COURSES OF STUDIES FOR THE M.Sc. EXAMINATION IN CHEMISTRY

Semester	Course	Course Name	Total marks
I	PAPER-I (CH-1.1.1)	INORGANIC CHEMISTRY	10+ 40 = 50
	PAPER-II (CH-1.1.2)	ORGANIC CHEMISTRY	10+ 40 = 50
	PAPER-III (CH-1.1.3)	PHYSICAL CHEMISTRY	10+ 40 = 50
	PAPER-IV (CH-1.1.4)	PHYSICAL CHEMISTRY	10+ 40 = 50
	PAPER-V (CH-1.1.5)	INORGANIC CHEMISTRY PRACTICAL	20 +80 =100
			300
II	PAPER-VI (CH-1.2.6)	INORGANIC CHEMISTRY II	10+ 40 = 50
	PAPER-VII (CH-1.2.7)	ORGANIC CHEMISTRY	10+ 40 = 50
	PAPER-VIII (CH-1.2.8)	PHYSICAL CHEMISTRY	10+ 40 = 50
	PAPER-IX (CH-1.2.9)	ORGANIC SPECTROSCOPY	10+ 40 = 50
	PAPER-X (CH-1.2.10)	ORGANIC CHEMISTRY PRACTICAL	20 +80 =100
			300
III	PAPER-XI (CH-2.3.11)	INORGANIC CHEMISTRY III	10+ 40 = 50
	PAPER-XII (CH-2.3.12)	INORGANIC CHEMISTRY IV	10+ 40 = 50
	PAPER-XIII (CH-2.3.13)	ORGANIC CHEMISTRY	10+ 40 = 50

	PAPER-XIV (CH-2.3.14)	PHYSICAL CHEMISTRY-III, INTERDISCIPLINARY-I	10+ 40 = 50
	PAPER-XV (CH-2.3.15)	GENERAL CHEMISTRY-IV: PRACTICAL	20 +80 =100
			300
IV	PAPER-XVI (CH-2.4.16)	MATERIALS CHEMISTRY	10+ 40 = 50
	PAPER-XVII (CH-2.4.17)	BIOCHEMISTRY	10+ 40 = 50
	PAPER-XVIII (CH-2.4.18)	BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY	10+ 40 = 50
	PAPER-XIX (CH-2.4.19)	MODERN ORGANIC CHEMISTRY	10+ 40 = 50
	PAPER-XX (CH-2.4.20)	Dissertation	100
			300
		TOTAL	**1200**

COURSES OF STUDIES FOR THE M.Sc. EXAMINATION IN CHEMISTRY

SEMESTER -I

PAPER-I (CH-1.1.1)

INORGANIC CHEMISTRY

***Learning Objectives*:** This paper aims to introduce the students to stereochemistry and bonding in main group compounds, symmetry, group theory and chemistry of main group elements.

***Learning Outcomes*:** This paper will ensure that the students learn to predict structures of main group compounds, do symmetry operations & predict point groups. Students will learn to apply the great orthogonality theorem and use of character tables. Students will gain a sound knowledge about some industrially important compounds of main group like Boranes, Carboranes, Silicones, Silicates, Boron nitride, Borazines, Phosphazenes etc. and also about Hydrides, Oxides and Oxoacids of pnictogens (N, P), chalcogens (S, Se & Te) and halogens, Xenon compounds, Pseudo halogens and Interhalogen compounds

UNIT-I Stereochemistry and Bonding in main group compounds

VSEPR, Walsh diagram (tri molecules), d_{π}-P_{π} bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

UNIT-II Symmetry and Group Theory

Symmetry elements and Symmetry operation, Groups and Subgroups, Symmetry point group. Schonflies symbols, Matrix representations of groups. Character of a representation. The Great Orthogonality theorem (without proof) and its importance. Character tables and their uses. Derivation of character table for C_{2v} , C_{3v}.

UNIT-III Chemistry of Main Group elements A

General characteristics, Allotropes, Structure and Reactions of simple and industrially important compounds: Boranes, Carboranes, Silicones, Silicates, Boron nitride, Borazines and Phosphazenes.

UNIT-IV Chemistry of Main Group elements B

General characteristics, Structure and Reactions of simple and industrially important compounds: Hydrides, Oxides and Oxoacids of pnictogens (N, P), chalcogens (S, Se &Te) and halogens, Xenon compounds, Pseudo halogens and Interhalogen compounds.

PAPER-II (CH-1.1.2)

ORGANIC CHEMISTRY

***Learning Objectives*:** The main objective of this paper is to introduce the students to the reaction dynamics i.e., the study of reaction mechanism.

***Learning Outcomes*:** The outcome of the course is to ensure that the students develop a critical understanding of reaction mechanism, kinetics and thermodynamics of organic reaction.

UNIT-I Reaction Mechanism: Structure and Reactivity: (a) Types of mechanism, 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, isotope effects. Hard and soft acids and bases. **(b)** Generation, structure, stability and reactivity of carbocations, carbanions, free radicals. Carbenes and nitrenes. Effect of structure on reactivity: resonance and field effect, steric effect, quantitative treatment. The Hammett equation and linear free energy relationships, substitutent and reaction constants. Taft equation.

UNIT-II (a) Aliphatic Nucleophilic substitution: The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by σ and π bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

The SN1 mechanism: Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

(b) Selective organic name reactions: Favorski reaction, stock enamine reaction, Mannich reaction, Sharpless asymmetric epoxidation, ene reaction, barton reaction, Baeyer-Villiger reaction, Chichibabin reaction, Claisen condensation, Claisen reduction, Curtius Rearrangement, Demjanov rearrangement, Dieckmann condensation, Favorskii rearrangement, Horner-Wadsworth-Emmons olefination, Wittig olefination, Wolff- kishner reduction, Mitsunobu reaction, Fries rearrangement, Peterson olefination, Macmurry Coupling

UNIT-III (a) Aromatic Nucleophilic Substitution: The SNAr, SN^{i} benzyne and SRN1 mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

(b) Aromatic Electrophilic Substitution: The areniun 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, Vilsmeier reaction, Gattermann- Koch reaction.

UNIT–IV (a) Free Radical Reactions: Types of free radical reactions: Free radical substitution, mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

(b) Elimination Reactions: The E2, EI and E1cB mechanisms. Orientationof the double bond. Reactivity: Effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

PAPER-III (CH-1.1.3)

PHYSICAL CHEMISTRY

***Learning Objectives*:** This course is intended to introduce students to the quantum chemistry, approximation methods and structure and bonding.

***Learning Outcomes*:** After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about structure and bonding

UNIT-I Quantum Chemistry: The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

UNIT-II Approximation Methods: The Helium atom. The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

UNIT-III Electronic Structure of Atoms: Multielectron atom. Electronic configuration. Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman splitting.

UNIT-IV Molecular Orbital Theory: H_2^+ and H_2 molecules: Valance bond theory (VBT) and molecular orbital theory (MOT) approaches. Homonuclear and Heteronuclear diatoms. Huckel theory of conjugated systems, bond order and charge density calculation. Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene.

PAPER-IV (CH-1.1.4)

PHYSICAL CHEMISTRY

***Learning Objectives*:** This course is intended to introduce students to the various facets of thermodynamics and chemical dynamics, which deals with the laws of thermodynamics, the concept of chemical potential and partial molar properties, Phase, concepts of thermodynamic probability and chemical dynamics.

***Learning Outcomes*:** The outcome of the course is to ensure that the students develop a critical understanding of thermodynamic systems, statistical thermodynamics and chemical dynamics

UNIT-I Classical Thermodynamics: Brief resume of concepts of laws of thermodynamics, entropy and free energy. The concept of chemical potential and partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and determination of fugacity. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients, ionic strength.

UNIT-I Classical Thermodynamics: Brief resume of concepts of laws of thermodynamics, entropy and free energy. The concept of chemical potential and partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and determination of fugacity. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients, ionic strength.

UNIT-II Phase Diagram: Phase behavior of one and two component systems (solid-solid, solid-liquid, solid-vapor, liquid-liquid, liquid-vapor equilibrium). Ehrenfest classification of phase transitions.

UNIT–III 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 function. Fermi-Dirac statistics, distribution law and application to metal. Bose-Einstein statistics - distribution law and application to helium.

UNIT–IV Chemical Dynamics: Potential energy surfaces. Collision theory of reaction rates, Conventional transition state theory (CTST); CTST as applied to ionic reactions, kinetic salt effects. steady state kinetics. Kinetic and thermodynamic control of reactions.

Treatment of unimolecular reactions. dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice Ramps Berger - Kassel Marcus (RRKM) theories of unimolecular reactions).

Dynamics chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen -bromine and hydrogen - chlorine reactions) and oscillatory reactions (Belousov- Zhabotinski reaction), homogeneous catalysis, kinetics of enzyme reactions. General features of fast reactions, study of fast reactions by flow methods, relaxation methods, Flash photolysis. Dynamics of barrier less chemical reactions in solution.

PAPER-V (CH-1.1.5)

INORGANIC CHEMISTRY PRACTICAL

***Learning Objectives*:** This course aims to explain the students how to classify acid and basic radicals into different groups and their chemical analysis. Synthesis of some selected inorganic complexes is also covered under this course.

***Learning Outcomes*:** After completion of this course students should be able to analyze mixture of inorganic salts and insoluble inorganic samples. Able to identify acid and basic radicals in a sample of unknown mixtures. They should be able to handle air and moisture sensitive chemicals for the synthesis and study of complexes and inorganic reactions.

1. Qualitative analysis of mixtures containing not more than eight radicals [less common metal ions Mo, W, Ti, V, Zr, U (two metal ions in cationic / anionic forms), insoluble- oxides, sulphates and halides may be included].
2. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.
3. Synthesis of bulky Schiff base (Ketimine/ diketimine/ phenolate) transition metal complexes.
4. Preparation of some selected inorganic compounds and their study. Handling of air and moisture sensitive compounds.
   a) Mn(acac)3

b) $K_3[Fe(C_2O_4)_3]$.

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

d) [Ni(dimg)$_2$.

e) $[Cu(NH_3)_4].SO_4.H_2O$

f) Cis - and Trans $[Co(en)_2]Cl_2$.

5. Wilkinson's catalyst, $(PPh_3)_3RhCl$:

a) Synthesis of Wilkinson's catalyst

b) Reaction of Wilkinson's catalyst with Cyclohexene

c) Reaction of Wilkinson's catalyst with Hydrogen.

SEMESTER –II

PAPER – VI (CH-1.2.6)

INORGANIC CHEMISTRY

***Learning Objectives*:** The objective of this course is to introduce students to chemistry of transition and inner transition elements and chemistry of lanthanides and actinides. This course deals with the electronic spectra of transition metal complexes, the nature of metal- ligand bonding and coordination chemistry of metal ions.

***Learning Outcomes*:** This course shall ensure that students get a thorough knowledge on CFT and MOT of transition metal complexes. Students will have a firm understanding of Orgel and Jahn-Teller diagrams, structure of mixed metal oxides and chemistry of inner transition elements.

UNIT-I: Electronic Spectra of Transition Metal Complexes: Spectroscopic ground states, Orgel diagrams for d^1-d^9 states in Oh and Td symmetry, Tanabe-Sugano diagrams for d^2 configuration in Oh and Td symmetry. Calculations of Dq, B and β parameters.

UNIT-II Metal-Ligand Bonding: Crystal-Field Theories: Limitation of Crystal Field Theory, Molecular orbital theory for Octahedral, Tetrahedral and Square Planar Complexes, σ and π bonding in Molecular Orbital Theory. Application of MOT to Correlation diagrams.

UNIT-III: Chemistry of Transition Transition Elements: Coordination chemistry of Transition Metal ions, Stabilization of Unusual oxidation states, Stereochemistry of coordination compounds, splitting of d-orbitals in Low symmetry environment, Jahn-Teller effect, Interpretation of Electronic Spectra including Charge Transfer Spectra, Spectrochemical series, Nephelauxetic series, Fluxional molecules, Iso and Hetero Poly acids. Structures of Mixed Metal Oxides: Spinel & Inverse Spinel, lleminite and Perovskite structure, Coloured Minerals and Gem quality crystals.

UNIT-IV: Chemistry of Inner Transition Elements: Chemistry of Lanthanides and Actinides: Lanthanide Contraction, Separation of Lanthanide elements, Oxidation state, Spectral and Magnetic Properties, Stereochemistry, Use of Lanthanide Compounds as Shift reagents, Actinide contraction, Oxidation states, Comparisons between Lanthanides andActinides.

PAPER -VII (CH-1.2.7)

ORGANIC CHEMISTRY

***Learning Objectives*:** This course deals with brief understanding of nature of bonding in organic compounds and stereochemical aspects. Different types of addition reaction to carbon-carbon double bonds and carbon-hetero multiple bonds, different classes of pericyclic reactions are introduced in this course. Students are also introduced to target oriented synthesis through retrosynthetic approaches.

***Learning Outcomes*:** This course will ensure that the students shall understand the bonding of complex polyenes, aromaticity and will gain a sound knowledge about stereochemistry of organic compounds. They should also get a clear idea of reaction mechanism of carbonyl compounds and get an insight into different theories and application of pericyclic reactions. After completing this course, they should be able to design logical synthetic steps toward synthesis of a target molecule.

UNIT-I (a) Nature of Bonding in Organic Molecules: Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and nonbenzenoid compounds, alternant and non-alternant hydrocarbons. Huckel's rule, energy level of π-molecular orbitals, annulenes, antiaromaticity, ψ- aromaticity, homoaromaticity, Fullerene (C60)

(b) Stereochemistry: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotropic and diastereotropic atoms, groups and faces, stereospecifjc and, steroselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helicalshape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

UNIT–II (a) Addition to Carbon-Carbon Multiple Bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, selectivity, orientation and reactivity, Electrophilic cyclization, Baldwin's rule. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction. Sharpless asymmetric epoxidation.

(b) Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates, Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. **UNIT-III Pericyclic Reactions:** Molecular orbital symmetry, Frontier orbitals ofethylene, 1,3-butadiene, 1, 3, 5 – hexatriene and allyl system. Classification of pericyclic reactions. WoodWard –Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions, conrotator and disrotatory motions; 4n, 4n+2 and allyl systems.Cycloadditions, antarafacial and suprafacial additions; 4n and 4n+2 systems, 2+2 additionof ketenes. 1, 3 - dipolar cycloadditon and cheletropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3 - and 5, 5 – sigmatropic rearrangements: Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

UNIT-IV (a) Disconnection approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two groups C-X disconnections, chemoselectivity, reversal of polarity (umpolung reaction), cyclisation reactions, amine synthesis.

(b) Protecting groups: Principle of protection of alcohol, amine, carbonyl, carboxyl groups and Umpolung Reaction

(c) One group C-C disconnection: Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

(d) Two group C – C disconnection: Diels-Alder reaction, 1,3 – difunctionalized compounds, alpha, beta- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5 – difunctionalized compounds, Michael addition and Robinson annelation.

(e) Chemistry of Natural Products: Application of Disconnection approach in the construction of biomolecules like Synthesis of Camphor, Longifoline & Juvabione.

PAPER VIII (CH-1.2.8)

PHYSICAL CHEMISTRY

***Learning Objectives*:** This course introduces students to surface chemistry including adsorption and surface tension. An outline on micelles is provided here. The course also deals with electrochemistry and ion-ion, ion-solvent interactions and electrodics. Lastly, an introduction to error analysis is given

Learning Outcomes: After successful completion of this course students should be able to understand statistical methods in chemical analysis. They should have a proper understanding of micellar systems, CMC, solubilization and reverse micelles. The students are also expected to gain insights into adsorption isotherms and catalytic activity in surfaces.

UNIT-I Surface Chemistry: (a) Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces.

(b) Micelles: Surface active agents, classification of surface-active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMCof surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, solubilization, micro emulsion, reverse micelles. **UNIT-II Electrochemistry: (a) Ion-Solvent interactions:** Nonstructural treatment ofion- solvent interaction, quantitative measure of ion solvent interactions. The Born model,Electrostatic potential at the surface of a charged sphere. The electrostatics of charging anddischarging spheres. The Born expression for the free energy of ion-solvent interactions,the interaction of a single ionic species with the solvents. Experimental evaluation of theheat of interaction of a salt and solvent, limitation of Born theory.

Structural treatment of the ion-solvent interactions, structure of water near an ion, Ion-dipole model of ion solvent interaction, ion-dipole approach to the heat of salvation, limitation of ion-dipole theory of salvation, water molecule as electrical quadrupole, ion-quadrupole model of ion-solvent interaction, Ion-induced dipole interactions in the primary salvation sheath, Limitation of ion-quadrupole theory of salvation.

(b) Ion-Ion interactions: Debye-Huckel-Onsager treatment and its extension. Debye- Huckel-Jerrum model.

UNIT-III Electrodics: Thermodynamics of electrified interface equations. Derivation of electrocapillarity; Lippmann equations (surface excess), methods of determination,Structure of electrified interfaces. Overpotentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, interfaces-theory of double layer at semiconductor- electrolyte solution interfaces. Effect of light at semiconductor solution interface. Electrocatalysis-influence of various parameters. Diffusion layer. The limiting current density and its practical application. Corrosion, Battery and Fuel cell.

UNIT-IV Error Analysis: Statistical methods in chemical analysis: Theory of error and treatment of quantitative data, accuracy and precision, ways of expressing accuracy and precision, Normal error curve and its equation. Useful statistical tests with equation, test of significance, the F-test, the students t-test, the Chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values,regression analysis (least square method for linear plots).

PAPER-IX (CH-1.2.9) ORGANIC SPECTROSCOPY

Learning Objectives: This course is basically focused on structure determination of organic molecules using spectroscopic method such as ultra violet (UV), infrared (IR), nuclear magnetic resonance (NMR) spectroscopy of ^{1}H and ^{13}C and mass spectroscopy (MS). This course introduces the basic principles of electronic transition, selection rule, molecular vibrations and absorption of electromagnetic radiation. Also nuclear spin and interaction of radiation with nucleus and fundamental principle of NMR spectroscopy is discussed. 2D NMR is also discussed such as COSY, NOESY, DEPT, APT for structure determination. Basic principles, instrumentation and application of MS are also covered.

Learning Outcomes: After successful completion of this course students should be able to elucidate the structure and molecular mass of small organic molecules using UV, IR, NMR, MS. Calculate the absorption maxima of conjugated molecules using Woodward rule. To gain firmidea of functional groups present in a molecule from IR spectroscopic idea.

UNIT-I (a) Ultraviolet and Visible Spectroscopy: Various electronic transitions, Beer Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, steric effect in biphenyls.

(b) Infrared spectroscopy: Instrumentation and sample handling, characteristics vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, Detail study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, amides, acids, anhydrides, lactones, lactams,and conjugated carbonyl compounds), Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FTIR, IR of gaseous, solid and polymeric materials.

UNIT II: Nuclear Magnetic Resonance Spectroscopy (NMR): General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic, and aromatic compounds) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, and mercapto), chemical exchange, effect of deuterium, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry, hindered rotation, karplus curve- variation of coupling constant with dihedral angle, simplification of complex spectra, nuclear magnetic double resonance, NMR shift reagents, solvent effects, Fourier transform technique, nuclear overhauser (NOE). Resonance of other materials.

UNIT III Carbon-13 NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two-dimension NMR spectroscopy – COSY, NOESY, DEPT, APT and INADEQUATE techniques.

UNIT IV Mass spectrometry: Introduction, ion production – EI, CI and FAB factors affecting fragmentation, ion-analysis, ion analysis, ion abundance, mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule, high resolution mass spectrometry, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

PAPER-X (CH-1.2.10) ORGANIC CHEMISTRY PRACTICAL

***Learning Objectives*:** This course is designed to introduce students to basic separation techniques
and purification of organic samples using TLC and column chromatography. Synthesis of certain derivatives of amino group and hydroxyl groups and some aromatic nitro compounds are also included in this course.

***Learning Outcomes*:** This course ensures that the students shall be able to purify and separate a mixture of organic samples. They should be able to perform synthesis of derivatives of simple functional groups and purify them.

1. Separation, purification and identification of compounds of binary mixtures (solid- solid, solid-liquid, liquid-liquid) using TLC and column chromatography, Chemical tests.

2. Quantitative Analysis:

(a) Determination of amino group by acetylation method.

(b) Detennination of hydroxyl group by acetylation method.

(c) Estimation of Keto group.

(d) Determination of iodine value and saponification value of an oil sample.

3. Organic Synthesis:

(a) Preparation of adipic acid, p-chlorotoluene, p-nitroaniline, p-bromoaniline, triphenylmethanol.

(b) Preparation of PDC (Pyridinium dichromate) & PCC(Pyridinium chloro chromate) reagentsand its application on benzyl alcohol.

(c) Grignard reagent preparation and reactions on aldehyde.

SEMESTER – III

PAPER-XI (CH-2.3.11)

INORGANIC CHEMISTRY III

Learning Objectives: This course is basically focused on synthesis, structure and bonding of metal π-complex and metal clusters. It also discusses the metal-ligand equilibrium in solution and factors affecting stability of metal complexes. Reaction mechanism inorganic complexes and different theories related to this are also covered under this course.

Learning Outcomes: After successful completion of this course students should be able to gain an insight into the structure and bonding involved in metal complexes and their kinetic and thermodynamic stability. They can also predict the mechanism of reactions involved in transition metal complexes.

UNIT –I (a) Metal π –Complex: Metal Carbonyls, Structure and Bonding, Important reactions of metal carbonyls; Preparation, Bonding, Structure and Important Reactions of Transition Metal Nitrosyl, Dinitrogen and Dioxygen Complexes ligands.

(b) Metal clusters: Metalloboranes, Metallocarboranes, Metal carbonyls and Metal halideclusters.

UNIT –II Metal -Ligand Equilibria in Solution: Stepwise and Overall formation constants and their interaction, trends in stepwise constants. Factors affecting the Stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect, Macrocyclic effect and its thermodynamic origin. Determination of Binary Formation Constants by pH-metry and Spectrophotometry.

UNIT-III Reaction Mechanism of Transition Metal Complexes (Part-A): Energy profile of a reaction, Reactivity of metal complexes, Inert and Labile complexes, Kinetic application of Valence Bond and Crystal field theories, Kinetics of Octahedral substitution, Acid hydrolysis, Factors affecting acid hydrolysis and base hydrolysis, Conjugate base mechanism, direct and indirect evidences in favour of conjugate basemechanism.

UNIT-IV Reaction Mechanism of Transition Metal Complexes (Part-B): Anation reactions, k-exchange, reaction without metal ligand bond cleavage. Substitution reactions in squareplanar complexes. The trans effect, mechanism of one electron transfer reactions, Outer sphere reactions, Marcus-Hush Theory, Inner sphere type reactions.

PAPER-XII (CH-2.3.12)

INORGANIC CHEMISTRY IV

Learning Objectives: This course is basically focused on homogeneous and heterogenous catalysis, nuclear chemistry and magneto chemistry.

Learning Outcomes: The outcome of this course will enable students to have a proper understanding of organometallic chemistry and nuclear chemistry. This course also deals with EPR spectroscopy and application in inorganic systems.

UNIT-I Organometallic Chemistry: 18-Electron Rule, Ligands in Organomettallics, Synthesis, bonding and reactions of Alkyl, Aryl, Alkylidenes, Alkylidynes, Allyl, Dienyl, Arene & Trienyl complexes, Cyclic π systems (3 to 8 membered rings) and Fullerene complexes. Spectral analysis of Organometallic Complexes.

UNIT –II Homogenous and Heterogenous catalysis: Stiochiometric reactions for Organometallic catalysts: Dissociation & Substitution, Oxidative addition & carbonylation, Oxygen transfer from Peroxo and Oxo Species, Reductive & Hydride elimination, Insertion, Displacement and Isomerization reaction.

Hydrogenation, Hydrosilation and Hydrocynation of unsaturated compounds, Hydroformylation, Wacker (Smidt) Process, Olefin Metathesis, Fischer-Tropsch synthesis, Zeigler-Natta polymerization, Water gas reaction.

UNIT –III Nuclear Chemistry: Radioactive Decay, Radioactive Equilibria, Nuclear Reactions, Q-Value, Reaction Cross- sections, Nuclear Fission, Fission Yield, Nuclear Fusion, Pinch Effect, Tracer Techniques, Neutron Activation Analysis (NAA), Counting Techniques, Ionization Counter, GM Counter, Proportional Counter.

UNIT –IV Magneto Chemistry & EPR: (a) Induction and susceptibility. Lande interval rule, calculation of g-values, Van Vleck's equation and its use. Effect of spin orbit coupling. Magnetic properties of A.E.T terms with reference to Co(I) and Ni(II) complexes.

(b) Electron Paramagnetic Resonance Spectroscopy: Hyperfine splitting, Spin orbit coupling, Significance of g-tensor, Zero field splitting, Kramer's degeneracy, Application to inorganic systems

PAPER-XIII (CH-2.3.13)

ORGANIC CHEMISTRY

***Learning Objectives*:** This course designed to get a brief idea about reagents used in oxidation and

reduction of various organic functional molecules, photo chemistry of alkenes and carbonyl compounds, synthesis of saturated and unsaturated heterocyclic rings. It also covers properties and application of organometallic reagents and basic principles of asymmetric synthesis.

***Learning Outcomes*:** The outcome of this course is to ensure that the students should get a comprehensive idea of controlled transformation of functional groups with desire stereochemistry. They should be able to synthesise three to six membered heterocyclic rings as well as benzo fused rings of pharmaceutical importance. They should also learn the synthetic application of various organometallic reagents.

UNIT- I (a) Oxidation: Introduction, different oxidative processes, hydroborations alkanes, alkenes, aromatic rings, saturated C-H groups (active and unactivated), alcohols, diols, aldehydes, ketones, ketals, and carboxylic. Amines, hydrazines and sulphides, Oxidation with ruthenium tetraoxide, iodobenzene diacetate and thallium III) nitrate, oxidation with IBX, Dess-martin periodinane, PDC (Pyridinium Dichromate), PCC (Pyridinium Chlorochromate). Swern oxidation. **(b) Reduction:** Introduction: Different reductive processes, hydrocarbons- alkanes, alkenes, alkynes and aromatic ring, Carbonyl compounds: aldehydes, ketones, acids and their derivatives. Epoxides, Nitro, nitroso, azo, oxime groups, hyrogenolysis, Clemmenson's reduction,Wolff kishner reduction & Luche reduction.

UNIT- II (a) Photo-chemistry: Cis-Tran Isomerisation, Paterno-Buchi Reaction, Norish type I & II reactions, Photo reductions of ketones, Di-π methane rearrangement, Photochemistry of Arenes. **(b) Asymmetric synthesis:** Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution– optical and kinetic.

UNIT-III (a) Heterocyclic Chemistry Principles of heteroclic synthesis involving cyclisation reactions and cycloadditions. (i) **Three-membered and four-membered heterocycles:** Synthesis and reactions of Aziridines, Oxiranes, thiranes, azetidines, Oxetanes and thietanes.

(ii) **Benzo fused Five-Membered Heterocycles:** Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes. (iii) **Nitrogen Containing heterocyclic:** Synthesis and reactivity of pyridine, quinoline, Isoqunoline and Indole.

Skraup Synthesis, Fisher Indole Synthesis.

(b) Carbohydrate: Chemistry of life, Primary metabolisim, Glycosides, Synthesis Compounds (Vitamin C and Inositols) derived from sugar, Hydrolysis of Polysaccharide, Amino Sugars.

UNIT- IV (a) Organometalic reagents: Principle, Preparations, properties and application of the following in organic Synthesis with mechanistic details. (i) **Group I and II Metals:** Li, Mg, Hg, Cd, Zn, (ii) **Transition metals:** Cu, Pd, Ni, Co (iii) **Group I and II metal Organic Compounds:** Li, Mg, Hg, Cd, Zn

(b) Organo main group chemistry-Boron, Silicon and Tin

PAPER-XIV (CH-2.3.14)

(PHYSICAL CHEMISTRY-III, INTERDISCIPLINARY-I)

Learning Objectives: This course deals with molecular spectroscopy such as rotational, vibrational, electronic and ESR. This course also introduces instrumental methods of analysis in XRD, IR, polarography, thermal analysis

Learning Outcomes: After course completion, students will have a knowledge on various spectroscopic instruments and the analysis of data. The students will also have a proper understanding of molecular spectroscopy and their application to different molecules.

UNIT-I Spectroscopy: (a) Rotational Spectroscopy The rigid diatomic rotor, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the roleof nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and thenon-rigid rotor. **(b) Vibrational Spectroscopy:** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration- rotation spectroscopy. Breakdown ofOppenheimer approximation, vibrations of polyatomic molecules, Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities; metal-ligand vibrations.

UNIT-II (a) Electronic Spectroscopy: Electronic transitions, Franck-Condon principle. Vertical transitions. Selection rules, parity, symmetry and spin selection rules. Polarization of transitions. Fluorescence and phosphorescence.**(b) Raman Spectroscopy:** Classical and quantum theories of Raman effect Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, Mutual exclusion principle.

UNIT-III Electron Spin Resonance (ESR) spectroscopy: g-factor, electron-nuclear coupling, double resonance in ESR electron-electron coupling. Techniques of ESR spectroscopy **Mössbauer Spectroscopy:** Basic principles, instrumentation, spectral parameter and displays, applications. Mossbauer parameters- isomer shift, quodropole splitting, Magnetic hyperfine interaction, Doppler effect. Applications of Mossbauer spectroscopy.

UNIT-IV Instrumental Method of Analysis: X-ray diffraction: Crystals and the diffractions of X-ray, Bragg's law concept of symmetry in crystals, lattice planes and Miller indices, systematic absence of reflections, multiplicities, the x-ray diffraction experiment, powder method, single crystal method, x-ray intensities, structure factor, particle size measurement by x-ray diffraction. **Polarography:** Current-voltage relationship, theory of polarographic waves, instrumentation, qualitative and quantitative applications. **Thermal analysis:** Theory, methodology, instruments and applications of theromogravimetric analysis (TGA), and differential scanning calorimetry (DSC).

PAPER-XV (CH-2.3.15) (GENERAL CHEMISTRY-IV: PRACTICAL)

Learning Objectives: This course is designed to introduce students with chemical kinetics, energy of activation, saponification experiments and Adsorption experiments. Determination of acid and basic strength by electrochemistry is also included.

Learning Outcomes: This course ensures that the students shall be able to study surface tension.They should be able to perform electrochemical analysis of acids and bases.

Chemical Kinetics:

1. Saponification of ethylacetate with sodium hydroxide by chemical method.
2. Comparison of strength of acids by ester hydrolysis
3. Determination of energy of activation of acid catalyzed hydrolysis of methyl acetate.
4. Determination of velocity constant of hydrolysis of an ester/ionic reaction in micellarmedia.

Adsorption:

1. Adsorption of acetic acid and oxalic acid on animal charcoal and verification of Freundlichisotherm.

2. Study of the surface tension – concentration relationship for solutions (Gibb's equation)

Phase equilibria:

1. Determination of critical solution temperature of phenol-water system.
2. Construction of phase diagram for a three component system (chloroform-acetic acid –water).

Electrochemistry:

1. Determination of strength of strong acid and weak acid in given mixture conductometrically.
2. Determination of solubility and solubility product of a sparingly soluble salt (i.e., PbSO4,BaSO4) conductometrically.
3. Determination of strength of halides in a mixture potentiometrically.
4. Determination of the formation constant of silver amine complex and stochiometry of thecomplex potentiometrically.
5. Estimation of ferrous iron in ferrous ammonium sulphate potentiometrically.
6. Potentiometric titration of a strong acid with strong base using quinhydrone electrode.
7. Determination of partial molar volume of solute (e.g. KCl) and solvent in binarymixture.
8. Determination of stoichiometry and stability constant of inorganic (e.g. ferric-salicylicacid) and organic (amine-iodine) complex.
9. Verification of Beer's law.
10. Determination of first and second ionization constants of phosphoric acid by pH meter.
11. Determination of hydrolysis constant of aniline hydrochloride by pH meter.
12. Verification of Debye-Huckel-Onsagar equation of conductance.
13. Determination of hydrolysis constant of aniline hydrochloride conductometrically.

SEMESTER-IV

PAPER-XVI (CH-2.4.16)

MATERIALS CHEMISTRY

Learning Objectives**:** The prime objective of this course is to introduce students to nanomaterials, their synthesis by different routes and characterization. This course also deals with introduction to plasma chemistry, surface treatment of polymers with plasma.

Learning Outcomes**:** After course completion, the students are expected to be able to synthesize thin films, nanomaterials and various polymeric composites. They will also have a knowledge on dealing with various plasma reactors for treatment of polymers using different carrier gases.

Unit-I: Materials Synthesis: Solid state synthesis, preparation of thin films, Growth of single crystals, synthesis of nanomaterials (Top-down and bottom-up approach).

UNIT II Characterization and Properties: X-ray diffraction, Scanning probe microscopy, Electron microscopy. Electrical, Magnetic and Optical properties of Materials. **Unit-III Plasma Materials:** Introduction to theoretical and application of plasmachemistry, Plasma temperature, Thermal and non thermal plasma, Plasma chemistry& gas discharge,Elementary plasma chemical reaction, ionization process.

Unit-IV Polymer Materials (B): Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods),sedimentation. electrically conducting, fire resistant, liquid crystal polymers

PAPER-XVII (CH-2.4.17)

BIOCHEMISTRY

Learning Objectives**:** The prime objective of this course is to introduce students to biophysical and bioorganic chemistry. The subject deals with enzyme catalysis, their mechanism and applications in different living systems. This coursed also focusses on the importance of various common enzymes, cofactors and apoenzymes

Learning Outcomes**:** After completion of this course, the students will gain insights into chemical and biological catalysts, enzyme catalysis and mechanism. Further, the studentswill be able to understand the structure and biological importance of enzymes.

UNIT-I Biophysical Chemistry 1: Introduction, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification. Fishers lock and key and koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity, labeling and enzyme modification by site directed mutagenesis.

UNIT-II Biophysical Chemistry 2: Enzyme kinetics, michaelismenten and lineweaver- burk plots, reversible and irreversible inhibition. Transition-state theory, orientation and steric effect,acid base catalysis, covalent catalysis, strain or distortion.

UNIT-III Bioorganic Chemistry 1: Example of some typical enzyme mechanism: chymotrypsin, ribonuclease, lysozyme, carboxypeptidase A. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, Thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NaDP^+$, FMN, FAD, lipoic acid, Vitamin B12.

UNIT-IV Bioorganic Chemistry 2: Mechanism of reactions catalyzed by cofactors. Nucleophilic displacement on a phosphorous atom, multiple displacement reaction and coupling of ATP cleavage to endergonic processes, transfer of sulphate, addition and elimination reactions, enolic intermediates in the isomerization reactions, β cleavage and condensation, isomerization, rearrangement, carboxylation, decarboxylation.

PAPER-XVIII (CH-2.4.18)

BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY

***Learning Objectives*:** This course deals with the importance of metal ions in biologicalsystems. It addresses the relevance and toxicity of metals ion along with their function. An introduction to supramolecular chemistry of cyclodextrin, calixarene etc is also provided in this course.

Learning Outcomes: After completion of this course the students should be able to understand the biologically relevant metal ions and their functions. The students should be able to design cyclodextrin inclusion complexes for their potential use in medicinal chemistry**.**

UNIT -I Biological roles of metal ions, Calcium Biochemistry, Oxygen Transport and storage: Hemoglobin, Myoglobin, Cobalt containing models of oxygen binding, Iron containing models of oxygen carrier, Hemocyanin; Iron storage and transport: Ferritin,Transferrin, Siderophores.

UNIT-II Enzymes exploiting acid catalysis: Carbonic anhydrase, Carboxypeptidases, Superoxide dismutase, Xanthine oxidase. Redox catalysis: Iron-sulfur proteins: Ferredoxins and Rubbredoxins, Non-heme iron, Cytochromes, Cytochrome P-450 enzymes, Blue Copper Proteins, Coenzyme B12 Nitrogen Fixation, Photosynthesis.

UNIT-III Metals in medicine: Ionophores, Importance of Na and K, Metal deficiency and diseases, Toxic effects of metals, Metals used for diagnosis and chemotherapy, Anticancer drugs.

UNIT-IV Supramolecular Chemistry: Host guest chemistry, chiral recognition and catalysis, molecular recognition, biomimetic chemistry, crown ethers, cryptates. Cyclodextrine, cyclodextrinbased enzyme models, calixarenes, Ionophores.

PAPER-XIX (CH-2.4.19)

MODERN ORGANIC CHEMISTRY

Learning Objectives: The prime objective of this course is to introduce students to medicinally important molecules and their mode of action as well as some important class of natural products like steroids and terpenoids and conceptual idea about modern asymmetric synthesis and organocatalysis. Application of modern spectroscopic methods for structure elucidation is alsocovered.

Learning Outcomes**:** After completion of this course the students should be able to understand the biophysical action of certain classes of drugs such as antipyretics, analgesics and antimalarials. They should have a thorough idea of kinetic resolution, chirality transfer, organocatalysis and asymmetric synthesis. Students should also be able to characterize a molecule using modern spectroscopic technique like UV, IR, ^{1}H, ^{13}C NMR and MS.

UNIT – I Organic compounds in Medicine and their mode of action (a) Synthesis of antipyretics, analgesics (Aspirin, Paracetamol, Ibuprofen) (b) Antimalarial drugs (Chloroquine and Artesunate)

UNIT – II Modern Asymmetric Synthesis: (a) Principles of asymmetric reaction and synthesis; Kinetic resolution, Dynamic kinetic resolution (DKR) and autocatalytic reactions; Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer and relay; Asymmetric inductions; Chiral pools, auxiliaries and templates. (b) Asymmetric oxidations and Reductions: Sharpless asymmetric epoxidation, dihydroxylation, Reduction of ketones, imines and olefins. (c) Asymmetric C-C bond forming reaction: aldol reaction and alkylation based on Evans method, Mukaiyama aldol reaction, Baylis-Hillman-Morita reactions, Asymmetric hydroformylation. (d) Organocatalysis: α-functionalization of aldehyde and ketones, 1,4-conjugate addition (β-functionalization and α,β- bifunctionalization of α,β-unsaturated carbonyl compounds).

UNIT-III Natural Products (a) Steroids: Cholesterol and Progesterone (b) Alkaloids: Morphine and Nicotine (b) Terpenoids and Carotenoids: Menthol, Citral, Lycopene and Carotene (Biosynthetic aspects should be addressed)

UNIT-IV: Spectroscopic Identification of Organic Molecules: Identification of organic compounds using modern techniques like UV, IR, ^{1}H NMR, ^{13}C NMR (DEPT, COSEY, NOSEY) & Mass spectrometry.

PAPER-XX (CH-2.4.20)

Dissertation

Learning Objectives: The main objective of this course is that the students can have an idea about a small project while doing a research work under faculty members of the department. The students will learn about doing literature survey and basing upon that carrying out different experiments to execute their project work.

Learning Outcomes**:** After completion of this course the students should be able to understand the concept of experimental investigation and analyzing the results by discussing with their supervisor which will benefit the students for higher studies.

The dissertation shall comprise of conducting a small project under faculty members of the department. The title and execution of the project work shall be decided in consultation with the faculty members of the department by a committee constituting HOD and other senior faculty members. The committee may also extend the provision of co- opting the external guide as per the provision provided by the Ravenshaw University.

In general, the student is expected to do literature survey in the assigned topic, andto do some kind of experimental investigation, and result analysis. However, final decision regarding the execution of project work rests with the supervisor/co-supervisor and the committee on mutual discussion to the best benefit of the student for academic career. The guideline provided by UGC shall be also taken into account in this regard.

VALUE ADDED COURSES

Medicinal Plants: Phytochemistry and Biological Activities

Learning objectives: To learn about phytochemistry and biological activities of medicinal plants

Learning Outcomes: Upon successful completion students should be able to understand the concepts of phytochemistry, able to appreciate the medicinal values of plants, know the various techniques involved in the phytochemistry and familiarize with the bio-active components present in the plants.

Unit I: Extraction and purification of bio-active compounds from plants by cold & hot extraction, Soxhlet extraction, and purification of crude extracts by solvent systems.

Unit II: Isolation of bioactive compounds by different chromatographic techniques such as thin layer, column, and high pressure liquid chromatography. Characterisation of isolated compounds by FTIR, Mass, andNMR spectroscopy.

Unit III: Clinical research and traditional uses of Indian medicinal plants - Eclipta alba, Gymnema Sylvestre, Ocimum sanctum, Curcuma longa. Phytopharmaceuticals and their health benefits: Anthocyanins, carotenoids, lycopene, isoflavones, polyphenols, omega 3 - fatty acids, biological effects of resveratrol.

Molecular Identification by Spectroscopic and computational Methods

***Learning objectives**:* To learn about various analytical instruments and hands on training.

***Learning Outcomes**:* After completion of the course, student will understand the basic principles, instrumentation processes, sampling techniques, data collection methods and data analysis. Students will gain a hands-on experience.

Unit-I: Use of computational tools in chemistry: Introduction to Microsoft excel and other equivalent tools, curve fitting, data analysis and error estimation, 3D data visualization, surface plotting, etc. Computational freewares (Avogadro, Gabedit, MOPAC, VMD, GROMACS etc.) for estimation of molecular properties such as optimization of molecular geometries, conformational analysis, calculation of vibrational spectra, thermochemical calculation using semiempirical tools.

Unit-II: Principles of FTIR and UV-Visible spectroscopies, Instrument details, Spectral data collection for some organic molecules, Interpretation and analysis of the acquired data.

Unit-III::Principle of Nuclear Magnetic Resonance (NMR) Spectroscopy, Instrument details, ^{1}H and ^{13}C Spectral data collection for some organic molecules.Interpretation, analysis of the acquired data and molecular identification.

ADD-ON COURSES

Nanomaterials and Sensors

Learning objectives*:* The course main objective is to build a sound idea about Nanomaterials, their fabrication methods, develop understanding about their property and few of their applications in modern day technology.

Learning Outcomes*:* The course is set to encourage the understanding of: 1. The importance of nanoscale materials for sensing applications. 2. Approaches used for characterizing sensors-based nanomaterials. 3. Approaches used for tailoring nanomaterials for a specific sensing application. 4. Metallic and semiconductor nanoparticles. 5. Organic and inorganic nanotubes and nanowires. 6. Optical, mechanical and chemical sensors based on nanomaterials. 7. Hybrid nanomaterial-based sensors.

Unit-I: Definition of Nanomaterials, materials in different size ranges, surface are to volume ratio and its importance in material property. 1D, 2D and 0D Nanostructures, and their electronic structures.

Unit-II, Fabricationof nanomaterials by Top Down and bottom up techniques. Synthesis of nanoparticles, nanowires and nanofilms; a case study with Ag/ Cu. Hand-on synthesis of Ag nanowires. Characterization of the synthesised nanomaterial by UV spectroscopy, X-ray diffraction (XRD), (Debye Scherrer analysis), and Scanning Electron Microscopy (SEM)(particle size distribution), and energy dispersive x-ray spectroscopy (EDAX) .

Unit-III: Definition of sensors, main elements of sensors, similarity between living organism and artificial sensor, quantum dot as sensors, nanowire based sensors, carbon nanotube bases sensors, sensors based on nanostructure of metal oxide.