COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-24 BATCH

DIT UNIVERSITY
DEHRADUN

DETAILED COURSE STRUCTUREOF
M.SC. IN CHEMISTRY

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Year: 1st **Semester: I**

Course Category	Course Code	Course Title	L	P	Credit
CC	CH616	Inorganic Chemistry -I	3	0	3
CC	CH617	Organic Chemistry - I	3	0	3
CC	CH618	Physical Chemistry - I	3	0	3
CC	CH616P	Inorganic Chemistry -I Lab	0	4	2
CC	CH617P	Organic Chemistry - I Lab	0	4	2
CC	CH618P	Physical Chemistry - I Lab	0	4	2
CC	CH619	Analytical Chemistry-I	3	0	3
AEC		AEC Basket	2	0	2
		Total	**14**	**12**	**20**

Ability Enhancement Course Basket

Course Category	Course Code	Course Title	L	P	Credit
AEC	CH646	Biology for Chemist (for Mathematics student)	2	0	2
AEC	CH647	Mathematics for Chemist (for Biology student)	2	0	2

Year: 1st **Semester: II**

Course Category	CourseCode	Course Title	L	P	Credit
CC	CH626	Inorganic Chemistry -II	3	0	3
CC	CH627	Organic Chemistry - II	3	0	3
CC	CH628	Physical Chemistry - II	3	0	3
CC	CH626P	Inorganic Chemistry -II Lab	0	4	2
CC	CH627P	Organic Chemistry – II Lab	0	4	2
CC	CH628P	Physical Chemistry – II Lab	0	4	2
CC	CH629	Analytical Chemistry-II	3	0	3
AEC	CH648	Research Methodology and Ethics	3	0	3
		Total	**15**	**12**	**21**

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

COURSE STRUCTURE

Year: 2nd **Semester: III**

Course Category	Course Code	Course Title	L	P	Credit
CC	CH706	Molecular Spectroscopy	3	0	3
CC	CH707	Group Theory and Structure of Metal Complexes	3	0	3
CC	CH***	Elective-I	3	0	3
CC	CH***	Elective-II	3	0	3
GEC	CH746	Computer Applications in Chemistry	3	2	4
PJCT	CH736	Project - I	0	8	4
		Total	**15**	**10**	**20**

Elective-I Basket

Course Category	Course Code	Course Title	L	P	Credit
CC	CH716	**Organic Spectroscopy** (Organic Chemistry-III)	3	0	3
CC	CH717	**Micro analytical Techniques** (Analytical Chemistry-III)	3	0	3

Elective-II Basket

Course Category	Course Code	Course Title	L	P	Credit
CC	CH718	**Heterocyclic Compounds** (Organic Chemistry-IV)	3	0	3
CC	CH719	**Separation Techniques** (Analytical Chemistry-IV)	3	0	3

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Year: 2nd **Semester: IV**

Course Category	CourseCode	Course Title	L	P	Credit
CC	CH***	Elective-III	3	0	3
CC	CH***	Elective-IV	3	0	3
PJCT	CH737	Project-II	0	20	10
SEM	CH738	Seminar	0	8	4
		Total	**6**	**28**	**20**

Elective-III Basket

Course Category	Course Code	Course Title	L	P	Credit
CC	CH726	**Natural product and Medicinal Chemistry** (Organic Chemistry-V)	3	0	3
CC	CH727	**Advanced spectroscopy and diffraction methods** (Analytical Chemistry-V)	3	0	3

Elective-IV Basket

Course Category	Course Code	Course Title	L	P	Credit
CC	CH728	**Synthetic Strategies** (Organic Chemistry-VI)	3	0	3
CC	CH729	**Electroanalytical Methods** (Analytical Chemistry-VI)	3	0	3

Summary of the Credit

Year	Semester	Max Credit
1	1	20
	2	21
2	3	20
	4	20
Total		**81**

Category wise classification of the Credit

Category		Credit	Number of Subjects
CC	Departmental Core Course	54	20
GEC	Generic Elective Course	4	1
AEC	Ability Enhancement Course	5	2
PRJT/THESIS	Project	14	2
SEM	Seminar	4	1
Total		**81**	**26**

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Semester I

Course Category	Course Code	Course Title	L	P	credit
CC	CH616	Inorganic Chemistry -I	3	0	3
CC	CH617	Organic Chemistry - I	3	0	3
CC	CH618	Physical Chemistry - I	3	0	3
	CH616P	Inorganic Chemistry -I Lab	0	4	2
	CH617P	Organic Chemistry - I Lab	0	4	2
	CH618P	Physical Chemistry - I Lab	0	4	2
CC	CH619	Analytical chemistry-I	3	0	3
AEC	CH646	Biology for Chemist (for Mathematics student)	2	0	2
	CH647	Mathematics for Chemist (for Biology student)	2	0	2
		Total	**14**	**12**	**20**

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH616	Subject Title	INORGANIC CHEMISTRY -I						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	1st	**Semester**	I

Course Objective
- Understanding structure, bonding and reaction mechanism involved in inorganic solids and metal complexes.
- Applying practical aspects of inorganic chemistry in research and development.

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: Introduction to d- and f-block elements: 10 lectures
Survey to transition and inner-transition elements. Properties and compounds of various transition elements.
Structure, bonding and properties of transition metal complexes:
Different types of ligands and coordination geometry (symmetry considerations), coordination number, isomerism (recapitulation), HSAB concept, thermodynamic stability, successive and overall stability constants, determination of stoichiometry (Job's method) and stability constants by spectrophotometric, potentiometric and polarographic methods, Irving-William series, chelate and macrocyclic effect.

Unit 2: Stereochemical aspects of coordination complexes: 10 lectures
Stereoisomerism in inorganic complexes, isomerism arising out of ligand and ligand conformation, chirality and nomenclature of chiral complexes, optical rotatory dispersion (ORD) and circular dichroism (CD).
Metal-ligand bonding:
Overview of crystal field and ligand field theories of 4-, 5- and 6-coordinated complexes, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral, square pyramidal, trigonal- bipyramidal and cubic complexes, measurement of CFSE (d1 to d10) in weak and strong ligand fields, Jahn-Teller distortion, nephelauxetic series, variation of lattice energy, ionic radii and heat of hydration across 1st row transition metal ions.

Unit 3: Molecular orbital theory (MOT) of coordination compounds: 5 lectures
Composition of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ and π bonding, angular overlap model.

Unit 4: Electronic spectra of coordination compounds: 7 lectures
Energy states from spectral terms of dn configurations, selection rules for ligand-field and charge transfer transitions in metal complexes, band intensities, factors influencing band widths, splitting of various terms, Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral dn complexes, calculation of ligand field parameters, luminescence, phosphorescent complexes.

Unit 5: Magnetic properties of coordination compounds: 7 lectures

Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects (L-S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over phenomenon, spin admixed states, metal-metal direct spin interaction and super exchange spin-spin interaction through bridging ligands, ferromagnetic, anti-ferromagnetic, ferrimagnetic behaviour of transition metal compounds, effect of temperature on their magnetic properties, single molecule magnets.

Course outcomes: -

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

CO1: Compare the trends in the properties of main group elements and discuss the chemistry of Si, B, C- based compounds.

CO2: Examine and apply the structural arrangement in metals, ionic, covalent compounds and inorganic solids

CO3: Understand and differentiate different theories of coordination chemistry

CO4: Explain the reaction mechanism of different metal complex reactions

REFERENCE BOOKS:

1. Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., “Advanced Inorganic Chemistry”, 6th Ed., John Wiley & Sons, 1999.
2. Douglas, B.E., McDaniel,D.H. and Alexander, J.J., “Concepts and Models in Inorganic Chemistry”, 3rd Ed., John Wiley & Sons, 2001.
3. Figgis, B.N., and Hitchman, M.A “Ligand Field Theory and Its Applications”, Wiley Eastern Ltd., 1999.
4. Huheey, J.E., Keiter, E.A. and Keiter, R.L., “Inorganic Chemistry Principle of Structure and Reactivity”, 4th Ed, Pearson Education, Inc., 2003.
5. Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., “Shriver and Atkins' Inorganic Chemistry”, 4th Ed, Oxford university press, 2009.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH616P	Subject Title	INORGANIC CHEMISTRY -I LAB						
LTP	0 0 4	**Credit**	2	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

List of Experiments:

1. Qualitative analysis of inorganic mixture containing 6 and 8 radicals including interfering radicals.
2. Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods:
3. Ag^+ (gravimetrically) and Cu^{2+}(Volumetrically)
4. Cu^{2+} (gravimetrically) and Zn^{2+}(Volumetrically)
5. Fe^{3+} (gravimetrically) and Ca^{2+}(Volumetrically)
6. Mg^{2+} (gravimetrically) and Ca^{2+}(Volumetrically)

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COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH617	Subject Title	ORGANIC CHEMISTRY - I						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	1^{st}	Semester	I

Course Objective

Understanding the basic concepts about how the organic reactions are carried out and also to make the students understand the mechanisms of different organic reactions including various stereo chemical, mechanistic and conformational aspects

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course content

Unit 1: Reaction mechanism: Structure and reactivity: 8 lectures

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopic effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, and nitrenes. Effect of structure on reactivity – resonance and field effects, steric effect, quantitative treatment. Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

Unit 2: Aliphatic Nucleophilic and Electrophilic Substitution: 9 lectures

SN1, SN2, mixed SN1 and SN2, SNi, and SET mechanisms. Nucleophilic substitution at allylic, aliphatic and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambient nucleophile, regioselectivity.

Bimolecular mechanisms – SE1, SE2, and SEi. Electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on reactivity.

Unit 3: Aromatic Nucleophilic and Electrophilic Substitution: 13 lectures

SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smile rearrangements.

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Unit 4: Stereochemistry: 5 lectures

Molecular symmetry and chirality: Symmetry operations and symmetry elements, point group classification and symmetry number.

Stereoisomerism: Classification, racemic modification, molecules with one, two or more chiral centres; Configuration nomenclature, D L, R S and E Z nomenclature. Axial and planar chirality and helicity (P & M); Stereochemistry and configurations of allenes, spiranes, alkylidine cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.

Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres. Simple chemical correlation of configurations with examples, quasiracemates.
Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (mono-, di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

Unit 5: Asymmetric induction: 4 lectures
Cram's, Prelog's and Felkin-Ahn model; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett principle.
Molecular dissymmetry and chiroptical properties: Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

Learning outcomes:
At the end of the course, the student should be able to
CO1: Recall the fundamental principles of organic reactions.
CO2: Understand the concepts related to nomenclature, isomerism and stereochemistry.
CO3: Apply their understanding about the organic reactions of industrial significance with respect to the chemo selectivity, regioselectivity and enantioselectivity.
CO4: Analyze the product distribution and the stereochemistry of various organic products.

REFERENCE BOOKS:

1. Advanced Organic Chemistry by J. March, John Wiley & Sons, 1992
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill
3. Organic Chemistry by S. H. Pine, McGraw Hill, 1987.
4. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley, 1994.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	**CH617 P**	**Subject Title**	**ORGANIC CHEMISTRY – I LAB**						
LTP	0 0 4	**Credit**	2	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

List of Experiments:

1. Separation of mixture of organic compounds by water separation and bicarbonate separation method.
2. Analysis of organic compounds separated by above experiment and confirmation by derivative preparation.
3. Preparation of organic compounds using condensation, diazotization, bromination, nitration, and oxidation.

REFERENCE BOOKS:

1. Mann, F.G. and Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).
3. Vogel's Text book of quantitative analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
4. Experiments and techniques in organic chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.
5. Systematic qualitative organic analysis, H. Middleton, Adward Arnold.
6. Handbook of organic analysis – qualitative and quantitative, H. Clark, Adward Arnold.
7. Vogel's text book of practical organic chemistry, A.R. Tatchell, John Wiley.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH618	Subject Title	PHYSICAL CHEMISTRY - I						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	1st	Semester	I

Course Objective

1. To study the fundamentals and applications of classical mechanics and quantum chemistry
2. To understand the structure of an atom and different approximation methods
3. To learn the concept of Molecular Orbital Theory and its applications.
4. Understand about thermodynamics and Non-ideal systems
5. Study the classical Maxwell-Boltzman and quantum statistics
6. Know about partition functions and determining thermodynamic properties
7. Describe the type of defects in metals and about semiconductors.

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: Quantum Chemistry : 20 lectures
Quantum Chemistry and Approximate Methods Postulates of Quantum mechanics, Linear and Hermitian operators, Turn-over rule, Commutation of operators and Uncertainty principle.
Some exactly soluble problems: Particle in a box (1-D, 2-D & 3-D) and ring. Concept of degeneracy and Jahn-Teller distortion. Simple harmonic oscillator problem and its solution using series solution or factorization method. Calculation of various average values. Angular momentum operators, Eigenvalues and eigen-functions, Rigid rotator and hydrogen atom Complete solution. Radial distributions.
Approximate methods: First order time-independent perturbation theory for non-degenerate states. Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).
HMO method and its applications: π-Electron approximation, Huckel Molecular Orbital Theory of conjugated systems, Calculation of properties- Delocalization energy, electron density, bond order, non-alternant hydrocarbons. Pairing theorem. Electronic and ESR spectra. Effect of substituents on spectra. Reactivity and electro-cyclic ring closures.

Unit 2: Advanced Chemical Thermodynamics: 15 lectures
Concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities. Concept and determination of fugacity. Non-ideal solutions: Excess functions for non-ideal solutions. Activity, activity coefficients, Debye-Huckel theory for activity coefficients, ionic strength.
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 functions – translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behavior of solids – chemical 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.

Non-equilibrium thermodynamics: Thermodynamic criterion for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction, etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's thermodynamics for biological systems, coupled reactions.

Unit 3: Solids: 4 lectures

Crystallography, powder X-ray diffraction – Bragg's peak, absences, indexing of simple systems. Structural classification of binary (AX, AX_2, etc.) and ternary (ABX, ABX_2, ABX_3, AB_2X_4, etc.) compositions. Packing of constituent particles in crystals, packing of crystals and coordination number, limiting radius ratio and geometry of crystals, lattice energy, void space in closed packing of spheres, imperfections for defects in solids. Bonding in solids – introduction to metals, insulators and semiconductors, electronic structure of solids. Electrical conductivity, mobility, thermal conductivity, and specific heat of solids. Magnetic properties of solids, magnetization and susceptibility. Amorphous and liquid crystals, polymorphism, transition temperature.

COURSE OUTCOMES: -

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

1. Differences between classical and quantum mechanics. The limitations of classical mechanics.
2. Describe about the connection of quantum mechanical operators to observables probabilities, amplitudes, averages, expectation values, and observables
3. Analyses the probabilities, amplitudes, averages, expectation values and observables
4. Differentiate between common approximation methods and standard chemical frameworks (Born-Oppenheimer approximation, molecular orbitals, for example)
5. Gain and understanding of solids, crystals, diffraction, bonding in solids, electronic structure of solids, magnetic properties of solids, superconductivity

REFERENCE BOOKS

1. Prasad, R. K. (2014). Quantum Chemistry (IV Revised Edition). New Delhi: New Age International Publishers Pvt. Ltd.
2. Chandra, A. K. (2017). Quantum Chemistry (IV Edition). New Delhi: Tata McGraw – Hill Publishing Company Ltd.
3. House, J. E. (2004). Fundamental of Quantum Chemistry (II Edition). New Delhi: Academic Press.
4. Levine, I. N. (2016). Quantum Chemistry (VII Edition). New Delhi: Pearson Education Pvt. Ltd.
5. Elementary Quantum Chemistry by F. L. Pilar, Dover Publications, Inc. NY,
6. 1990. 2nd Ed.
7. Puri, B. R., Sharma, L. R., Pathania, M. S. (2013). Principles of Physical Chemistry (46th Edition). Jalandar: Vishal Publishing Co.
8. Atkins, P., & De Paula, J. (2014). Atkins Physical Chemistry (X Edition). Oxford: Oxford University Press.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	**CH618P**	**Subject Title**	**PHYSICAL CHEMISTRY – I LAB**						
LTP	0 0 4	**Credit**	2	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

Course Content: Chemical Kinetics

1. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate by the Initial Rate Method. Study the reaction at two different temperatures and calculate the thermodynamic parameters.
2. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.

Study the saponification of ethyl acetate with sodium hydroxide volumetrically. Conductometry

(i) Determine the Cell Constant of the given conductivity cell at room temperature and study the equivalent conductance versus square root of concentration relationship of a strong electrolyte (KCl or NaCl) and weak electrolyte (acetic acid).
(ii) Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions
(iii) Determine the equivalent conductance, degree of dissociation and dissociation constant (K_a) of acetic acid.

(i) Study the conductometric titration of hydrochloric acid with sodium carbonate and determine the concentration of sodium carbonate in a commercial sample of soda ash.
(ii) Study the conductometric titration of potassium sulphate solution vs. barium chloride solution
(iii) Study the conductometric titration of
(iv) Acetic acid vs. sodium hydroxide,
(v) Acetic acid vs. ammonium hydroxide,
(vi) HCl vs. NaOH Comment on the nature of the graphs.

3. Study the stepwise neutralization of a polybasic acid e.g. oxalic acid, citric acid, succinic acid by conductometric titration and explain the variation in the plots.

Potentiometry

(i) Titrate hydrochloric acid and sodium hydroxide potentiometrically.
(ii) Determine the dissociation constant of acetic acid potentiometrically.
(iii) Titrate oxalic acid and sodium hydroxide potentiometrically.

Titrate a mixture of

(i) Strong and weak acids (Hydrochloric and acetic acids)
(ii) Weak acid (acetic acid) and dibasic acid (oxalic acid)
(iii) Strong acid (hydrochloric acid) and dibasic acid (oxalic acid) versus sodium hydroxide.

(i) Titrate a solution of Mohr's salt against potassium permanganate potentiometrically.
(ii) Titrate a solution of Mohr's Salt and potassium dichromate potentiometrically.

Computational Methods

Familiarity with word processing, electronic spreadsheets, data processing, mathematical packages, chemical structure drawing and molecular modelling.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH619	Subject Title	ANALYTICAL CHEMISTRY – I						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	1^{st}	Semester	I

Course Objective

1. Making students understand the importance of absorption and emission spectroscopic analysis.
2. Learn the principles and usage of Electroanalytical techniques.
3. Get insight into basics of different chromatographic techniques.
4. Discuss the concept of nuclear chemistry
5. Justify the implication of nuclear chemistry in energy generation

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: Spectral methods: 7 lectures
Spectrophotometry– Beer-Lambert law, its applications and limitations, single and double beam spectrophotometer, analysis of mixtures, fluorimetry, nephelometry, turbiditmetry. Atomic absorption spectrometry– principle and applications, flame emission spectrometry (flame photometry).

Unit 2: Electroanalytical methods: **6 lectures**
Polarography, amperometric and bio-amperometric titrations.

Unit 3: Nuclear methods: 7 lectures
Fundamentals of radioactivity and decay, preparation of radioisotopes for tracers, applications with radiotracers, radiometric titration, radioactivity measurements by gas filled and scintillation detectors.

Unit 4: Solvent extraction: **6 lectures**
Partition law and its limitations, distribution ratio, separation factor, factors influencing extraction, multiple extractions. Extraction of metal chelates.

Unit 5: Advanced Chromatographic Techniques: 13 lectures
Introduction and classification, theory of column chromatography, retention time, retention volume, capacity factor, concept of plate and rate theory, resolution, column performance, normal and reverse phase chromatography, paper and thin layer chromatography, gas phase chromatography, ion-exchangers. GC, LC and HPLC

Course outcomes: -
After the completion of this course, the learner will be able to:
CO1: Understand the basics of spectrophotometry
CO2: Solve problems related to UV-Visible Spectroscopy, fluorimetry, nephelometry, turbiditmetry and
Flame atomic absorption and emission spectrometry
CO3: Analyze Electroanalytical and nuclear methods of analysis

CO4: Understand the methods of separations.
CO4: Perform chromatographic analysis

REFERENCE BOOKS:

1. Ewing, G.W., "Instrumental Methods of Chemical Analysis", 5th Ed. McGraw Hill, 2004.
2. Mendham, J., Denny, R.C., Barnes, J.D. and Thomas, M.J.K., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed. Pearson Education, 2004.
3. Christian, G.D., "Analytical Chemistry" 6th Ed. Wiley, 2008.
4. Sood, D.D., Reddy, A.V.R. and Ramamoorthy, N., "Fundamentals of Radiochemistry", IANCAS, BARC, Mumbai, 2004.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH646	Subject Title	BIOLOGY FOR CHEMIST (FOR MATHEMATICS STUDENT)						
LTP	2 0 0	Credit	2	Subject Category	CC	Year	1st	Semester	I

Course Objective: To introduce molecular structure and interactions present in various bio-molecules that help in functioning and organization of living cell.

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Objective: To introduce molecular structure and interactions present in various bio-molecules that help in functioning and organization of living cell.

Unit 1: Introduction: 8 lectures
Cell structure and functions, Scales of biological systems, Dimensions of bio-molecules and assemblies, Times of biological processes and biologically important energies, ATP. Water – physical properties and structure of water molecules, Interactions in aqueous solutions, Role of water in life, Biological buffers, Henderson-Hasselbalch equation.

Unit 2: Amino Acids and Peptides: 8 lectures
Classification of amino acids and their properties, Polypeptides, Primary Structures, N-terminal and C-terminal determinations. Structure of peptide bond, synthesis of peptides, Solid phase peptide synthesis.

Unit 3: Nucleic Acids: 8 lectures
Purine and pyrimidine bases, Nucleotides, Nucleosides, Base pairing via H-bonding, Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), Double helix model of DNA, Chemical and enzymatic hydrolysis of nucleic acids, The chemical basis for heredity, An overview of replication of DNA, Transcription, Translation and genetic code.

Unit 4: Carbohydrates: 8 lectures
Biologically important monosaccharides, disaccharides and polysaccharides, Glycoproteins, Role of sugars in biological recognition, Blood group substances, Carbohydrate metabolism - Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenesis, Pentose Phosphate pathway.

Unit 5: Lipids: 7 lectures
Lipid classification, Lipid Bilayers, Membrane Proteins - integral membrane proteins, Lipid linked proteins, peripheral proteins, Overview of membrane structure and assembly. Liposomes, their biological functions.

Course outcomes:
CO1: Understand the characteristics and classifications of amino acids, peptides, nucleic acid, carbohydrate, lipids.
CO2: Know the methods of quantitative and qualitative analysis of biological molecules.
CO3: Understand the basic principles of protein-protein and protein-nucleic acid interactions

RECOMMENDED BOOKS

1. Voet, D.J., Voet, J.G., Pratt, C.W., Principles of Biochemistry, John Wiley, (2008) 3rd ed.
2. Berg, J.M., and Tymoczko, J.L., Stryer, L., Biochemistry, W.H. Freeman (2007) 6th ed.
3. Garrett, R.H., Grisham, C.M., Biochemistry, Brooks/Cole, Cengage Learning, (2010)4th ed.
4. Conn, E.E., and Stump, F., Outlines of Biochemistry, John Wiley (2006) 5th ed.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH647	Subject Title	MATHEMATICS FOR CHEMIST (FOR BIOLOGY STUDENT)						
LTP	2 0 0	Credit	2	Subject Category	CC	Year	1st	Semester	I

Course Objective
To study the fundamentals and uses of vector, matrix, differential calculus, differential equations, permutation and probability in chemistry.

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Content: Vectors and Matrix Algebra:
Unit 1: Vectors: 3 lectures
Vectors, dots, cross and triple products, etc. The gradient, divergence, and curl. Vector calculus, Gauss' theorem, divergence theorem, etc.

Unit 2: Matrix Algebra: 10 lectures
Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (symmetric, skew-symmetric, Hermitian, Skew-Hermitian, unit, diagonal, unitary, etc.) and their properties. Matrix equations: Homogenous, non-homogenous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization determinants (examples from Huckel theory). Introduction to tensors; polarizability and magnetic susceptibility as examples.

Unit 3: Differential Calculus: 10 lectures
Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution, etc.), exact and inexact differentials with their applications to thermodynamic properties.
Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus.
Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar)), curve sketching.

Unit 4: Elementary differential equations: 8 lectures
Variables-separable and exact first-order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry, etc. Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and Legendre equation, etc., spherical harmonics, second order differential equations and their solutions.

Unit 5: Permutation and Probability: 8 lectures
Permutations and combinations, probability and probability theorems, probability curves average, root mean square and most probable errors, examples from the kinetic theory of gases, etc., curve fitting (including least squares fit, etc.) with a general polynomial fit.

Learning outcomes:

CO1: The students will acquire knowledge of importance of mathematics in chemistry.

CO2: Different curve fitting methods are necessary for chemist.

Books Suggested

1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
2. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
4. Chemical Mathematics, D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Semester II

Course Category	CourseCode	Course Title	L	P	Credit
CC	CH626	Inorganic Chemistry -II	3	0	3
CC	CH627	Organic Chemistry - II	3	0	3
CC	CH628	Physical Chemistry - II	3	0	3
CC	CH626P	Inorganic Chemistry -II Lab	0	4	2
CC	CH627P	Organic Chemistry – II Lab	0	4	2
CC	CH628P	Physical Chemistry – II Lab	0	4	2
CC	CH629	Analytical Chemistry-II	3	0	3
AEC	CH648	Research methodology and Ethics	3	0	3
		Total	**15**	**12**	**21**

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH626	Subject Title	INORGANIC CHEMISTRY II						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	1st	Semester	I

Course Objective

1. To understand the basic concepts about how the metal mediated reactions are carried out and also to make the students understand the mechanisms of different organometallic reactions
2. To be able to get familiarized with almost all the basic organometallic concepts
3. To learn and understand the synthetic and mechanistic aspects
4. To impart knowledge in the theory and applications of various organometallic reagents.

Course Pre/Co- requisite (if any): no restricted pre-requisite

Unit 1: Organometallic Chemistry: 14 lectures

Types of ligands in organometallic compounds - eighteen Electron rule and its application to π-acceptor ligands, limitations of 18 electron rule, description of bonding models for π-acceptor ligands including CO, alkyl compounds, alkenes (Dewar-Chatt-Duncanson model) and tertiary phosphines, physical evidences and consequences of bonding. Metallocenes: Ferrocene.

Main group organometallics: Introduction, review of comparative aspects of synthetic methods, reactivity and bonding in ionic, covalent, electron deficient and electron rich organometallic compounds. Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands.

π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cyclohepta-trienyls and cyclooctatetraenes, reactions and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxionalty, bimetallic and cluster complexes.

Unit 2: Stability constants of metal complexes and their applications: **14 lectures**

Stoichiometric and thermodynamic equilibrium constants, stepwise formation of complexes, formation functions, φ, n and α_C and relationship between different functions. Calculation of stability constants. Graphical Methods: using sets of data {φ, [A]}; {α_C, [A]} and { n , [A]}. Curve fitting method, Elimination method, Numerical method, Potentiometric method, Method of corresponding solutions, Ion exchange method, Solvent extraction, Polarographic method and Spectrophotometric methods, which include Job's method of continuous variation, Logarithmic method, Bent and French mole ratio method. Turner and Anderson methods and Yatsimirskiis method.

Analytical applications of complex formation; gravimetric analysis, complexometric titrations (Conditional constants, titration curves, titration error, detection of end point using metal indicators and instrumental methods. Indicator errors, Indicator correction, etc. Simultaneous titrations, stepwise titrations, back titrations). Use of masking and demasking agents in complexometric titrations.

Unit 3: Inorganic chains, rings, cages and clusters: 11 lectures

Chains– catenation and hetero-catenation, structural aspects of silicate minerals and silicones, one- dimensional conductors: (SN)x chains, chalcogenide glasses, iso- and heteropolyanions. Rings– borazines, boron nitride, phosphazenes–structural models, phosphazene polymers, and other homocylic and heterocyclic inorganic ring systems. Cages– Boron cage compounds– structural aspects (boranes-styx number and Wade's rule) of higher boranes, carboranes, metallacarboranes, phosphorous cage compounds with P–P, P–O, P–S. Clusters– metal clusters, metal carbonyl clusters, di-, tri-, tetra- and hexanuclear clusters.

Course outcomes:

CO1: Know the synthesis, mechanisms and the functions of various organometallic reagents or catalysts.

CO2: Learn the requirement of new organometallic compounds.

CO3: Analyze the spectral data of organometallic complexes.

RECOMMENDED BOOKS

1. Basic Organometallic Chemistry: Concepts, Syntheses and Applications Paperback – Dr. B.D. Gupta, Dr. Anil J. Elias, Universities Press; 2 editions, 2013.
2. Applied Homogeneous Catalysis with Organometallic Compounds: A Comprehensive Handbook in Four Volumes Hardcover – Import, 8 Nov 2017, by Boy Cornils, Wolfgang Herrmann, Matthias Beller, Rocco Paciello (Eds), 2017.
3. The Organometallic Chemistry of the Transition Metals by Crabtree, 6th edition, 2014, ISBN: 978-1-118-13807-6.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	**CH626 P**	**Subject Title**	**INORGANIC CHEMISTRY II LAB**						
LTP	0 0 4	**Credit**	2	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

Course content

1. Qualitative analysis of inorganic mixture containing 8 radicals including interfering radicals.

2. Separation of cations and anions by:

- **(i)** Paper chromatography
- **(ii)** Column chromatography

3. Synthesis of selected coordination compounds from the following, characterization and metal content determination by suitable route:

1. $[Cu(NH_3)_4.H_2O]SO_4$
2. $[Fe(acac)_3]$
3. $[Mn(acac)_3]$
4. $[Mn(C_2O_4)_3]$
5. $VO(acac)_2$
6. $TiO(C_9H_8NO)_2.2H_2O$
7. Cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
8. $Na[Cr(NH_3)_2(SCN)_4]$
9. $K_3[Fe(C_2O_4)_3]$
10. Any other suitable coordination compound

REFERENCE BOOKS:

- Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J., “Vogel’s Text Book of Quantitative Chemical Analysis”, 6th Ed., ELBS Longman Group UK Ltd., 2004.
- Srivastava T.N. and Kamboj P.C., “Analytical Chemistry”, Vishal Publications, 2000.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

<table>
<tr><td>Subject Code</td><td>CH627</td><td>Subject Title</td><td colspan="7">ORGANIC CHEMISTRY II</td></tr>
<tr><td>LTP</td><td>3 0 0</td><td>Credit</td><td>3</td><td>Subject Category</td><td>CC</td><td>Year</td><td>1st</td><td>Semester</td><td>I</td></tr>
</table>

Course Objective

1. Imparting knowledge in the theory and applications of various aspects of photochemistry and pericyclic reactions.
2. Understanding the synthesis and mechanisms of various reactions related to the synthesis by cycloaddition, photochemistry.
3. To impart knowledge in the theory and applications of various organometallic reagents.

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course content

Unit 1: Reagents and Methods in Organic Synthesis: 20 lectures
Organosilicone Compounds: Preparation and applications in organic synthesis. Applications of Pd(0) and Pd(II) complexes in organic synthesis: Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling. Preparation and applications of lithium organocuparates. Reductions: Stereochemistry, stereoselection and mechanism of catalytic hydrogenation and metal- liquid ammonia reductions.
Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithium aluminium hydride and alkoxy substituted LAH reducing agents, DIBAL; Applications of hydroboration (reductions, oxidations and cabonylations): diborane, diisoamylborane, thexylborane, 9-BBN, isopinocamphenyl and diisopinocamphenyl borane.
Homogeneous hydrogenations: Mechanisms and applications using Rh, Ru and other metal complexes.
Oxidations: Scope of the following oxidizing reagents with relevant applications and mechanisms: DDQ, SeO_2, $Tl(NO_3)_3$, Sharpless Asymmetric epoxidation, Asymmetric hydroxylation and aminohydroxylation.

Unit 2: Photochemistry & Pericyclic Reactions: 19 lectures
Photophysical processes: Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects, Stern-Volmer plot, delayed fluorescence, etc. Photochemistry of alkenes: cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes; dimerizations.
Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic); α,β-unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno–Buchi reactions; photoreductions.
Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar and prismanes in isomerization. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loefller-Freytag reaction.
Pericyclic reactions: Electrocyclic, cycloaddition, sigmatropic and chelotropic reactions; General Orbital Symmetry rules, Frontier Orbital approach, PMO approach, Correlation diagrams for different systems, Hückel–Mobius approach, General pericyclic selection rule and its applications, 1,3- dipolar additions, Ene reaction.

Course outcomes:

At the end of the course, students should be able to

CO1: Recall the fundamental principles of photochemical reactions.

CO2: Understand the concepts related to light induced organic synthesis, mechanisms and the functions of various reagents.

CO3: Apply their understanding about the photochemical reactions of industrial significance.

CO4: Analyse the product distribution and the stereochemistry of various organic products derive photochemistry.

CO5: Evaluate the photochemical reactions based on the influence of the substituents on sul molecules.

CO6: Design new photochemical reactions in order to achieve the required product(s).

CO7: Learn the requirement of new organometallic compounds.

Reference Books

1. Pericyclic reactions-A Textbook: Reactions Applications and Theory. S
    a. Sankararaman, iley-VCH 2015.
2. Organic Photochemistry and Peri Cyclic Reactions, S. Kalaivanai, MJP Publishers, 2011.
3. Pericyclic reactions, Sunil Kumar, Vinod Kumar, S.P. Singh, Elsevier, 2016.

Subject Code	**CH627 P**	**Subject Title**	**ORGANIC CHEMISTRY II LAB**						
LTP	0 0 4	**Credit**	2	**Subject Category**	CC	**Year**	**1^{st}**	**Semester**	**I**

List of Experiments:

1. Separation of mixture of organic compounds by HCl separation and NaOH separation method.
2. Analysis of organic compounds separated by above experiment and confirmation by derivative preparation.

3. Multi step synthesis including photochemical methods; representative examples (minimum two):
   a. Hydroquinone→ Hydroquinone Diacetate → 2, 5 -Dihydroxyacetophenone → 2, 5 -Dibenzoxyacetophenone →Dibromocinnamic acid→ cis & Trans
   b. Benzaldehyde→ Cinnamic acid → α, β α-Bromo Cinnamic acid
   c. Chalcone→ Chalcone epoxide→ α-Benzoyl phenyl acetaldehyde
   d. Benzaldehyde → Benzoin → Benzil → Benzilic acid
   e. Resorcinol →7-Hydroxy-4-methylcoumarin→7-Acetoxy-4-methylcoumarin → 4-Methyl-7-hydroxy-8-acetylcoumarin

4. Multi-component synthesis (minimum two):
   a. Mannich Reaction (reaction of primary amine, formaldehyde and carbonyl compound)
   b. Organic synthesis in water (Preparation of Hydroxy methyl benzotriazole)
   c. Synthesis of Benzimidazole (Condensation of diamines and aldehydes)
   d. Synthesis of chromenes and xanthene's

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	**CH628**	**Subject Title**	**PHYSICAL CHEMISTRY II**						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

Course Objective

1. It is central to the discipline of chemistry and yet is of enormous practical importance.
2. To impart knowledge of applications of reaction kinetics, surface reaction, adsorption and catalysis.
3. Understanding the facts and theories relating to the rates at which chemical reactions occur in the gas phase, liquid phase, and on surfaces is the objective of this course.
4. To acquire knowledge of photochemistry and photophysical principles, their applications on simple and macromolecules.

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: Electrochemistry: 6 lectures
Solutions: Activity coefficients and ion-ion interactions. The physical significance of activity coefficients, mean activity coefficient of an electrolyte, and its determination. Derivation of the Debye-Hückel theory of activity coefficients (both point ion size and finite ion size models). Excess functions.

Unit 2: Surface chemistry: 10 lectures
Adsorption of gases on solid surface, difference between physical and chemical adsorption, adsorption isotherms, adsorption from solution, surface tension and surface energy, capillary action, formation of surface films, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibb's adsorption isotherm, estimation of surface area (BET equation).
Micelles: Surface active agents and their classification, micellization, hydrophobic interaction, critical miceller concentration (CMC), factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, reverse micelles, solubilisation, and micro-emulsion.

Unit 3: Macromolecules: 7 lectures
Polymer: Definition, types of polymers and applications, mechanism and kinetics of polymerization, liquid crystal polymers, conducting polymers.
Molecular mass and its distribution, number and mass average molecular mass, determination of molecular mass by osmometry, viscosity, light scattering and size exclusion chromatography methods. Glass transition temperature, the Flory-Huggins theory of polymer solutions, living radical polymerization, polymer nanocomposite.

Unit 4: Catalysis and Chemical kinetics: 10 lectures
Introduction, positive and negative catalysis, homogenous and heterogenous catalysis, promoters and anti-catalysis, autocatalysis, biological/ enzyme catalysis, mechanism of enzyme reaction, characteristics of catalytic action, theories of catalysis, catalysis in industry.

Theories of reaction rates: Collision theory, Transition state theory, theory of unimolecular reactions, Lindemann mechanism and RRKM theory. Steady state approximation (SSA). Complex reactions: parallel reactions, reversible reactions, and consecutive reactions. Kinetic and thermodynamic control of reactions. Kinetics of chain reactions, detections of radical and kinetics of HBr, H_2O_2 reactions, explosion limits. Application of following to the reaction kinetics− solvent effect, kinetic isotope effect and salt effect, experimental technique for studying the fast reaction kinetics, kinetics of homogenous and heterogenous catalysis, kinetics of polymerization and enzyme reactions.

Unit 5: Photochemistry: 6 lectures

Quantum efficiencies of photochemical and photophysical processes, experimental techniques for continuous photolysis. Primary and secondary photochemical processes, Franck-Condon principle and its applications, rates of absorption and emission, lifetimes of electronically excited states and their fate, quenching of excited states species – dynamic and static quenching, radiationless transition and pre-dissociation, energy transfer processes, FRET analysis, mechanistic analysis and reaction dynamics. Radiation chemistry–Interaction with ionizing radiation with matter, dosimetry, generation of free radicals and intermediates, comparison between photo- and radiation chemistry.

Course Outcomes

The student will have knowledge of

CO1: Photochemistry and photophysical principles.
CO2: application of photochemistry and photophysical principles on simple and macromolecules.
CO3: Debye-Huckel theory and determination of activity and activity coefficient.
CO4: Mechanism for chemical reactions for optimizing the experimental conditions.
CO5: Application of homogeneous and heterogeneous catalysis in chemical synthesis
CO6: Importance of adsorption process and catalytic activity at the solid surfaces

REFERENCE BOOKS:

1. Laidler, K.J., “Reaction Kinetics”, Anand Sons, New Delhi, 2005.
2. Amis, E.S.,“Solvent Effect of Reaction Rates and Mechanism”, Academic Press, 2005.
3. Mukherjee, K.K., “Fundamentals of Photochemistry”, New Age, 2004.
4. Physical chemistry, PW Atkins, ELBS.
5. Chemical kinetics, KJ Laidler, McGraw-Hill.
6. Kinetics and mechanism of chemical transformations, J Rajaraman and J Kuriacose, McMillan.
7. Micelles, theoretical and applied aspects, V Moroi, Plenum.
8. Modern electrochemistry, Vol. I and Vol. II, JOM Bockris and AKN Reddy, Plenum.
9. Introduction to polymer science, VR Gowarikar, NV Vishwanathan and J Sridhar, Wiley Easter.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH628 P	Subject Title	PHYSICAL CHEMISTRY II LAB						
LTP	0 0 4	**Credit**	2	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

Course Content:

1. Chemical kinetics:

1. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
2. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
3. Study the kinetics of the iodination of acetone in the presence of acid by the Initial Rate Method.

2. Potentiometry:

1. To determine the solubility and solubility product of an insoluble salt, AgX (X=Cl, Br or I) potentiometrically.
2. To titrate phosphoric acid potentiometrically against sodium hydroxide.
3. To titrate potentiometrically solutions of
   i. KCl/ KBr/ KI
   ii. mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
4. To titrate Fe^{2+} with Ce^{4+} potentiometrically.
5. To determine zinc in the presence of calcium by potentiometric titration.

3. Distribution law:

To determine distribution coefficient of I2 between two immiscible solvents.

4. Solution:

a. Molecular weight determination of a non-volatile and non-electrolyte/ electrolyte by cryoscopic method.

b. Molecular weight determination of a non-volatile and non-electrolyte/ electrolyte by ebuloscopic method.

5. Adsorption:

To study the adsorption of acetic acid on activated charcoal.

REFERENCE BOOKS:

1. Vogel's textbook of quantitative analysis, revise, J Basset, RC Denney, GH Jeffery and J Mendham, ELBS.
2. Practical physical chemistry, AM James and FE Proichad, Longman.
3. Findley's practical physical chemistry, BP Levitt, Longman.
4. Experimental physical chemistry, RC Das and B Behera, Tata McGraw Hill.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH629	Subject Title	ANALYTICAL CHEMISTRY-II						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	**1st**	**Semester**	**I**

Course Objective

1. Learning the importance of thermal analysis as well as absorption and emission spectroscopic analysis.
2. Understand the principles and applications of surface analytical techniques.
3. Learn the principles and usage of Electroanalytical techniques.
4. To understand and familiarize with the basic principles, theory and instrumentation of Mass spectrometry.
5. To impart knowledge in the theory and applications of mass spectroscopic techniques which are very important characterization techniques to understand the structure of the molecules in chemistry.

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Content:

Unit 1: Electroanalytical methods: 5 lectures

Instrumentation, theory and applications of polarography−normal DC, pulse and differential pulse polarography, AC polarography. Linear and cyclic voltammetry, square wave voltammetry, coulometry at controlled potential, chronopotentiometry, anodic stripping voltammetry. Sensors−different types of solid and liquid sensors, nano material and chemically modified sensors, applications in environmental and biological sample analysis.

Unit 2: Nuclear and X-ray methods: 12 lectures

Radiotracers– choice and synthesis of radiotracers, isotope dilution methods, neutron activation analysis. Material science studies using positron emitters and Mössbauer source. Principles of X-ray spectra, X- ray absorption, emission fluorescence and diffraction methods and applications. Ion beam analysis, proton induced X-ray emission, Rutherford backscattering spectrometry, elastic recoil detection analysis for hydrogen measurement, nuclear microprobe.

Unit 3: Mass spectrometry: 8 lectures

Different types of ion sources, mass analyzers and detectors, resolution and resolving power, interpretation of mass spectra, hyphenated systems like LC-MS, GC-MS, MS-MS.

Unit 4: Atomic spectroscopy and hyphenation: 7 lectures

Atomic absorption spectroscopy with electro thermal atomizers, cold vapor technique, inductively coupled plasma atomic emission methods − principle and instrumentation, hyphenation with mass spectrometry (ICP-MS), laser ablation and HPLC.

Unit 5: Thermal Analysis: 7 lectures

Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

Knowledge of Lab Safety and Software: Introduction to lab safety rules, Material safety datasheet, and norms, software (Excel, ACD/ ChemSketch)

Course outcomes:

At the end of the course, the student should be able to

CO1: Analyse thermal behaviour of different organic and inorganic materials using TGA, DTA and DSC

CO2: Apply absorption and emission techniques for trace element analysis from different matrices.

CO3: Students will be skilled in the interpreting the Mass spectroscopy to derive the information regarding the structure, the molecules.

CO4: Students will apply the learned fundamental instrumental techniques in the physical characterization of organic molecules.

REFERENCE BOOKS:

1. Meites, L., “Polarographic Techniques”, 3rd Ed., Interscience publishers, N.Y., 1990.
2. Sane, R.T. and Joshi, A.P., “Electroanalytical Chemistry: Theory and Applications”, Quest Publications, 1999.
3. Loveland, W., Morrissey, D. and Seaborg, G.T., “Modern Nuclear Chemistry”, John Wiley and Sons, New Jersey, 2006.
4. Sood, D.D., Reddy, A.V.R. and Ramamoorthy N., “Fundamentals of Radiochemistry”, IANCAS, BARC, India, 2004.
5. Skoog, D.A., Holler, F.J. and Crouch, S.R., “Principles of Instrumental Analysis”, Thomson Brooks/Cole, Canada, 2007.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

<table>
<tr><td>Subject Code</td><td>CH648</td><td>Subject Title</td><td colspan="7">RESEARCH METHODOLOGY AND ETHICS</td></tr>
<tr><td>LTP</td><td>3 0 0</td><td>Credit</td><td>3</td><td>Subject Category</td><td>CC</td><td>Year</td><td>1st</td><td>Semester</td><td>II</td></tr>
</table>

Course Objective

1. Impart skills to develop a research topic and design
2. Define a purpose statement, a research question or hypothesis and a research objective
3. Analyze the data and arrive at a valid conclusion
4. Compile and present research findings

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Content:

Unit 1: Introduction: 3 lectures

Meaning, objective and importance of research methodology, types of research (basic, applied and patent oriented), defining research problem, research design including various methods, research process and steps involved. Literature survey and documentation.

Unit 2: Use of encyclopaedias and tools in research: 3 lectures

Research Guides, Handbook, Academic Databases for chemistry. Methods to search required information effectively.

Unit 3: Fundamentals of research: 7 lectures

Technical writing and reporting of research: Types of research report: Dissertation and thesis, research paper, review article, short communication, conference presentation, meeting report etc.

Structure and organization of research reports: Title, abstract, key words, introduction, methodology, results, discussion, conclusion, acknowledgement, references, footnotes, tables and illustrations. Impact factor, rating, indexing and citation of journals. Detailed study of 'Instruction to Authors' of any research journal, a thorough understanding of steps involved in submitting articles electronically to any research journal (Registration, new article submission, tracking process, submitting revised articles).

Problem identification and formulation:

Scientific Research: Problem, Definition, Objectives, Types, Purposes and components of Research problem.

Unit 4: Research design and sampling: 13 lectures

Measures of central tendency, Data collection, analysis and hypothesis testing: Classification of data, methods of data collection, sample size, sampling procedure and methods.

Data analysis and reporting:

Data processing and graphical representation of data. Collection, Classification and Tabulation of data, Bar diagrams and Pie diagrams, Histogram, Frequency curve and frequency polygon, Ogives.

Correlation and Regression analysis:

Correlations and regressions-: Relation between two variables, scatter diagram, definition of correlations, curve fitting, principles of least square, Two regression lines, Karl Pearson's coefficient of correlation, Rank correlation, Probability theory: Random experiments, sample space, probability theory, conditional probability. Baye's theorem.

Variables:

Random variable, (discrete and continuous), Probability density function (discrete and continuous), Distribution function for discrete random variable. Distribution function for continuous random variable, Joint probability distribution, Standard distributions. Binomial distribution, Poisson distribution, Normal distributions. Standard normal distributions.

Statistical inference and hypothesis:

Types of hypothesis (experimental and non-experimental), hypothesis testing (Parametric and non- parametric tests), generalization and interpretation of results.

Unit 5: Research ethics and Plagiarism: 13 lectures

Ethical consideration during animal experimentation including CPCSEA guidelines. Plagiarism and use of plagiarism detection softwares such as Turnitin.

Hands-on experience:

Practice on identification of research problem, identifying gaps, searching journals, report writing, analysis and other concepts covered in above topics.

Course outcome:

After the end of this course, students shall be able to:

CO1: Carry out effective research

CO2: Write good research papers

CO3: Understand the importance of intellectual property rights and the consequences of plagiarism

CO4: Understand how to write doctoral-level research

REFERENCE BOOKS:

1. Catherine Dawson, Introduction to research methods: a practical guide for anyone undertaking a research project, Oxford: How to Books, Reprint 2010.
2. Julius S. Bendat, Allan G. Piersol, Random Data: Analysis and Measurement Procedures, 4thEdition, ISBN: 978-1-118-21082-6, 640 pages, September 2011.
3. Research in Medical and Biological Sciences, 1st Edition, From Planning and Preparation to Grant Application and Publication, Editos: Petter Laake Haakon Benestad Bjorn Olsen, ISBN: 9780128001547, Academic Press, March 2015.
4. John Creswell, Research Design: Qualitative, Quantitative, and Mixed Methods Approaches, Fourth Edition (March 14, 2013).
5. Kothari C.R., Research Methodology Methods and Techniques, Wishwa Prakashan, New Delhi.
6. Lokesh K., Methodology of Educational research, Vikash Publishing House Pvt. Ltd., New Delhi.
7. Kumar R., Research Methodology, Dorling Kindersley (India) Pvt. Ltd., New Delhi.
8. Rao G.N., Research Methodology and Qualitative Methods, B.S. Publications, Hyderabad.
9. Saunders M., Lewis P. and Thornhill A., Research Methods for Business Students, Dorling Kindersley (India) Pvt. Ltd., New Delhi.
10. Bolton S. and Bon C., Pharmaceutical Statistics: Practical and Clinical Applications, Marcel Dekker, New York.
11. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, An introduction to Research Methodology, RBSA Publishers, Jaipur.
12. Fisher R.A. Statistical Methods for Research Works, Oliver and Boyd, Edinburgh.

13. Chow S.S. and Liu J.P., Statistical Design and Analysis in Pharmaceutical Sciences, Marcel Dekker, New York.

14. Buncher C.R., Statistics in the Pharmaceutical Industry, Marcel Dekker, New York.

15. Fundamentals of Biostatistics. by Irfan A Khan.

16. An introduction to Biostatistics. by PSS Sunder Rao.

17. Introduction to the Practice of Statistics by Moore and McCabe.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Semester III

Course Category	Course Code	Course Title	L	P	Credit
CC	CH706	Molecular Spectroscopy	3	0	3
CC	CH707	Group Theory and structure of metal complexes	3	0	3
CC	CH708	Organic chemistry-III (**Organic spectroscopy**)	3	0	3
	CH709	Analytical chemistry-III (Microanalytical techniques)	3	0	3
CC	CH716	Organic chemistry-IV (**Heterocyclic compounds**)	3	0	3
	CH717	Analytical chemistry-IV (Separation techniques)	3	0	3
GEC	CH746	Computer applications in Chemistry	3	2	4
PJCT	CH736	Project - I	0	8	4
		Total	**15**	**10**	**20**

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH706	Subject Title	MOLECULAR SPECTROSCOPY						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	**2^{nd}**	**Semester**	**III**

Course Objective

1. To impart the knowledge of electronic, rotation, vibration. NMR, FTIR, ESR, spectroscopy and their applications.
2. To apply the different aspects of NMR spectroscopy to predict the structure of compounds.
3. To analyze about the Mossbauer spectroscopy.
4. To evaluate about the invaluable tools in synthetic chemistry for the confirmation of known molecules and elucidation of shape and structures of unknown compounds of high complexity with a high degree of certainty.

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Contents

Unit 1: Spectroscopic methods: 7 lectures
Characterization of electromagnetic radiation. Born- Oppenheimer approximation. Heisenberg's Uncertainty Principle. Basic elements of spectroscopy. Time dependent perturbation. Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra:
Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Unit 2: Rotational and vibrational spectroscopy: 12 lectures
Rotational: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/ or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First order Stark effect.
Vibrational: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands. Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect. Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules.

Unit 3: Raman spectroscopy: 5 lectures
Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

Unit 4: Electronic spectroscopy: 10 lectures

Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N2) and simple polyatomic molecules (H2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem. Polyatomic molecules. Oscillator strengths. Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde). Qualitative ideas of solvent effects-viscosity, polarity, hydrogen bonding.

Excited states: Deactivation. Jablonskii diagram. Fluorescence and phosphorescence and factors affecting these. Calculation of excited state life-times from absorption data. Quenching of fluorescence, Stern-Volmer equation.

Unit 5: NMR spectroscopy: 5 lectures

Larmor precession. Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation. Quantum mechanical treatment of the AB system. Selection rules and relative intensities of lines.

Principles of Mossbauer spectroscopy: Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Course outcomes

The students will acquire knowledge of

CO1: Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis

CO2: Electronic spectroscopy of different elements and simple molecules.

CO3: Nuclear Magnetic and Electron Spin Resonance Spectroscopy for organic compounds analysis, medical diagnostics.

RECOMMENDED BOOKS:

1. Hollas. J. M. Modern Spectroscopy 4th Ed., John Wiley & Sons (2004)
2. Barrow, G. M. Introduction to Molecular Spectroscopy McGraw-Hill (1962).
3. Kakkar, R., Atomic & Molecular Spectroscopy Cambridge University Press (2015)
4. Brand, J. C. D. & Speakman, J. C. Molecular Structure: The Physical Approach 2nd Ed., Edward Arnold: London (1975).
5. Chang, R. Basic Principles of Spectroscopy McGraw-Hill, New York, N.Y. (1970). 6. Moore, W. J. Physical Chemistry 4th Ed. Prentice-Hall (1972).
6. Warren, B. E. X-Ray Diffraction Dover Publications (1990).
7. Bacon, G. E. Fifty Years of Neutron Diffraction Hilger (1987).

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH707	Subject Title	GROUP THEORY AND STRUCTURE OF METAL COMPLEXES						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	**2^{nd}**	**Semester**	**III**

Course Objective

1. Applying practical aspects of symmetry and group theory in different research problems.
2. Understanding structure, bonding and reaction mechanism involved in inorganic solids and metal complexes.
3. Applying practical aspects of inorganic chemistry in research and development.

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Contents

Unit 1: Molecular symmetry: **9 lectures**

Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation.

Products of symmetry operations, equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups and classification.

Unit 2: Symmetry: 15 lectures

Optical activity and dipole moment. Representation of groups, reducible and irreducible representations. The Great Orthogonality theorem, character tables, position vector and base vector as basis for representation. Wavefunctions as bases for irreducible representations (p- and d-orbitals). Direct product.

Spectral transition probability, vibrionic coupling, non-centrosymmetric complexes, polarization of allowed transitions.

Application of Group Theory in Infrared and Raman Spectroscopy.

SALCs, projection operators, illustrative examples.

Unit 3: Hybridization and its applications: 5 lectures

Hybrid orbitals as Linear Combinations of Atomic Orbitals. Selected examples. MO diagram using Group Theory. Symmetry and chemical reactions.

Unit 4: Chemistry of d-and f-block elements: 10 lectures

Term-symbols, Russel-Saunders states, Crystal field theory and splitting in O_h, T_d, D_{4h} and C_{4v} systems, Orgel and Tanabe-Sugano diagrams, determination of Dq and Racah parameters, oxidation states and electronic absorption spectra of complex ions. Spectrochemical series and effects of covalency. Nephelauxetic series, magnetic properties of transition metal complexes and lanthanides, metal-metal bonds, cluster compounds of d-block elements, poly-oxo metallates of Ru, Os, Mo. Structure and bonding in complexes containing π-acceptor ligands. Relativistic effects affecting the properties of heavier transition elements.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Course outcomes:

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

- **CO1.** Remember the concepts of symmetry and symmetry operations in molecules.
- **CO2.** Explore the applications of group theory in molecular spectroscopy.
- **CO3.** Use of character tables and projection operator techniques.
- **CO4.** Apply the group theory and molecular spectroscopy to solve real world problems.

RECOMMENDED TEXTS:

1. Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
2. Jaffe, H. H. & Orchin, M. Symmetry in Chemistry Dover Publications (2002).
3. Hatfield, W. F. & Palmer, R. A. Problems in Structural Inorganic Chemistry W. A. Benjamin, Inc.: N.Y (1971).
4. Hatfield, W. E. & Parker, W. E. Symmetry in Chemical Bonding & Structure C. E. Merrill Publishing Co.: USA (1974).
5. Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973).
6. Shriver, D. F., Atkins, P. W. & Langford, C. H. Inorganic Chemistry, 2^{nd} Ed., Oxford Univ. Press (1998).
7. Purcell, K. F. & Kotz, J. C. Inorganic Chemistry, W. B. Saunders and Co.: N. Y. (1985).
8. Wulfsberg, G. Inorganic Chemistry Univ. Science books: USA (2000); Viva Books: New Delhi.
9. Sutton, D. Electronic Spectra of Transition Metal Complexes McGraw-Hill: New York (1968).
10. Mabbs, F. E. & Machin, D. J. Magnetism and Transition Metal Complexes Chapman and Hall: U.K. (1973).
11. Drago, R. S. Physical Methods in Chemistry W. B. Saunders Co.: U.K. (1977).

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH746	Subject Title	COMPUTER APPLICATIONS IN CHEMISTRY						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	2nd	Semester	III

Course Objective

1. Provides essential theoretical background of computational chemistry and practical/programming skills to perform
2. scientific computations to solve chemical problems.
3. Students will have exposure on a variety of computational tools in chemical science esp related to research

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: Introduction to computers and computing: 9 lectures
Basic structure and functioning of computer, computer languages, operating systems, introduction to UNIX and WINDOWS. Data processing, principles of programming.

Unit 2: FORTRAN Programming: 10 lectures
Types of Constants and Variables in Fortran, Dimension, Data, Type, COMMON and EQUIVALENCE statements, Arithmetic and Logical IF, IF-THENELSE constructs, 'DO' statement, Various types of 'I/O' statements, Library functions, Statement functions, Function subprograms and subroutine subprograms.

Unit 3: Programming in chemistry: 10 lectures
Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, Ph titration, kinetics, and radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations with the Huckel's theory. Elementary structural features, such as bond lengths, bond angles, dihedral angles, etc. of molecule extracted from a database, such as Cambridge database.

Unit 4: Use of computer programmes: 10 lectures
Running standard programmes and packages. Any suitable software, such as CHEMDRAW, MATLAB, LOTUS, EASYPLOT, FOXPRO, and word processing software, such as WORDSTAR/MSWORD.

Leaning outcomes:
CO1: Critically assess the applicability of computational methods to specific problems in chemistry and successfully apply appropriate computational techniques in their academic and scientific careers.
CO2: Hands on training in the context of currently available computational chemistry software and high-performance computer hardware.

List of experiment:

1. Exposure to available standard application packages like: Chemdraw, generation of graphs, data sheets creation, and tables using Excel Programme.
2. Some typical exercises based on the above:
3. Decimal-binary conversion
4. Numerical differentiation, quadrature and finding roots
5. pH of a weak acid
6. Roots of cubic equations (e.g. van der Waals' equation)- iterative, Newton-Raphson, Binary bisection, Regula-Falsi methods.
7. Titration curves and end-point location
8. Numerical integration (Trapezoidal, Simpson's rule)
9. H and S from Cp data
10. Chemical kinetics simulations
11. Least-squares fit including graphics
12. Numerical solution of differential equations (e.g. in kinetics)
13. Interpolation & interpolation of data
14. Gauss-Siedel method and its use in solving simultaneous equations (e.g. Lambert-Beer's law)

REFERENCE BOOKS:

1. V. Rajaraman, Fortran 77, Prentice Hall (India), New Delhi (1997).
2. Xavier, Fortran 77 and Numerical Methods, New Age International Pvt. Ltd. Publishers, New Delhi (1994).
3. S. Lipschutz and A. Poe, Schaum's Outline Series – Theory and Problems of Programming with Fortran including structured Fortran, Mc Graw Hill Book Company, Singapore (1982).
4. K. V. Raman, Computers in Chemistry, Tata McGraw Hill (1993).
5. Computers and common sense, R Hunt and J Shelley, Prentice Hall.
6. Computational chemistry, AC Norris.
7. Microcomputer quantum mechanics, JP Killingbeck, Adam Hilger.
8. Computer programming in FORTRAN IV, V Rajaraman, Prentice Hall.
9. An introduction to digital computer design, V Rajaraman and T Radhakrishnan, Prentice Hall.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

<table>
<tr><td>Subject Code</td><td>CH716</td><td>Subject Title</td><td colspan="7">ORGANIC CHEMISTRY-III (ORGANIC SPECTROSCOPY)</td></tr>
<tr><td>LTP</td><td>3 0 0</td><td>Credit</td><td>3</td><td>Subject Category</td><td>CC</td><td>Year</td><td>2nd</td><td>Semester</td><td>III</td></tr>
</table>

Course Objective

1. To understand and familiarize with the basic principles, theory of IR, 1H NMR, 13C NMR, 2D and Mass spectrometry.
2. To impart knowledge in the theory and applications of these spectroscopic techniques whi very important

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Content:

Unit 1: IR: 8 Lectures

Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups. Effect of H- bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

Unit 2: PMR: 10 Lectures

Natural abundance of 13C, 19F and 31P nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, spin-spin coupling, splitting theory, magnitude of coupling constant; Simple, virtual and complex spin-spin coupling; Chemical and magnetic equivalence, proton exchange, factors affecting the coupling – First and non-first order spectra; Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents) and NOE experiments (NOESY, HOESY, ROESY, etc.)

Applications of PMR in structural elucidation of simple and complex compounds.

Unit 3: CMR:8 Lectures

Resolution and multiplicity of 13 C NMR, 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and INEPT experiments; Introduction to 2D-NMR; COSY, HMQC and HETEROR spectra.

Unit 4: MASS: 13 Lectures

Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ion peak; Ionization methods (EI, CI, FAB, ESI, APCI and MALDI), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-, β-, allylic and benzylic cleavage; McLafferty rearrangement, ortho effect etc.

Structure elucidation of organic compounds using IR, NMR and Mass Spectra

Course outcomes:

CO1: Students will be skilled in the interpreting the IR, one, two-dimensional NMR spectroscopy, and Mass spectroscopy to derive the information regarding the structure, stereochemistry of the molecules.

CO2: Students will apply the learned the physical characterization of organic molecules

REFERENCE BOOKS:

1. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
2. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds John Wiley & Sons (1981).
3. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy Cengage Learning (2014).
4. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH717	Subject Title	ANALYTICAL CHEMISTRY III						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	2^{nd}	Semester	III

Course Objective

1. Understanding the insights of soil analysis, soil based waste management.
2. Learning the different aspects of pollutants in water, food, blood, and drugs and their analysis.
3. Identifying the different industrial pollutants and their prevention methods.
4. Evaluate errors in chemical analysis through statistical treatment of data

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Content:

Unit 1: Introduction: 5 lectures

Role of analytical chemistry, classification of analytical methods: classical and instrumental. Types of instrumental analysis. Selection of analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware: cleaning and calibration of glassware. Sample preparations: dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in analytical laboratory.

Unit 2: Errors and evaluation: 5 lectures

Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error. Types of errors in experimental data-determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods of reporting analytical data. Statistical evaluation of data-indeterminate errors. The use of statistics.

Unit 3: Food analysis: 8 lectures

Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration: common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

Unit 4: Analysis of water pollution: 10 lectures

Origin of waste water, types, water pollutants and their effects. Sources of water pollution: domestic, industrial, agricultural soil and radioactive wasts as source of pollution. Objectives of analysis, parameters of analysis: color, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulfate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution: public health, significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.

Unit 5: Analysis of soil, fuel, body fluids and drugs: 11 lectures

Analysis of soil:

Moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, Sulphur and alkali salts.

Fuel analysis:

Solid, liquid and gas. Ultimate and proximate analysis, heating values, grading of coal. Liquid fuels: flash point, aniline point, octane number and carbon residue. Gaseous fuels: producer gas and water gas, calorific value and its determination.

Clinical chemistry:

Composition of blood, collection and preservation of samples. Clinical analysis, serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis: trace elements in the body.

Drug analysis:

Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Course outcomes:

CO1: Analyze different trace elements.in soil by Chemical analysis.

CO2: Evaluate parameters to be controlled in solid waste and adopt methods for reduction and recycling of solid waste.

CO3: Analyze water quality through different analytical methods.

CO4: Apply absorption and emission and chemical analysis analyzing water pollutants and understand their impact.

CO5: Evaluate the industrial pollutants, understand their effects and adopt methods to reduce them.

CO6: Demonstrate their knowledge in evaluating different contaminants in food through water, pesticides and additives.

REFERENCE BOOKS:

1. Analytical chemistry, GD Christian, J Wiley.
2. Fundamentals of analytical chemistry, DA Skoog, DM West and FJ Holler, WB Saunders.
3. Analytical chemistry – principles, JH Kennedy, WB Saunders.
4. Analytical chemistry – principles and techniques, LG Hargis, Prentice Hall.
5. Principles of instrumental analysis, DA Skoog and JL Loary, WB Saunder.
6. Principles of instrumental analysis, DA Skoog, WB Saunders.
7. Quantitative analysis, RA Day, Jr. and AL Underwood, Prentice Hall.
8. Environmental solution analysis, SM Khopkar, Wiley Eastern.
9. Basic concepts of analytical chemistry, SM Khopkar, Wiley Eastern.
10. Handbook of instrumental techniques for analytical chemistry, F Settle, Prentice Hall.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH718	Subject Title	ORGANIC CHEMISTRY-IV (HETEROCYCLIC COMPOUNDS)						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	2nd	Semester	III

Course objectives: Understanding basic concepts about synthesis and reaction mechanisms of various heterocyclic organic reactions.
Course Pre/Co- requisite (if any): no restricted pre-requisite

Unit 1: Nomenclature of heterocycles: 9 lectures
Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.

Aromatic heterocycles:
General chemical behaviour of aromatic heterocycles, classification (structural type), criterion of aromaticity (bond length, ring current and chemical shifts in 1H NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

Non-aromatic heterocycles:
Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects – anomeric and related effects. Attractive interactions – hydrogen bonding and intermolecular nucleophilic-electrophilic interactions.

Unit 2: Heterocyclic synthesis: 20 lectures
Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

Small ring heterocycles:
Three-membered and four-membered heterocycles – synthesis and reactions of aziridines, oxiranes, thiiranes, oxetanes and thietanes.

Benzo-fused five-membered heterocycles:
Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, and benzothiophenes.

Meso-ionic heterocycles:
General classification, chemistry of some important meso-ionic heterocycles of type-A and –B and their applications.

Six-membered heterocycles with one heteroatom:
Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium and thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones. Six-membered heterocycles with two or more heteroatoms: 4 lectures Synthesis and reactions of diazines, triazines, tetrazines and thiazines.

Seven- and large-membered heterocycles:
Synthesis and reactions of azepines, oxepines, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

Unit 3: Heterocyclic systems containing P, As, Sb and B: 10 lectures
Heterocyclic rings containing phosphorus: Introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systems – phosphorinanes, phosphorines, phospholanes and phospholes. Heterocyclic rings containing as and Sb: Introduction, synthesis and characteristics of 5- and 6-membered ring systems. Heterocyclic rings containing B: Introduction, synthesis, reactivity and spectral characteristics of 3-, 5- and 6-membered ring systems.

Course outcome:
At the end of the course, students should be able to
CO1: Recall the fundamental principles of heterocyclic reactions.
CO2: Understand the concepts related to synthesis, mechanisms and the functions of various reagents.

REFERENCE BOOKS:
1. Heterocyclic chemistry Vol. 1-3, RR Gupta, M Kumar and V Gupta, Springer Verlag.
2. The chemistry of heterocycles, T Eicher and S Hauptmann, Thieme.
3. Heterocyclic chemistry, JA Joule, K Mills and GF Smith, Chapman and Hall.
4. Heterocyclic chemistry, TL Gilchrist, Longman scientific Technical.
5. Contemporary heterocyclic chemistry, GR Newkome and WW Paudler, Wiley-Inter Science.
6. An introduction to the heterocyclic compounds, RM Acheson, John Wiley.
7. Comprehensive heterocyclic chemistry, AR Kartrizky and CW Rees, eds. Pergamon Press

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH719	Subject Title	ANALYTICAL CHEMISTRY-IV (SEPARATION TECHNIQUES)						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	2nd	Semester	III

Course Objective

1. Making students understand the insights of statistical methods in qualitative and quantitative analysis and usage of different analytical instruments for chemical analysis.
2. Get insight into basics of different chromatographic techniques.

Course Pre/Co- requisite (if any): no restricted pre-requisite

Unit 1: Introduction to chromatography: 5 lectures
Principle & Classification of Chromatographic Methods. Interaction Mechanism (Ion-Exchange, Adsorption, Partition, Ion association, Gel Permeation and Molecular Sieving) - Chromatographic Resolution - Van Deemter Equation - Band Broadening and Non-Ideal Behavior - Optimizing Chromatographic Separation - Capacity Factor, Peak Capacity, Column Efficiency and Resolution - Calibrations and Standardizations.

Unit 2: Gas Chromatography: 7 lectures
Instrumentation - Carrier Gas – Packed and Capillary Column, Types of Stationary Phases and Column Selection). Injection Methods (On-column, Split/Split-less and Programmed Temperature Vaporiser) Temperature Control - Common detector systems.
Sampling Methods - Sample Selection & Preparation and Injection -. GC Method Development - Troubleshooting - Quantitative and Qualitative Applications – Hyphenated Systems (GC/MS).

Unit 3: Liquid Chromatography: 10 lectures
Instrumentation - HPLC/UPLC Columns - Types, Packing Characteristics and Modern Column Trends of HPLC Columns - Specialty Columns (Chiral and Bio-Separation).
Stationary Phases (Normal and Reverse-phase) - Mobile Phases (Selection of Mobile Phase, Isocratic and Gradient Elution) - Sample Preparation and Introduction- HPLC Method Development – Preparative HPLC - Troubleshooting – Quantitative and Qualitative Applications – Hyphenated Systems (LC/MS).
Super-critical Fluid Chromatography:
Concepts of Super-Critical Fluid Extraction (SFE) / Chromatography (SFC) - Properties of Supercritical Fluids – Selection of Solvents - Instrumentation – Working Mechanism - Applications.

Unit 4: Liquid – liquid extraction: 12 lectures
Principle, significance of various terms, batch and counter current extraction, classification of extraction systems, extraction equilibria of metal chelates, ion association extraction systems, extraction with high molecular weight amines, synergism, stripping, backwashing, salting out agents, masking agents, emulsion formation, identification of extracting species, analysis of organic phase, analysis of raffinate, environmental considerations, solid phase extraction.

Unit 5: Membrane and allied methods of separation: 5 lectures

Fundamentals and various terms, Liquid membranes, Cloud point extraction, Micellar enhanced separation processes, external field induced membrane separation processes.

Separation Techniques Based on Rate Processes:

(a) Barrier-separation methods: Membrane Separation-Ultra-filtration, dialysis, electro-dialysis, electro-osmosis, reverse Osmosis

(b) Field separation methods: Electrophoresis, Ultracentrifugation.

Course outcomes:

CO1: Identify and Separate different fragment from organic compounds using GC and HPLC techniques.

CO2: Apply GC and GC-MS techniques for the analysis of volatile organic compounds in predicting the fragments and structures of compounds.

CO3: Evaluate different chiral and bio molecules by separating them using HPLC, UPLC and hyphenated techniques like LC-MS.

CO4: Apply the principles and working of super critical fluid chromatography for extraction of super critical fluids.

CO5: Purify biological molecules using affinity chromatography.

REFERENCE BOOKS:

1. Richard G. Compton and Craig E. Banks, Understanding Voltammetry, 2nd Revised Edn., World Scientific Publishers, 2011.
2. Konstantin N. Mikhelson, Ion-Selective Electrodes, Springer-Verlag, 2013.
3. Gary D. Christian, Purnendu K. Dasgupta and Kevin A. Schug, Analytical Chemistry, 7th Edn., John Wiley & Sons, Inc., 2014.
4. Daniel C. Harris and Chucky Lucy, Quantitative Chemical Analysis, 9th Edn., W.H. Freeman, 2015.
5. Mark F. Vitha, Chromatoraphy: Principles and Instrumentation, John Wiley & Sons, Inc., 2017.
6. Danilo Corradini, Handbook of HPLC, CRC Press Taylor and Francis, 2011.
7. C.F. Poole, Gas Chromatography, Elsevier Inc., 2012.
8. Yuki Saito and Takumi Kikuchi, Voltammetry – Theory, Types and Applications, Nova Science Publishers, Inc. 2014.
9. M. Anderson, A. Fitch and J. Stickney, Chemically Modified Electrodes, Electrochemical Society, 2015
10. Douglas A. Skoog, F. James Holler and Stanley R. Crouch, Principles of Instrumental Analysis, 7th Edn., Cengage Learning Publishers, 2018.
11. Rousseau, R.W.,“Handbook of Separation Process Technology”, John Wiley & Sons, 1989.
12. Fifield, F.W. and Kealey, D., “Principles and Practice of Analytical Chemistry”, 5th Ed., Blackwell Science, 2000.
13. Li, N.N., Fane, A.G., Winston, W.S. and Matsuura, H. T., (Eds.), “Advanced Membrane Technology and Applications”, Wiley, 2008.
14. Mitra, S. (Ed.), “Sample preparation techniques in Analytical Chemistry”, John Wiley and Sons, New Jersey, 2003.
15. Madou, M.J.,” Fundamentals of Microfabrications and Nanotechnology”, 3rd Ed., CRC Press, 2011.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Semester IV

Course Category	Course Code	Course Title	L	P	Credit
CC	CH726	Organic chemistry-V(**Natural product and Medicinal chemistry**)	3	0	3
	CH727	Analytical chemistry-V (Advanced spectroscopy and diffraction methods)	3	0	3
CC	CH728	Organic chemistry-VI (**Synthetic strategies**)	3	0	3
	CH729	Analytical chemistry-VI (Electroanalytical methods)	3	0	3
PJCT	CH737	Project	0	20	10
SEM	CH738	Seminar	0	8	4
		Total	**6**	**28**	**20**

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH726	Subject Title	ORGANIC CHEMISTRY-V (NATURAL PRODUCT AND MEDICINAL CHEMISTRY)						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	**2nd**	**Semester**	**IV**

Course objectives:

1. To understand the chemistry aspects of alkaloids, steroids, and carotenoids and their sources and also related to methods of isolation.
2. To develop thorough knowledge of natural products relating with its synthesis, properties, medicinal applications and their metabolic activities and biological functions

Course Pre/Co- requisite (if any): no restricted pre-requisite

Unit 1: Alkaloids: 12 lectures

Definition, nomenclature, and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic rings, role of alkaloids in plants. Structure, stereochemistry, synthesis, and biosynthesis of Ephedrine, (+)-Coniine, Nicotine, Atropine, Quinine, and Morphine.

Unit 2: Steroids: 12 lectures

Occurrence, nomenclature, basic skeleton, Diel’s hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone. Biosynthesis of steroids.

Unit 3: Plant pigments and Carotenoids: 7 lectures

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Asigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin. Zingiberene, Santonin, Phytol, Abietic acid, and β-Carotene.

Unit 4: Porphyrins and Prostaglandins: 4 lectures

Porphyrins: Structure and synthesis of Haemoglobin and Chlorophyll.

Prostaglandins: Occurrence, nomenclature, classification, biogenesis, and physiological effects. Synthesis of PGE2 and PGF2α.

Unit 5: Antibiotics: 4 lectures

Mechanism of action of lactam antibiotics, non-lactam antibiotics and quinilones; antiviral and anti-AIDS drugs.

Neurotransmitters: classes of neurotransmitters, Drugs affecting collingeric and adrenergic mechanisms.

Anti-histamines, anti-inflammatory, anti-analgesics, anticancer and anti-hypertensive drugs.

Learning outcomes:

CO1: Understand the chemistry, degradation, synthesis and biosynthesis of natural products like steroids, alkaloids, terpenoids, flavonoids and pigments.

REFERENCE BOOKS:

1. Natural products: Chemistry and biological significance, J Mann, RS Davidson, JB Hobbs, DV Banthrope and JB Harborne, Longman, Essex.
2. Organic chemistry, vol. 2, IL Finar, ELBS.
3. Stereoselective synthesis: A practical approach, M Nogradi, VCH. • Rodd's chemistry of carbon compounds, Ed. S Coffey, Elsevier.
4. Chemistry, biological and pharmacological properties of medicinal plants from the Americas, ed. Kurt Hostettmann, MP Gupta and A Marston, Harwood Academic Publishers.
5. Introduction to flavonoids, BA Bohm, Harwood Academic Publishers.
6. New trends in natural product chemistry, Atta-ur-Rahman and MI Choudhary, Harwood Academic Publishers.
7. Insecticides of natural origin, Sukh Dev, Harwood Academic Publishers.
8. Gringauz, A. *Introduction to Medicinal Chemistry: How Drugs Act and Why?* John Wiley & Sons (1997).
9. Patrick, G. L. *Introduction to Medicinal Chemistry* Oxford University Press (2001).
10. Lemke, T. L. & William, D. A., *Foye's Principles of Medicinal Chemistry*, 5th Ed., USA, (2002)

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

<table>
<tr><td>Subject Code</td><td>CH727</td><td>Subject Title</td><td colspan="7">ANALYTICAL CHEMISTRY-V (ADVANCED SPECTROSCOPY AND DIFFRACTION METHODS)</td></tr>
<tr><td>LTP</td><td>3 0 0</td><td>Credit</td><td>3</td><td>Subject Category</td><td>CC</td><td>Year</td><td>2nd</td><td>Semester</td><td>IV</td></tr>
</table>

Course Objective

1. To impart knowledge of advanced spectroscopic techniques for structural analysis of organic compounds and its applications.
2. Understand the basic physical aspects of NMR and Photoacoustic spectroscopy
3. Understand the basic physical aspects of X-ray, electron and neutron diffraction

Course Pre/Co- requisite (if any): no restricted pre-requisite

Course Content:

Unit 1: Magnetic resonance: 12 lectures

Introduction to magnetic resonance spectroscopy and classification.

Nuclear Magnetic Resonance Spectroscopy (NMR): Nuclear spin, spin angular momentum, nuclear resonance, basic principles and relaxation times, saturation, intensity of NMR signals, electronic shielding and deshielding, NMR in liquids: chemical shift and its measurement, spin-spin couplings, factors affecting coupling constant 'J', NMR spectra of AX, A3X and AB systems, spin decoupling, basic idea about instrumentation, NMR studies of nuclei other than proton: ^{13}C, ^{19}F, and ^{31}P.

FT-NMR: Rotating frame of reference, effect of RF pulses, FID, Multipulse operation, measurement of T1 by inversion recovery method, spin echo and measurement of T2, 2-D NMR, NMR hardware, advantages.

Electron spin resonance spectroscopy: Basic principle, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

Nuclear quadrupole resonance spectroscopy: Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

Unit 2: Photoacoustic spectroscopy: 5 lectures

Basic principles of photoacoustic spectroscopy (PAS), PAS-gases and condensed systems, chemical and surface applications.

Unit 3: X-ray diffraction: 10 lectures

Bragg's condition, miller indices, Laue method, Bragg's 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, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

Unit 4: Electron diffraction: 4 lectures

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

Unit 5: Neutron diffraction: 8 lectures

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

Learning outcomes:

CO1: The students will acquire knowledge of

CO2: Electronic spectroscopy of different elements and simple molecules.

CO3: Nuclear Magnetic and Electron Spin Resonance Spectroscopy for organic compounds analysis, medical diagnostics.

CO4: Understand the principle of X-ray, electron and neutron diffraction technique.

REFERENCE BOOKS:

1. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 3rd Edition, Springer.
2. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, (1979), Chapman and Hall, London.
3. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, (1986), Addison Wesley, Longman Ltd, London.
4. Modern spectroscopy, JM Hollas, John Wiley.
5. NMR, NQR, EPR and Mossbauer spectroscopy in inorganic chemistry, RV Parish, Ellis Harwood.
6. Physical methods in chemistry, RS Drago, Saunders College.
7. Basic principles of spectroscopy, R Chang, McGraw Hill.
8. Introduction to photoelectron spectroscopy, PK Ghosh, John Wiley.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	CH728	Subject Title	ORGANIC CHEMISTRY-VI (SYNTHETIC STRATEGIES)						
LTP	3 0 0	Credit	3	Subject Category	CC	Year	2nd	Semester	IV

Course objective:
Providing various methodologies used in organic synthesis, which enable the student to think different possible ways to synthesis an organic compound including ring synthesis and understanding about the disconnection approach for the organic synthesis and asymmetric synthesis

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: Disconnection and synthetic approach: 9 lectures
Introduction to synthons and synthetic equivalents, disconnection approach, one group and two group disconnections, reversal of polarity, chemo-selectivity, functional group inter-conversions, selectivity rules, one group C-X disconnection, two group C-X disconnections, 1,3-difunctional and 1,5- difunctional compounds. Tandem reactions, Domino reactions and multi-component reactions.

Unit 2: Asymmetric synthesis: 3 lectures
Development of methodologies for asymmetric synthesis: regioselectivity, stereoselectivity, dia-stereoselectivity and stereospecificity.

Unit 3: One group C-C disconnection: 6 lectures
Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic and nitro compounds in organic synthesis. Examples of other relevant groups.
Two-group C-C disconnections: 6 lectures
Diels-Alder reaction, 1,3-difunctionalized compounds, α, β-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difucntionalized compounds, Micheal addition and Robinson annelation.

Unit 4: Ring synthesis: 5 lectures
Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

Unit 5: Synthesis of some complex molecules: 10 lectures
Total synthesis of the following compounds using disconnection approaches: Camphor, Longifoline, Cortisone, Reserpine, Vitamn-D, Juvabione, Aphidicolin, Fredericamycin A, Gingerol, (z)-Jasmone, Prostaglandins E2, F2α, Menthol, Taxol and Gandriol.

Course outcomes:
At the end of the course, students should be able to
CO1: Recollect the fundamental principles of organic reactions.
CO2: Understand the concepts related to synthesis, mechanisms and the functions of various reagents.

REFERENCE BOOKS:

1. Warren, S. Organic Synthesis: The Disconnection Approach John Wiley & Sons (1984).
2. Lehn, J-M, Supramolecular Chemistry: Concepts & Perspectives. A Personal Account Vch Verlagsgesells chaft Mbh (1995).
3. Vögtle, F. Supramolecular Chemistry: An Introduction John Wiley & Sons (1993).
4. Designing organic synthesis, S Warren, Wiley.
5. Organic synthesis – concepts, methods and starting materials, J Fuhrhop and G Penzillin, Verlage VCH.
6. Some modern methods of organic synthesis, W Carruthers, Cambridge Univ. Press.
7. Modern synthetic reactions, HO House, WA Benjamin.
8. Advanced organic chemistry: Reactions, mechanisms and structure, J March, Wiley.
9. Principles of organic synthesis, R Norman and JM Coxon Blackie Academic & Professional.
10. Advanced organic chemistry Part B, FA Carey and RJ Sundberg, Plenum Press.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Subject Code	**CH729**	**Subject Title**	**ANALYTICAL CHEMISTRY-VI (ELECTROANALYTICAL METHODS)**						
LTP	3 0 0	**Credit**	3	**Subject Category**	CC	**Year**	**2^{nd}**	**Semester**	**IV**

Course Objective

1. Learn the principles and usage of Electroanalytical techniques.
2. Understanding different types of nanomaterials, syntheses and characterization
3. Applying the knowledge of nanomaterials in science and technology

Course Pre/Co- requisite (if any): no restricted pre-requisite
Course Content:

Unit 1: General Introduction: 3 lectures
Electrocapillary curve and electrocapillary maximum potential, Mercury electrodes (DME, SME, HMDE), Rotating platinum electrode. Three-electrode system.

Unit 2: Polarographic techniques: 9 lectures
Operational amplifiers concept and design of polarographic circuit using op-amps. Ilkovic equation, theory of diffusion, kinetic, adsorption and catalytic currents. Controlled potential electrolysis and coulometry. 2 and 3 electrodes systems. Polarography versus voltammetry, determination of number of electrons. Theory of reversible, quasi-reversible and irreversible electrode processes. Pulse and differential pulse polarography and their superiority over DC polarography. A.C. polarography.

Unit 3: Voltammetric techniques: 14 lectures
Linear and cyclic sweep voltammetry, Randles Sevcik equation, effect of sweep rate and evaluation of adsorption characteristics of reactant or product using CV. Coupled chemical reactions and their characterization. Characteristics of commonly used working electrodes such as glassy carbon, platinum, pyrolytic graphite and reference electrodes SCE and Ag/AgCl. Enzyme catalysed oxidations of biomoleules viz., uric acid, guanine, adenine and their comparison with electrochemical reactions. Anodic and cathodic stripping and determination of metal ions, pollutants and biomolecules using stripping voltammetry.

Unit 4: Sensors: 7 lectures
Amperometric and voltammetric sensors. Modified electrodes and their advantages over conventional electrodes in sensing variety of metals and biomolecules. Nanomaterials in electrode modification– C60, single wall and multi wall carbon nanotubes. Preparation and characterization of modified surfaces. Applications of sensors in determining cases of doping.

Unit 4: Ion-selective electrodes: 6 lectures
Working principles and applications– Theoretical considerations - Types of ion-selective electrodes – Properties of ion-selective electrodes – Sources of errors – Construction and working of cation specific electrodes for analysis of cadmium, lead, arsenic and anion specific electrodes for fluoride, chloride and sulphide ions.

COURSE STRUCTURE & SYLLABUS OF M.SC. CHEMISTRY APPLICABLE FOR 2022-2024 BATCH

Course outcomes:

At the end of the course, the student should be able to

CO1: Analyze electroactive species using different voltammetric techniques.

CO2: Define different types of nanomaterials based on dimensionality and structure

CO3: Propose preparation methods for different nanomaterials

CO4: Analyse nanomaterials using characterization techniques

CO5: Explain the structural and chemical properties of carbon based nanomaterials

REFERENCE BOOKS:

1. Meites, L., “Polarographic Techniques”, 3rd Ed., Interscience publishers, N.Y., 1990.
2. Lund and Baizer, “Organic Electrochemistry”, Marcel Dekker, New York, 2000.
3. Bard, A.J. and Faulkner, L.R., “Electrochemical Methods-Fundamentals and Applications”, John Wiley, 2000.
4. Sane, R.T. and Joshi, A.P., “Electroanalytical Chemistry: Theory and Applications”, Quest Publications,1999.
5. Richard G. Compton and Craig E. Banks, Understanding Voltammetry, 2nd Revised Edn., World Scientific Publishers, 2011.
6. Konstantin N. Mikhelson, Ion-Selective Electrodes, Springer-Verlag, 2013.
7. Gary D. Christian, Purnendu K. Dasgupta and Kevin A. Schug, Analytical Chemistry, 7th Edn., John Wiley & Sons, Inc., 2014.
8. Daniel C. Harris and Chucky Lucy, Quantitative Chemical Analysis, 9th Edn., W.H. Freeman, 2015.
9. Mark F. Vitha, Chromatoraphy: Principles and Instrumentation, John Wiley & Sons, Inc., 2017.
10. Danilo Corradini, Handbook of HPLC, CRC Press Taylor and Francis, 2011.
11. C.F. Poole, Gas Chromatography, Elsevier Inc., 2012.
12. Yuki Saito and Takumi Kikuchi, Voltammetry – Theory, Types and Applications, Nova Science Publishers, Inc. 2014.
13. M. Anderson, A. Fitch and J. Stickney, Chemically Modified Electrodes, Electrochemical Society, 2015.
14. Douglas A. Skoog, F. James Holler and Stanley R. Crouch, Principles of Instrumental Analysis, 7th Edn., Cengage Learning Publishers, 2018.