M.Sc. Chemistry  
Syllabus 2019-2020

First Semester

Paper no. –1

Unit – I Symmetry and group theory in chemistry: Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schoenflies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables of C2v , C2h, C3v and their use in spectroscopy.

Unit – II Metal-ligand bonding: Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes. Bonding and molecular orbital theory. Metal-complexes: metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.


Paper No-2 Unit – I


UNIT-II Conformational analysis: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Stereochemistry: Elements of symmetry, chirality, molecules with more than one chiral center, methods of resolution, optical purity, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (Biphenyls, allenes and spiranes), chirality due to helical shape.

Unit – III Reaction intermediates: Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Sandmeyer reaction, Free radical rearrangement and Hunsdiecker reaction. Elimination reactions: the e2, e1 and e1c b mechanisms. Orientation of the double bond. Reactivity, effects of substrate structures, attacking base, the leaving group and the medium.

Unit – IV Pericyclic reactions: Classification of pericyclic reactions. Woodward- Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions - antarafacial and suprafacial additions, 4n and 4n+2 system, 2+2 addition of ketenes, 1, 3 dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatrophic shifts involving carbon moieties, 3, 3- and 5, 5-sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Paper NO.- 3

Unit - I

Mathematical concept in quantum chemistry: Vector quantities and their properties. Complex numbers and Coordinate transformation. Differential and Integral Calculus, Basic rules of differentiation and Integration Applications. The Schrodinger equation and postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems. Particle in a box the harmonic oscillator, the rigid rotator, the hydrogen atom.

Unit –II Basics of thermodynamics: Maxwell’s thermodynamic relations isotherm, vant’ Hoff hypothesis. Partial molar volume and partial molar heat content. Chemical potential, Gibbs Duhem equation, variation of chemical potential with temperature and pressure. Chemical potential of ideal gases,
pure solids, liquids and mixture of ideal gases. Activity and Fugacity, Determination of Fugacity, Variation of Fugacity with temperature and pressure.


**Unit –IV** Chemical dynamics –I: Methods of determining rate laws, consecutive reactions, collision theory of reaction rates, steric factor, Activated complex theory, kinetic salt effects, steady state kinetics, and thermodynamic and kinetic control of reactions. Dynamic chain (Hydrogen-bromine and Hydrogen-chlorine reactions) and Oscillatory reactions (Belousov - Zhabolinsky reaction)

**Paper No.-4 Unit-I**

Unifying principles-Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, dispersion, polarization and scattering, Uncertainty relation and natural line width and natural line broadening, transition probability, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

**Unit- II** Microwave spectroscopy:

Classification of molecules in term of their internal rotation mechanism, determination of rotation energy of diatomic and polyatomic molecules, effect of isotopic substitution on diatomic and polyatomic molecules. Intensities of rotational spectral lines and parameters of rotational and the transition frequencies, non-rigid rotors, Linear and symmetric top polyatomic molecules. Application in determination of bond length.

**Unit- III** Scattering spectroscopy: Electron Diffraction Spectroscopy : Principle, instrumentations and application of Auger spectroscopy and Scanning Electron Microscopy for chemical characterization, electron diffraction of gases and vapours, The Wierl equation and co-related method, application of electron diffraction theory, instrumentation and application of turbidimetry, nephelometry and fluorometry, fluorescence and phosphorescence and factors affecting them.

**Unit- IV** Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, Coherent anti Stokes Raman spectroscopy (CARS), Instrumentation, Application of Raman effect in molecular structures, Raman activity of molecular vibration, structure of CO$_2$, N$_2$O, SO$_2$, NO$_2$, CIF$_3$

**Second Semester**

**Paper-1 Unit-I**

Reaction mechanism of transition metal complexes: 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, anation reactions and reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

**Unit – II** Electronic spectra and magnetic properties of transition metal complexes:

Spectroscopic ground states, Selection rules, mechanism for breakdown of the selection rules, intensity of absorption, band width correlation, Orgel and Tanabe- Sugano diagram for transition metal complexes (d$^1$-$d^9$ states), spectra of d-d metal complexes of the type [M (H$_2$O)$_6$] n+, spin free and spin paired ML$_6$ complexes of other geometries, Calculations of D$q$, B and $\beta$ parameters, spin forbidden transitions, effect of spin-orbit coupling, Spectrochemical and Nephelouexitic series. Magnetic properties of complexes of various geometries based on crystal field model, spin free-spin paired equillibria in octahedral stereochemistry.
Unit – III Transition metal complexes: Transition metal complexes with unsaturated organic molecules, alkanes, allyl, diene dienyl, arene and trienyl complex, preparations, properties, nature of bonding and structure features. Important reaction relating to nucleophilic and electrophilic attack on ligands and organic synthesis. Transition Metal Complexes with Bond to hydrogen.

Unit-IV Alkyls and aryls of transition metals: Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis. Compounds of transition metal - Carbon multiple bonds : Alkylidenes, low valent carbenes, nature of bond and Structural characteristics. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as olefin, allyl and dienyl complexes.

Paper-2 Unit-1


Paper No.-3 Unit-1

Unit –II Statistical thermodynamics: probability, permutations and combinations, concepts of probability, maxwell boltzmann distribution. different ensembles and partition functions-translational, rotational, vibrational and electronic partition functions. thermodynamic function using appropriate partition functions. fermi-dirac and bose-einstein statistics and statistical basis of entropy. heat capacity of solids, debye and einstein models.


**Unit – IV** Chemical dynamics–II: General features of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrier less chemical reactions in solutions, dynamics of unimolecular reaction. [Lindemann – Hinshelwood, RRK and Rice-Rampsperger-Kassel-Marcus {RRKM}] theories of unimolecular reactions.

**Paper No.-4 Unit- I**  

**Unit – II** Infra red spectroscopy:Introduction, simple and anharmonic oscillators in vibrational spectroscopy, diatomic-vibrating rotor, Modes of vibration in polyatomic molecules, vibration-coupling, Fourier Transform IR spectroscopy: instrumentation, interferometric spectrophotometer, sample handling, Factors influencing vibrational frequencies, Application of IR spectroscopy: Interpretation of IR spectra of normal alkanes, aromatic hydrocarbons, alcohols and phenols aldehydes and ketones, ethers, esters, carboxylic acids, amines and amides.


**Unit– IV** Nuclear resonance spectrophotometry:theory of nmr spectroscopy, interaction of nuclear spin and magnetic moment, chemical shift, processional motion of nuclear particles in magnetic field, spin-spin splitting, coupling constants, factor affecting the chemical shift, shielding effect, effect of chemical exchange, hydrogen bonding, instrumentation of fourier transform nmr spectrometer, structure determination of organic compounds, carbon-13 nmr spectroscopy, multiplicity-proton (1h) decoupling-noise decoupling, off resonance decoupling, selective proton decoupling. chemical shift (aliphatic , olephinic, alkyne, aromatic and carbonyl carbon)

**Third Semester**

**Paper No.-13**

**Unit-1** Electron spin resonance spectroscopy: Introduction, principle, Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron). Nuclear quadrupole resonance spectroscopy: Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings, applications.

**Unit–II** Photoelectron spectroscopy: Basic principle for atoms and molecules;Photo-electric effect, ionization process, Koopman’s theorem, Auger electron spectroscopy,Determination of Dipolemoment. Photoelectron spectra of simple molecules-ESCA,Photoacoustic Spectroscopy: Basic principle of Photo acoustic Spectroscopy (PAS), PAS –gases and condensed system. Chemical and Surface applications.

**Unit–III** Photochemical reactions: Interaction of electromagnetic radiation with matter, Stern Volmer equation, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, Actinometry.


Paper No.-2 Unit-I


Paper No.-3 Unit-1


Unit – II Micelles and adsorption: Micelles: Classification of surface active agents,
micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of Surfactants. Thermodynamics of micellization - phase separation and mass action models. Reverse micells, micro-emulsion. Micellar Catalysis, Surface tension capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm.

**Unit –III** Solid state chemistry-I : Crystal defects and Non-stoichiometry - Perfect and imperfect crystals, intrinsic and extrinsic defects - point defect, line and plane defects, vacancies - Schottky defects and Frankel defects. Thermodynamics of Schottky and Frenkel defect, formation of color centres, non-stoichiometry and defects. Electronic properties and Band theory of semiconductors.

**Unit-IV** Polymer – Definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, average molecular mass, molecular mass determination (Osmometry, Viscometry, diffusion and light scattering methods), Sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

**Paper No.-4  Unit-1**
Sample preparation, digestion and statistical analysis Sampling - Collection, Preservation and preparation of sample, Techniques of sampling solids, liquids and gases, Operation of drying and preparing a solution of the analyte. Principle, methodology and application of different types of digestions such as acid digestion, base digestion, enzymatic and microwave digestion for liquid and solid materials. Evolution and procession of Analytical Data, Precision and Accuracy, Types of Errors, Propagation of errors, Normal Distribution Curve, Standard deviation, Confidence limit, Graphical presentation of result - Method of average, Method of Linear least square, Significant figures, Statistical aid to hypothesis testing - t-test, F-test, Correlation coefficient, Rejection of data.

**Unit –II** Separation techniques: Efficiency of extraction, Selectivity of extraction, Extraction system, Method of Extraction, applications. Principle, classification of chromatographic techniques, Technique and applications of paper chromatography, Thin-layer chromatography, HPLC, Column chromatography. Gas Chromatography

**Unit –III** Thermal and automated methods principle, instrumentation, application of tga, dta and dsc methods. Automated methods, principle, instrumentation and application of flow injection analysis.

**Unit –IV** Electrochemistry: Principles and instrumentation of pH potentiometry, coulometry and conductometry. Polarography: Basic principles, Diffusion current, polarized electrode, Micro electrode, Dropping Mercury Electrode, Ilkovic equation, Polarographic wave, Qualitative analysis Stripping methods, Cyclic Voltammetry, Amperometric titration: curves, Differential pulse polargraphy and Squarewave polarography.

**Fourth Semester**

**Paper-1 Unit-1**

**Advanced chromatography** : Ion chromatography: Ion exchange equilibrium, Ion-exchange packing and Inorganic Applications. Size exclusion chromatography: Column packing, Theory and applications. Supercritical fluid chromatography: Properties of supercritical fluid, SFC - Instrumentation and operating variables, comparison with other types of chromatography, applications. Capillary Electrophoresis and capillary electrochromatography: overviews and applications


**UNIT –III**
Atomic emission spectroscopy
Selectivity, sensitivity and interferences of atomic spectroscopy Theory, instrumentation and application of flame photometry, AES, ICP-AES and AFS.

Unit –IV Atomic absorption spectroscopy and hyphenated techniques Theory, instrumentation and applications of flame and graphite furnace AAS, cold-vapour and hydride generation AAS. Theory, instrumentation and application of hyphenated techniques i.e. GC/HPLC/MS/GC/IC/HPLC- ICP-MS.

Paper No-2


Unit- III Drug design development of new drugs procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (sar), factors affecting bioactivity, resonance, inductive effect. theories of drug activity: occupancy theory, rate theory, induced fit theory, quantitative structure activity relationship (qsar)-hansch approach-free wilson model, relationship between free wilson and hans analysis concepts of drug receptors, lipophilicity, pharmacophore, pharmacological activity and typical range of parameters related to drug likeness. General introduction of pharmacokinetics and pharmacodynamics.


Paper No.-3

Unit- I Non equilibrium thermodynamics: Fundamental concepts, Forces and Fluxes, Entropy production, Phenomenological Laws and Onsager’s theory for biological systems, coupled reactions.


Unit-IV Nuclear and radiochemistry nuclear theory: Nuclear cross section and nuclear radii,
nuclear shells and magic numbers, theory of nuclear shell model, nuclear potentials, square well and simple harmonic oscillator potentials, application, liquid drop model, semi-empirical mass equation, application and limitations.Nuclear fission: Mass, energy and charge distribution of fission products, decay chains, prompt and delayed neutrons, liquid drop model of nuclear fission. Nuclear energy: Nuclear fission, chain reaction, multiplication factor, nuclear reactors. Applied radiochemistry: Radioactive isotopes, purity and strength of radioisotopes. Radiochemical principle in the use of tracers, Application of Tracers in Chemical investigations, Physico-chemical methods, Analytical applications, Age determinations, Medical applications, Agricultural application.

Paper No.-4

Unit - I Air pollution monitoring and analysis Classification of air pollution monitoring levels, air quality, standards and index, monitoring and analysis of selected air borne pollutants: SO₂, NOₓ, SPM, Volatile organic compounds, Pb, CO₂, Persistent organic compounds, Hg, carbon and ozone. Air pollution control devices Viz ESP, scrubber technique, baghouse filters etc. Atmospheric chemistry of acid rains, photochemical smog, greenhouse effect, global warming, ozone hole.

Unit – II Soil and water pollution Soil and water quality standards, monitoring and analysis of selected soil and water contaminants: COD, pesticides, heavy metals, POP's, fluoride, cyanide, nitrate, phosphate, oil & grease, Geobiochemical impact of municipal solid waste, steel plants effluent, domestic sewage. Control devices of water pollutants.


Unit – IV Cosmetics, clinical and drug analysis Introduction of Cosmetics, evaluation of cosmetics materials, raw material and additives, Cosmetics colors, Perfumes in cosmetics, Cosmetics formulating, introduction, standards and methods of analysis- Creams, Face powders, Make-up, Shaving preparations, Bath preparations. Concepts and principles of analytical methods commonly used in the clinical species: i.e. ammonia, Nitrogen, Ca, Cl, CO₂, Fe, K, Li, Mg, Na, P, urea, glucose. Method for analysis of proteins (i.e. albumin, bilirubin, creatinine, cholesterol, HDL-cholesterol, triglycerides) and Enzymes (i.e. Alanine Aminotransferase, acid phosphatase, alkaline phosphatase, amylase, aspartate, aminotransferase, cholinesterase, lactate, and lipase)