocols.
- Integrate green chemistry principles into research design and evaluate their contribution to sustainable development and environmental safety.

Suggested Readings:

Books

1. Mukherjee, K.C., Rasashastra: The Science of Indian Alchemy and Chemistry, Motilal Banarsidass, Delhi.
2. Kothari, C.R., Garg, G., Research Methodology. Methods and Techniques, New Age International Publishers.
3. Gastel, B., Day, R.A., How to Write and Publish a Scientific Paper, Cambridge University Press.
4. Davis, M., Scientific Papers and Presentations, Academic Press.
5. Shamoo, A.E., Resnik, D.B., Responsible Conduct of Research, Oxford University Press.
6. Steneck, N.H., Introduction to the Responsible Conduct of Research, Office of Research Integrity (ORI).
7. UGC, Research and Publication Ethics (Available as e-book on ugc.ac.in).
8. Lewars, E.G., Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer.
9. Billo, E.J., Excel for Scientists and Engineers, Wiley-Interscience.
10. Mendham, J., Denney, R.C., Barnes, J.D., Thomas, M., Sivasankar, B.S., Vogel's Textbook of Quantitative Chemical Analysis, Pearson.
11. American Chemical Society (ACS), Safety in Academic Chemistry Laboratories, Vol. 1 and 2.
12. Mukherjee, J.C., A Textbook of Practical Chemistry, Orient BlackSwan.
13. Anastas, P.T., Warner, J.C., Green Chemistry: Theory and Practice, Oxford University Press.
14. Doxsee, K.M., Hutchison, J.E., Green Organic Chemistry Strategies, Tools, and Laboratory Experiments, Brooks/Cole
15. Benvenuto, M.A., Sustainable Green Chemistry: A Teaching Approach, De Gruyter. 16. ChemDraw and ChemSketch user manuals (Available from PerkinElmer and ACD/Labs)

Suggested equivalent online courses and Web Sources:

- https://archive.nptel.ac.in/course.html
- https://ugcmoocs.inflibnet.ac.in/index.php/courses/moocs
- https://swayam.gov.in/explorer

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Practical)*	*Marks*	
M.Sc. II SEM	Core	PC- 21	**Advanced Physical Chemistry**	Max: 100	Min: 40

Duration: 6 hours

Course Learning Outcomes (CLO)

Upon successful completion of this Education, learners will be able to:

- Analyze the temperature dependence of thermodynamic parameters like enthalpy of solution, solubility, and calculate the preparation and standardization of solutions
- Investigate the effects of ionic strength on reaction, temperature, catalysts, and sand mechanisms.
- Apply electrochemical techniques to estimate dissociation constants, identify metal ions and solubility product.
- Demonstrate accurate preparation and standardization of solutions along with precise serial dilution techniques.
- Utilize modern chemical drawing software to represent molecular structures and reaction pathways effectively.
- Apply statistical and graphical tools to analyse and present chemical with clarity.
- Operate and calibrate fundamental analytical instruments, ensuring reliable measurements.
- Perform eco-friendly synthesis of nanoparticles using natural plant extracts.
- Synthesize important organic compounds using classical organic reactions with practical understanding.
- Extract and isolate valuable organic compounds from natural sources using standard laboratory methods

Practical List:

1. Determination of partial molar volume of solute (e.g., KCl) and solvent in a binary mixture.
2. Determination of the temperature dependence of the solubility compound in two solvents having similar intramolecular (benzoic acid in water and in DMSO water mixture and calculation of the molar heat of solution.
3. Determination of energy and enthalpy of activation KMnO4 and benzyl alcohol in an acidic medium.
4. Determination of solubility and solubility product (e.g., PbSO4, BaSO4) conductometrically.. soluble salts
5. Determination of the strength of a strong conductometrically/ potentiometrically acidic in a given mixture pH metrically.
6. Determination of strengths of halides potentiometrically.
7. Determination of the rate constant: The reaction between potassium Persulfate and potassium iodide
8. Determination of the pka an acid using a pH meter. Gibbs free energy change) of an organic
9. Verification of Beer's law using a colorimetric method.
10. Investigation of the antogale satalytic reaction between potassium permanganate and oxalic acid and determination of the enthalpy change (AH) and activation energy (Ea).
11. Measurement of the surface tension of organic liquids using a stalagmometer.

12. Determination of the relative viscosity of organic liquids using an Ostwald Viscometer.
13. Investigation of the adsorption of oxalic acid on activated charcoal and examination of the validity of the Langmuir and the Freundlich adsorption isotherms.
14. Influence of ionic strength on the rate constant of the reaction between potassium iodide (KI) and potassium persulfate (KS2O).
15. Study of the kinetics of acid-catalysed hydrolysis of an ester by titrimetric.

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Practical)*	*Marks*	
M.Sc. II SEM	Core	PC- 22	**Research Methodology for Chemists**	Max: 100	Min: 40

Duration: 6 hours

Course Learning Outcomes (CLO)

Upon successful completion of this, the students will be able to:

- Demonstrate accurate preparation along with precise serial dilution and Standardization of solutions.
- Utilize modern chemical software to represent molecules.
- Apply statistical and graphical tools to analyse and present chemical data with clarity.
- Operate and calibrate fundamental analytical instruments, ensuring reliable measurements.
- Perform-Friendly synthesis of nanoparticles using natural plant
- Synthesize important organic compounds using classical organic reactions with practical understanding.
- Tract and isolate valuable organic compounds from natural sources using standard laboratory methods.

Practical List:

1. Preparation of primary and secondary standard solutions and performance of accurate serial dilutions using volumetric techniques.
2. Drawing of structures/schemes and reaction mechanisms using chemical drawing software such as ChemDraw, ChemSketch, and MarvinSketch, etc.
3. Analysis and graphical/statistical representation of chemical data using software like MS Excel, PowerPoint, and open-source alternatives.
4. Calibration and operation of analytical instruments such as pH meters, potentiometers, and conductometers using standard buffer and salt solutions.
5. Demonstration of green synthesis of nanoparticles using natural extracts such as tea, tulsi (basil), aloe vera, lemon juice, and ginger etc.
6. Synthesis of ZnO Nanoparticles via Sol-Gel Method.
7. Green Synthesis of CuO Nanoparticles.
8. Synthesis of Graphene Oxide (GO) using Hummers Method.
9. Characterization of Catalyst/ Compounds using spectral Education

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Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	Core	**Course MCH 301**	**Inorganic Chemistry**	Max: 40	Min: 14

COURSE OBJECTIVE:

To provide an overview of group theory, enhance the knowledge of reaction mechanism of transition metals, theory, principle, and applications of nanomaterials, ESR, and *Mössbauer Spectroscopy.*

UNIT-1

Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations

UNIT-2

Group theory and vibrational Spectroscopy. Group theory to symmetry, shapes, and molecular energy level diagrams of molecules like BF_3, NH_3 (AB_3 type), $[Pt(NH_3)_4]^{2+}$, $[Ni(CN)_4]^{2-}$ (AB_4 type), and $[Co(NH_3)_6]^{3+}$ (AB_6 type) molecules. Modes of bonding of ligands such as SCN^-, β-ketoenolate and related ligands, nitrate ion, and carboxylates

Application of group theory to Spectroscopy. Use of group theory in predicting IR and Raman active modes in some simple molecules of C_{2v}, C_{3v}, and $D_{\infty h}$ point groups.

UNIT- 3

Nanomaterials: Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms.

Ceramics- Ceramic Structures, mechanical properties, clay products. Refracrtories, characterization, properties, and applications.

Microscopic Composites dispersion strengthened and particle-reinforced composites, macroscopic composites.

UNIT- 4

Electron Spin Resonance Spectroscopy. Basic principles, hyperfine and superhyperfine splitting, g value, and factors affecting g values, applications to transition metal complexes.

UNIT-5

Mössbauer Spectroscopy. Basic principles, spectral parameters, and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds, including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds -nature of M-L bond, coordination number, structure, and (3) detection of oxidation state

COURSE OUTCOME:

By the end of this course student will be able to-

- Gain a thorough knowledge about Group theory and applications to molecules.
- Build the concept of Electron Spin Resonance and Mossbauer Spectroscopy and their application in structure elucidation.

Suggested Readings:

1. Jag Mohan. (2018). Organic Spectroscopy: Principles and Applications (II Edition). New Delhi: Narose Publishing House.

2. Kemp, W. (2017). Organic Spectroscopy (III Edition). New York: Palgrave Macmillan.

3. Sharma, Y. R. (2013). Elementary Organic Spectroscopy: Principles and Chemical Applications (Revised V Edition). New Delhi: S. Chand & Company Limited.

4. Silverstein, R. M., Webster, F. X., & Kiemle, D. (2014). Spectroscopy of Organic Compounds (VIII Edition). New York: John Wiley & Sons.

5. Levine, I. N. (2013). Quantum Chemistry (VII Edition). New Delhi: Pearson Education Pvt. Ltd.

6. Drago, R.S. (2012). Physical Methods in Inorganic Chemistry. New York: East- West Press Pvt. Ltd.

7. Banwell.,(2017). Fundamentals of Molecular & Spectroscopy (IV Edition), McGraw-Hill Education (India) Pvt. Limited

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	Core	Course MCH **302**	**Physical Chemistry**	Max: 40	Min: 14

COURSE OBJECTIVE:

To understand the concept of Molecular orbital theory, Crystal defects, *Electronic Properties, and Band Theory.*

UNIT- 1

Electronic Structure of Atoms. Electronic configuration, Russell-Saunders terms and coupling scheme, Slater parameters, magnetic effects. Zeeman splitting; virial theorem.

UNIT-2

Molecular Orbital Theory. Hückel theory of conjugated systems, bond order, and charge density calculations. Applications to ethylene, butadiene, and cyclobutadiene. Introduction to extended Hückel theory.

UNIT- 3

Homogeneous Catalysis. Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, and Zeigler-Natta polymerization of olefins.

Heterogeneous Catalysis. Thermodynamics of active centers, mechanism of heterogeneous catalysis; structural promotion and structural modification.

UNIT- 4

Crystal Defects. Perfect and imperfect crystals, stoichiometric and non-stoichiometric defects. Intrinsic and extrinsic defects, point defects, line and plane defects, Schottky and Frenkel defects.

Solid State Reactions. General principles, coprecipitation as a precursor to solid-state reactions, and factors affecting solid-state reactions.

UNIT V

Electronic Properties and Band Theory. Metals, insulators, and semiconductors. Electronic structure of solids: Band theory; band structure of metals, insulators, and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, and superconductors.

Course Outcome:

By the end of this course, students will be able to

- Develop concepts of Electronic Structure of Atoms and Molecular Orbital Theory and their applications.
- Enhance the knowledge about Homogeneous and Heterogeneous Catalysis.
- Develop an understanding of the Crystal defects and solid-state Reactions
- Build concepts of Electronic Properties and Band theory, types and applications on insulators, semiconductors, and superconductors.

Suggested Readings:

1. Bahl, A., Bahl, B. S., & Tuli, G. D, (2014). Essentials of Physical Chemistry (VEdition). New Delhi: S. Chand & Company.

2. Puri, B.R., Sharma, L.R., & Pathania, M.S. (2015). Elements of Physical Chemistry. Jalandhar: Vishal Publishing House.

3. Laidler, K. J. (2004). Chemical Kinetics (III Edition). New Delhi: Pearson Education Publishing. Indian Branch.

4. Gurdeep Raj, Chemical Kinetics, Goel Publishing House.

5. A.A.Frost and R.G.Pearson, Kinetics and Mechanism, Wiley Eastern, Pvt. Ltd.

6. Emmet, P. H. (1954). Catalysis (Vol I and II). Reinhold

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	Core	Course MCH 303	**Spectroscopy III**	Max: 40	Min: 14

COURSE OBJECTIVE:

To understand the principles, theories, instrumentation, and applications of C^{13}NMR, Mass, Electron diffraction, and neutron diffraction spectroscopic techniques

UNIT- 1

^{13}C-NMR Spectroscopy General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), wide band H-decoupled and off-resonance H-decoupled spectra. Calculation of chemical shift values for alkanes and substituted benzene. Two-dimensional NMR spectroscopy. COSY, and DEPT techniques. *Conjoint Spectroscopy Problems.* Application of UV, IR, Raman, NMR and Mass spectrometry for elucidation of the structure of organic compounds.

UNIT- 2

Mass Spectrometry-Part I. Ion production, electron ionisation (EI), chemical ionisation (CI), field desorption (FD), field ionisation (FI), and fast atom bombardment (FAB). Atmospheric pressure ionisation techniques. Electrospray ionisation, and atmospheric pressure chemical ionisation. Thermospray ionisation. Matrix-assisted laser desorption ionisation (MALDI). Mass analysers. Magnetic sector analysers. Quadrupolar analysers, ion trap, time-of-flight (TOF), ion cyclotron resonance (ICR).Electron multiplier. Tandem mass spectrometry (MS/MS).

UNIT- 3

*Mass Spectrometry-Part II.*Isotopic abundance. Electron ionisation and fragmentation (positive ions).Molecular ion peak, metastable peak. McLafferty rearrangement. Nitrogen rule. Parity rule. Mass spectral fragmentation of organic compounds containing common functional groups (alkanes, alkenes, alkynes, halo-compounds, alcohols, amines, carbonyl compounds, aromatic compounds).

High resolution mass spectrometry. Interpretation of mass spectra. Problems based on mass spectrometry of organic compounds.

UNIT- 4

X-ray Diffraction. Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor, and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis.

UNIT- 5

Electron Diffraction. Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of the structure of simple gas phase molecules. Low-energy electron diffraction and structure of surfaces.

Neutron Diffraction. Scattering of neutrons by solids and liquids, magnetic scattering, and measurement techniques. Elucidation of the structure of the magnetically ordered unit cell.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand C13 NMR and its application in structure elucidation.
- Build concepts of Mass spectrometry, its techniques, applications, and interpretation of spectra.
- Understand and apply the concepts of X Ray, Electron, and Neutron diffraction, their types, and applications for the structure elucidation of organic compounds
- Develop an understanding of Conjoint Spectroscopy for elucidation of the structure of organic compounds using UV, IR, Raman, NMR, and Mass Spectroscopy.

Suggested Readings:

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
3. Physical Methods in Chemistry, R.S. Drago, Saunders College.
4. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw-Hill.
5. Basic Principles of Spectroscopy, R. Chang, McGraw-Hill.
6. Introduction to Photoelectron Spectroscopy: P. K. Ghosh, John Wiley.
7. Macromolecules: Structure and Function, F. Wold, Prentice Hall.
8. Fundamentals of molecular spectroscopy, C.N. Banwell, Tata McGraw-Hill, New Delhi.
9. Instrumental Methods of Analysis, Willard, Meritt, and Dean.

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	**Elective** A	**Course MCH 304**	**Medicinal Chemistry**	Max: 40	Min: 14

COURSE OBJECTIVE

- To understand the basics of Medicinal chemistry, drug targets, drug metabolism, membranes, and receptors in the drug delivery process.
- To apply the various theories of Drugs, their mechanism, and modes of action for various kinds of drugs

UNIT- 1

Structure and activity. Relationship between chemical structure and biological activity (SAR).Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson analysis and Hansch analysis.

UNIT- 2

Pharmacodynamics. Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulfonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, and significance of drug metabolism in medicinal chemistry.

UNIT- 3

Antibiotics and antibacterials. Introduction, Antibiotic β-Lactam type - Penicillins, Cephalosporins, Antitubercular. Streptomycin, Broad-spectrum antibiotics.Tetracyclines, Anticancer – Dactinomycin (Actinomycin D)

UNIT- 4

Antifungal polyenes, Antibacterials. Ciprofloxacin, Norfloxacin, Antiviral. Acyclovir Antimalarials. Chemotherapy of malaria. SAR.Chloroquine, Chloroguanide, and Mefloquine

UNIT- 5

Non-steroidal Anti-inflammatory Drugs. Diclofenac Sodium, Ibuprofen, and Netopam Antihistaminic and antiasthmatic agents: Terfenadine, Cinnarizine, Salbutamol, and Beclomethasone dipropionate.

COURSE OUTCOME:

By the end of this course, students will be able to

- Understand Medicinal Chemistry and its application in pharmaceutical chemistry.
- Develop an understanding of Structure and Reactivity, Pharmacodynamics in Drug Design, Metabolism, and Development.
- Enhance the knowledge about Antibiotics, Antibacterials, Antifungals, and NSA Drugs, their structure, synthesis, mode of action, advantages, and disadvantages.

Suggested Readings:

1. Ahluwalia, V. K. (2012). Green Chemistry-Environmentally Benign Reactions. New Delhi: Ane Books Pvt Ltd.

2. Ghose, J. (2012). A Text book of Pharmaceutical Chemistry. New Delhi: S. Chand Pub Ltd.

3. Ilango, K., & Valentina, P. (2017). Text Book of Medicinal Chemistry. Vol II. Chennai: Keerthi Publishers.

4. Ashutosh Kar, (2018). Medicinal Chemistry (III Edition). New Delhi: New Age International Publishers. 5. Stanley E. Manahan, (2006). Green Chemistry and the Ten Commandments of Sustainability (II Edition). Columbia, Missouri U.S.A: ChemChar Research. Inc Publishers Columbia.

6. Chatterjea, M. N., & Shinde, R. (2012). Textbook of Medicinal Biochemistry. New Delhi: Jaypee Brothers. Medical Publishers (P) Ltd. 7. G.L. Patrick, (2013). Introduction to Medicinal Chemistry (I Edition). UK: Oxford University Pre

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	**Elective** B	**Course MCH 304**	**Chemistry of Natural Products**	Max: 40	Min: 14

COURSE OBJECTIVE

To understand the importance of natural products, their structure, synthesis, and applications.

UNIT- 1

Terpenoids. General methods of structure elucidation. Isoprene rule.Structure determination, stereochemistry, and synthesis of the following representative molecules: citral, geraniol, □-terpineol, menthol, □-pinene, camphor, and abietic acid. Biosynthesis of terpenoids.

UNIT- 2

Alkaloids. General methods of structure elucidation. Structure determination, stereochemistry, and synthesis of the following representative molecules: ephedrine, nicotine, atropine, quinine and morphine. Biosynthesis of alkaloids.

UNIT- 3

Steroids. Structure elucidation, stereochemistry, and chemical synthesis of cholesterol, bile acids, androsterone, testosterone, estrone, progestrone, and aldosterone. Biosynthesis of steroids.

UNIT- 4

*Plant Pigments.Carotenoids.*Structure and synthesis of □-carotene. *Flavonoids.*Nature, general methods for structure elucidation and synthesis of anthocyanins and flavones.Structure and synthesis of cyanidin chloride, cyanin, flavone, flavonol and quercetin.Biosynthesis of flavonoids.*Chlorophyll.*Chemistry of chlorophyll.

UNIT- 5

*Vitamins and Antibiotics.Vitamins.*Structure and synthesis of vitamin B_1 (thiamine), B_2 (riboflavin) and B_6 (pyridoxine). Chemistry of Vitamin B_{12}. *Antibiotics.*Structure and synthesis of penicillins and chloramphenicol.

Course Outcome:

By the end of this course, the student will be able to

- Understand the Chemistry of Natural Products and their application in pharmaceutical chemistry.
- Develop an understanding of Alkaloids, Steroids, Carotenoids, Vitamins, Flavonoids, and Antibiotics, their structure, synthesis, and applications.

Suggested Readings:

1. Chatwal, G. R. (2015). Organic Chemistry of Natural Products Vol. II. New Delhi: Himalaya Publishing House.

2. Finar, I. L. (2013). Organic Chemistry Vol. II: Stereochemistry and the Chemistry of Natural Products (V Edition). New Delhi: Pearson Education, Ltd.

3. Chatwal, G. R. (2015). Organic Chemistry of Natural Products. Vol. I. New Delhi: Himalaya Publishing House.

4. Saluja, M. P., Raj Kumar & Anuja Agarwal (2017). Advanced Natural Products (Revised IV Edition). Meerut: Krishna Prakashan Media (P) Ltd.

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Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	**Elective C**	**Course MCH 304**	**Polymers**	Max: 40	Min: 14

COURSE OBJECTIVE:

- To enable the student to get knowledge about the basic concepts of polymerization, and classification.
- To provide knowledge about properties, structure, processing techniques and applications of commercial polymers.

UNIT- 1

Basics of Polymers. Repeating units, degree of polymerisation, linear, branched and network polymers. Classification of polymers. Addition, radical, ionic, coordination and condensation polymerisation; their mechanism and examples.

Polymerisation conditions and polymer reactions. Polymerisation in homogeneous and heterogeneous systems.

UNIT-2

Polymer Characterisation. Significance of molecular weight of polymer. Polydispersive average molecular weight. Number, weight and viscosity average weights. Measurement of molecular weights. End group, viscosity, light scattering, osmotic and ultracentrifugation methods. Chemical and spectroscopic analysis of polymers.X-Ray diffraction study. Thermal analysis, tensile strength, fatique, impact. Tear resistance. Hardness and abrasion resistance.

UNIT- 3

Structure and Properties. Configuration of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers. Polymer structure and physical properties; crystalline melting point Tm, melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

UNIT- 4

Polymer Processing. Plastics, elastomers and fibres. Compounding. Processing techniques, Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

UNIT- 5

Properties of Polymers. Properties of polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers. Fire retarding polymers, and electrically conducting polymers. Biomedical polymers. Contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

COURSE OBJECTIVE:

By the end of this course student will be able to-

- Create an understanding Polymer Chemistry and its industrial applications.
- Develop an understanding of Polymer basics and characterization, its structure and properties.
- Understand the Polymer processing and their properties and applications in biomedical field.

Suggested Readings:

1. Billmeyer, F. W. (2003). Text Book of Polymer Science (III Edition). New York: John Wiley.
2. Alcock, H. R., Lampe, F. W., & Mark, J. E. (2003). Contemporary Polymer Chemistry (III Edition). NJ: Prentice Hall Englewood Cliffs.
3. Flory, P. J. (1953). Principles of Polymer Chemistry. New York: Cornell University Press.
4. Odian, G. (2004). Principles of Polymerization (IV Edition). New York: John Wiley & Sons.
5. Textbook of Polymer Science, F.W. Billmeyer, Jr., Wiley.
6. Polymer Science, V.R. Gwariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
7. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
8. Contomporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
9. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.

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Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. IV SEM	Core	**Course MCH 401**	**Inorganic Chemistry**	Max: 40	Min: 14

COURSE OBJECTIVE: To enable the students in understanding various Aspects of Bioinorganic chemistry, Electron Transfer in Biology, organic reagent in organic chemistry, Photosystems and energy transfer concept

Unit- 1

Organic Reagents in Inorganic Chemistry: Chelation, factors determining the stability of

chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use ofthe following reagents in analysis:

(a) Dimethylglyoxime (in analytical chemistry)

(b) EDTA (in analytical chemistry)

(c) 8-Hydroxyquinoline (in analytical chemistry)

(d) 1,10-Phenanthroline (in analytical chemistry)

(e) Thiosemicarbazones (in analytical chemistry)

(f) Dithiazone (in analytical chemistry)

UNIT- 2

Bioinorganic Chemistry. Metal containing enzymes: Carboxypeptidase-A, Carbonic anhydrase, arginase, urease, DNA polymerase, phosphoglucomutase (glucose storage): structure and reactivity

UNIT- 3

Bioinorganic Chemistry: Metal complexes in transmission of energy: Chlorophylls, photosystem-I and photosystem-II in cleavage of water, model systems.

UNIT- 4

/Electron Transfer in Biology: Structure and function of metalloproteins in electron transport processes-cytochromes and ion-sulphur proteins. Nitrogenase: Biological nitrogen fixation, molybdenum nitrogenase-structure and function.

UNIT- 5

Transport and Storage of Dioxygen Structure and function of haemoglobin, myoglobin, hemocyanin and hemerythrin. Poisoning towards haemoglobin and myoglobin.

COUSE OUTCOME:

By the end of this course student will be able to-

- Gain a thorough knowledge about Organic Reagents in Inorganic Chemistry, their structure and applications
- Develop the concept of Bioinorganic Chemistry, metal containing enzymes and metal complexes in energy transmission.
- Build the concept of Electron transfer in Biology, transport and storage of dioxygen.

Suggested Readings:

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. ed. G.L. Eichturn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley, Environmental Chemistry, S. E. Manahan, Lewis Publishers.

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. IV SEM	Core	Course MCH 402	Organic synthesis strategies	Max: 40	Min: 14

COURSE OBJECTIVE

- To enable students to know various strategies used in retro synthetic analysis, chemistry of various organic reagents and the chemistry of Oxidation and Reduction reactions
- To understand basics of asymmetric synthesis, chemistry of various reagents, reaction and mechanism of selected named reactions, the chemistry of protecting and deprotecting groups and synthesis of selected drug molecules.

UNIT- 1

Oxidation. Oxidation of carbon carbon double bond. Perhydroxylation, potassium permanganate, osmium tetroxide, iodine together with silver carboxylates, ozonolysis. Enantioselective epoxidation of allylic alcohols (Sharpless epoxidation).Oxidation of alcohols. Chromic acid, chromiun (VI) oxide-pyridine complexes, manganese (IV) oxide, silver carbonate, oxidation via alkoxy sulphonium salts. Baeyer-Villiger oxidation of ketones. Oxidation with ruthenium tetroxide, thallium(III) nitrate and iodobenzene diacetate.

UNIT- 2

Reduction. Catalytic hydrogenation (homogeneous and heterogenous).Stereochemistry and mechanism, selectivity of reduction.Reduction by dissolving metals. Metal and acid, metal and alcohol, metal and ammonia.

Reduction by hydride-transfer reagents.Aluminium alkoxides, lithium aluminium hydride, sodium borohydride, lithium hydrido-alkoxyaluminates.Wolff-Kishner reduction. Reduction with di-imide

UNIT- 3

Designing organic synthesis. The Disconnection Approach. Basic principles, synthons, functional group interconversions. Order of events in organic synthesis. One group CX disconnections and two group CX disconnections. Chemoselectivity. Reversal of polarity (umpolung). Amine synthesis

UNIT- 4

Organic Reagents: Reagents in organic synthesis: Willkinson catalyst, Lithium dialkylcuprates(Gilman's reagents), Lithium diisopropylamide (LDA), 1,3-Dithiane (Umpolung), Dicyclohexylcarbobiimide (DCC), and Trimethylsilyliodide, DDQ, SeO2, Baker yeast, Tri-nbutyltinhydride, Nickel tetracarbonyl, Trimethylchlorosilane

UNIT- 5

Rearrangement General mechanistic considerations-nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Backmann, Hofmann, Curtius, Schmidt, Benzidine, Baeyer-Villiger, Shapiro reaction, Witting rearrangement, and Stevens rearrangement.

COURSE OUTCOME

By the end of this course, students will be able to

- Create an understanding of Organic Synthesis Strategies and their application.
- Gain knowledge about concepts of Oxidation, Reduction, and Rearrangement reactions and their applications to some known reactions.
- Develop an understanding Disconnection approach, types, and chemoselectivity.

Suggested Readings:

1. Warren,S. (2010). Organic Synthesis the Disconnection approach, Wiley and sons,

2. Renuga,S. (2016). Name reactions and reagents in organic synthesis, Vishal Publishing Co. Jalandhar-Delhi.

3. Nasir Hussain and Saba Khan, (2016). Reactions and Reagents, Himanshu Publications, New Delhi.

4. Clayden, J., Greeves, N. & Warren, S. (2012). Organic Chemistry (II Edition). Oxford University Press, Oxford.

5. Sanyal, S. N. (2014). Reactions, Rearrangements and Reagents (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).

6. Smith, M. B. (2015). March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure(VII Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.

6. Warren, S., & Wyatt, P. (2008). Organic Synthesis: The Disconnection Approach (II Edition). John Wiley & Sons Ltd., Chichester.

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. IV SEM	**Departmental Elective**	Course **MCH 403 A**	**Environmental Chemistry**	Max: 40	Min: 14

COURSE OBJECTIVE:

To provide an overview of water, air, soil, radioactive, and noise pollution, including methods for the prevention of pollution and its control measures.

UNIT- 1

Environment Introduction. Composition of atmosphere, vertical temperature, temperature inversion, heat budget of the earth, atmospheric system, vertical stability atmosphere, Biochemical cycles of C, N, P, S and O. Biodistribution of elements.

Hydrosphere Chemical composition of water bodies-lakes, streams, rivers and wetlands etc. Hydrological cycle Aquatic pollution – Inorganic, organic, pesticide, agriculture, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and microorganisms. Water quality standards.Analytical methods of measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.

UNIT- 2

Soils-Composition, micro and macro nutrients, pollution – fertilizers, pesticides, plastics, and metals.Waste treatment.

Atmosphere Chemical composition of atmosphere – particles, ions, and radicals, and their formation. Chemical and photochemical reactions in the atmosphere, smog formation, oxides of N,C, S, O, and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Unit- 3

Industrial Pollution

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Environmental disasters – Chernobyl, Three Mile Island, Seveso, and Minamata disasters, Japan tsunami.

UNIT- 4

Environmental Toxicology Toxic heavy metals**:** Mercury, lead, arsenic, and cadmium. Causes of toxicity. Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound**:** Pesticides, classification, properties and uses of organochlorine and ionospheric pesticides, detection and damaging effects.

Unit-5

Aquatic Chemistry and Water Pollution. Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD, and COD. Aerobic and anaerobic reactions of organic sulphur and nitrogen compounds in water acid base chemistry of fresh water and sea water. Aluminum, nitrate, and fluoride in water. Petrification. Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification, and disinfection.

COURSE OUTCOME:

By the end of this course, students will be able to

- Understand Environmental Chemistry and its concepts.
- Build concepts of the Hydrosphere, Atmosphere and Soil, their composition, and the side effects of pollution.
- Understand and apply the concepts of industrial pollution and study of some famous environmental disasters.
- Understand and apply the concepts Water pollution, purification and treatment and study of some prime pollutants.
- Develop an understanding of environmental toxicology and some toxic Organic Compounds.

Suggested Readings:

1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
2. Chemistry of Atmospheres, R.P. Wayne, Oxford.
3. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
5. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.
6. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
7. Environmental chemistry, Sharma and Kaur, Krishna Publishers.
8. Environmental Chemistry, Analysis, S.M. Khopkar, Wiley Eastern.
9. Standard Method of Chemical Analysis, F.J.WelcherVol.III, VanNostr and ReinholdCo.
10. Environmental Toxicology, Ed.J.Rose, Gordon and Breach Science Publication. 7. Environmental Chemistry, C. Baird, W.H.Freeman

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. IV SEM	Departmental Elective	Course MCH 403 B	**Chemistry of Materials**	Max: 40	Min: 14

COURSE OBJECTIVE: To bridge the gap between fundamental ideas of chemistry to modern research and industry-related topics.

UNIT- 1

Ceramics, Composites and Nanomaterials. Ceramic structures, mechanical properties, clay products.Refractories, characterization, properties and applications. Microscopic composites, dispersion-strengthened and particle-reinforced composites, macroscopic composites.Nanocrystalline phase, preparation procedures, properties and applications.

UNIT- 2

Liquid Crystals. Thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases. Molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

UNIT- 3

Ionic Conductors. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors, phase transtions and mechanism of conduction in superionic conductors. Examples and applications of ionic conductors.

UNIT- 4

High Tc Materials. High-Tc superconductivity. Preparation and characterization of 1-2-3 and 2-1-4 materials. Normal state properties, anisotropy, temperature dependence of electrical resistance, and optical phonon modes. Superconducting state; heat capacity; coherence length, elastic constants, microwave absorption-pairing and multigap structure in high Tc materials. Applications of high Tc materials.

UNIT- 5

Organic Solids, Fullerenes, Molecular Devices. Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes, doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches, sensors. Non-linear optical materials, non-linear optical effects. Molecular hyperpolarisability.

Course Outcome:

By the end of this course student will be able to-

- Develop an understanding Chemistry of Materials and its application in chemistry.
- Develop an understanding of Ceramics, Composites and Nanomaterials, their structure, characterization, properties and applications.
- Understand and apply the concepts Liquid Crystals and Ionic conductors, their structure, types, properties and applications in wide variety of chemistry, physics and allied fields.
- Build the concept of Superconductors and its indepth study for understanding of their possible applications.
- Build concepts of Organic solids, Fullerenes and Molecular Devices and its applications.

Suggested Readings:

1. Materials Science and Engineering: An Introduction (Hardcover) by William D. Callister Jr.
2. Introduction to Materials Science for Engineers by James Shackelford
3. Foundations of Materials Science and Engineering by William Smith
4. The Science and Engineering of Materials by Donald Askeland and Wendelin Wright
5. Material Science and Metallurgy by OP Khanna

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. IV SEM	**Open Elective**	Course **MCH 404 A**	Biochemistry	Max: 40	Min: 14

COURSE OBJECTIVE: To provide a comprehensive introduction to biochemistry and to learn the chemistry of enzymes, structures of nucleic acids and biosynthesis of proteins.

UNIT-1

Carbohydrates: Types of naturally occurring sugars: Deoxy-sugars, amino sugars, branched chain sugars. General methods of structure and ring size determination with particular reference to maltose, lactose, sucrose, pectin, starch and cellulose, photosynthesis of carbohydrates, metabolism of glucose, Glycoside- (amygdalin).

UNIT-2

Amino acid, peptides and proteins: General methods of peptide synthesis, sequence determination. Chemistry of insulin and oxytocin.Purines and nucleic acid. Chemistry of uric acid, adenine, protein synthesis.

UNIT-3

Vitamins: A general study, detailed study of chemistry of thiamine (Vitamin B1), Ascorbic acid

(Vitamin C), Pantothenic acid, biotin (Vitamin H), α-tocopherol (Vitamin E), Biological importance of vitamins.

UNIT- 4

Enzymes: Nomenclature and classification, extraction and purification, Remarkable properties of enzymes like catalytic power, specificity and regulation, Proximity effects and molecular adaptation, Chemical and biological catalysis. Mechanism of enzyme action: Transition state theory, orientation and steric effect, acid base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms (chymotrypsin, ribo nuclease, lysozyme and carboxypetidase A). Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

UNIT-5

(A) Kinds of reactions catalyzed by Enzymes: Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate addition and elimination reactions, enolic intermediates in isomerization reactions, β- cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation reactions.

(B) Coenzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate

pyridoxal phosphate, NAD+, NADP+, FMN, FAD, Lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand Biochemistry and its application in chemistry.
- Gain knowledge about concept of Carbohydrates, Amino Acids, Vitamins and enzymes their structure, types, properties, metabolism, synthesis and uses in the human body.

Suggested Readings:

1. Biochemistry, D. Voet and J.G. Voet, John Wiley.
2. Principles of Biochemistry, A.L. Lehninger, D.L. Nelson and M.M. Cox, CBS Publishers, Delhi.
3. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.

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Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. IV SEM	**Open Elective**	Course **MCH 404 B**	**Bioorganic Chemistry**	Max: 40	Min: 14

COURSE OBJECTIVE

To Understand reactions Catalyzed by Enzymes, chemical strategies and mechanisms behind enzyme catalysis, enzyme models and Biotechnological Application of enzymes.

Unit-1

Introduction: Basic Consideration, Proximity effects and molecular adoption. Enzymes: Introduction, Chemical and Biological catalysis, remarkable properties of enzymes,Nomenclature and classification, concept and identification of active site by use of inhibitors, reversible& irreversible inhibition.

Unit-2

Kinds of Reactions Catalyzed by Enzymes: B-cleavage and consideration, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation. Mechanism of Enzyme action: Transition state theory, Orientation and steric effect, acid-base catalysis, covalent catalysis. Co-Enzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions of coenzyme A.

Unit-3

Enzyme Models :Host guest chemistry, Chiral recognition and catalysis, molecular recognition,

molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, cryptates, cyclodextrins, cyclodextrin based enzyme models, Calixarenes, ionophores, micelles synthetic

enzyme or synzymes.

Unit-4

Biotechnological Application of enzymes: Large scale production and purification of enzymes,techniques and methods of immobilization of enzyme activity, application of immobilized enzymes, effect of immobilization on Enzyme activity, application of immobilized enzymes. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Unit-5

Metalloenzymes Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin; Coenzymes; Molybdenum enzyme: xanthine oxidase; Zinc enzymes: carbonic anhydrase, carboxy peptidase and interchangeability of zinc and cobalt in enzymes; Vitamin B12 and B12 coenzymes; Iron storage, transport, biomineralization and siderophores, ferritin and transferrins..

Course Outcome:

By the end of this course student will be able to-

- Understand of Bioorganic chemistry and its applications.
- Gain knowledge about Enzymes, their nomenclature, classification, properties,, models and biotechnological and clinical applications.
- Apply knowledge of organic and bioorganic chemistry to predict chemical properties and reactivity in chemical and biological contexts and propose mechanistic hypotheses for reactions.

Suggested Readings:

1. Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi
2. Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding" by A R Fersht and W H Freeman.
3. "Bioorganic Chemistry" by H Dugas.
4. Bioorganic Chemistry: A Chemical Approach to Enzyme Action (Springer Advanced Texts in Chemistry)" by Hermann Dugas

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Department of Chemistry

Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	Practical	Course MCH 305	**Organic Chemistry**	Max: 50	Min: 18

Maximum Marks: 50 *Minimum Marks: 20*

Analysis

1. Estimation of protein by Lowry's method.
2. Estimation of carbohydrate by Anthrone's method
3. Isolation of caffeine and alkaloids from tea.
4. To determine the iodine value of the given oil or fat
5. To determine the Saponification value of the given oil or fat
6. Estimation of Ascorbic Acid i.e. vitamin C.
7. Estimation of Amino acid by Sorenson's method
8. Spectrophotometric estimation of Glucose with the help of Fehling solution

Multi Step Synthesis

1. Benzoin- benzyl- benzilic acid
2. Benzophenone –benzpinacole- benzpinacolone
3. Ethyl acetoacetate 3-methyl-1-phenylpyrazol-5-one antipyrin (phenazone)
4. Benzaldehyde benzoin benzil 5,5-diphenylhydantoin
5. Phenylhydrazine acetophenonephenylhydrazone 2-phenylindole
6. Chlorobenzene 1-chloro-2,4-dinitrobenzene 2,4-dinitrophenylhydrazine

Spectral Analysis

Interpretation of pre-recorded UV-Vis, IR, NMR, Mass, Raman spectrum and characterisation of one organic compound

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Class	*Course Type*	*Course Code*	*Course Title (Theory/Practical)*	*Marks*	
M.Sc. III SEM	Practical	Course MCH 306	**Physical Chemistry**	Max: 50	Min: 18

Maximum Marks: 50 *Minimum Marks: 20*

Conductometry

1. To determine the strength of an unknown (given weak) acid conductometrically using a standard alkali solution(strong).
2. To determine the strength of an unknown (given strong) acid conductometrically using a standard alkali solution(weak).
3. To determine the strength of an acid conductometrically using a standard alkali solution in a mixture of acids
4. To determine the dissociation constant of a weak electrolyte and to verify Ostwald's dilution law.
5. To determine the equivalent conductance of a strong electrolyte at several concentrations and hence verify the Onsager equation.
6. To find the solubility and solubility product of a sparingly soluble salt conductometrically.

pH metry

7. To determine the strength of an unknown (given weak) acid pHmetrically using a standard alkali solution(strong).
8. To determine the strength of an unknown (given strong) acid pHmetrically using a standard alkali solution(weak).
9. To determine the strength of an acid pH metrically using a standard alkali solution in a mixture of acids

Potentiometry

10. To determine the strength of an unknown (given weak) acid potentiometrically using a standard alkali solution (strong).
11. To determine the strength of an unknown (given strong) acid potentiometrically using a standard alkali solution (weak).
12. To determine the strength of an acid potentiometrically using a standard alkali solution in a mixture of acids

Spectrophotometry

13. To verify Lambert-Beer's law using a spectrophotometer.

Enzyme Kinetics

14. To study the effect of temperature on invertase enzyme activity and determine its optimum pH
15. To study of the effect of substrate concentration on enzyme activity.
16. Effect of enzyme concentration on enzyme activity