

Structure of Chemistry Major Course

Semester	Course Description with Marks				
	Theory				Practical
	Organic Chemistry	Inorganic Chemistry	Physical Chemistry	Total	
First	16	17	17	50 Chem 0101 (Credit 4)	Chem 0191 (50) Organic (Credit 6)
Second	17	17	16	50 Chem 0201 (Credit 4)	Chem 0291 (50) Inorganic (Credit 6)
Third	17	16	17	50 Chem 0301 (Credit 4)	Chem 0391 (50) Physical (Credit 6)
	17	16	17	50 Chem 0302 (Credit 4)	
Fourth	17	17	16	50 Chem 0401 (Credit 4)	Chem 0491 (50) Physical, Computer, Instrumentation (Credit 6)
	16	17	17	50 Chem 0402 (Credit 4)	
Fifth	50 Chem 0501 (Credit 4)	50 Chem 0502 (Credit 4)	50 Chem 0503 (Credit 4)	150	Chem 0591 (50) Organic (Credit 6) Chem 0592 (50) Inorganic (Credit 6)
Sixth	50 Chem 0601 (Credit 4)	50 Chem 0602 (Credit 4)	50 Chem 0603 (Credit 4)	150	Chem 0691 Combined Practical: 50 (Credit 6) Chem 0692 Project and Grand Viva: 50 (Credit 6)
Total	200	200	200	600	400

FIRST SEMESTER

Course No. CHEM0101 (FM=50; C=4)

Group A: Organic Chemistry (M=16)

General Introduction:

Functional group based classification and nomenclature. Sources / origin of different compounds. Molecular formula and IHD / DBE.

Bonding, Structure and Physical Properties of Organic Molecules:

Valence bond theory: Concept of hybridisation, resonance (including hyperconjugation), inductive effect, steric effect, steric inhibition of resonance. Orbital pictures of bonding (sp^3 , sp^2 , sp : C-C, C-N & C-O system).

MO theory: Sketch and energy levels of MOs of i) acyclic π orbital system (C=C, conjugated diene and allyl systems) ii) cyclic π orbital system (neutral system: [4], [6] annulenes; charged system: 3, 4, 5-membered ring system); Frost diagram, Huckel's rules for aromaticity, antiaromaticity; homoaromaticity.

Physical properties: Melting point, boiling point; solubility; dipole moment; acid and base strength.

Group B: Inorganic & Physical Chemistry (M=34)

Atomic Structure and Bonding (M=16)

Why study quantum mechanics; Double slit experiment, Heisenberg's uncertainty principle, Wave-Particle duality, idea of de Broglie matter waves. Schrodinger equation, Hydrogenic wavefunctions, Quantum numbers, introduction to the concept of atomic orbitals; shapes, radial and angular probability diagrams of s, p and d orbitals (qualitative idea). Many electron atoms and ions: Pauli's exclusion principle, Hund's rule, exchange energy, Aufbau principle and its limitation. Term symbols of atoms and ions for atomic numbers <30 . Linear combination of atomic orbitals, hybrid orbitals; orbital picture of bonding,

Radioactivity (M=9)

Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes. Basic instrumentation, measurement of radioactivity, principles of isotope dilution analysis, neutron activation analysis Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

Gaseous state (M=9)

Maxwell's distribution of speeds; kinetic energy distribution in one, two and three dimensions, calculation of number of molecules having energy $\geq \epsilon$; calculations of average quantities. Basic idea about beta, gama and error functions.

Deviation of gases from ideal behaviour (compressibility factor, Andrew's and Amagat's plots); van der Waals equation of state: derivation and characteristic features; existence of critical state; critical constants in terms of van der Waals constants, the law of corresponding states; virial equation of state and significance of the second virial co-efficient, Boyle temperature, the Dieterici equation of state (preliminary ideas only); intermolecular forces and potentials (Keesom, Debye and London).

Course No. CHEM0191 (FM=50; C=4)
PRACTICAL

Organic Chemistry Practical

Qualitative Analysis (solid & liquid)

Lassaigne's tests of special elements (N, S, X). Preliminary Tests: ignition, Beilstein, Br₂ & KMnO₄ test. Tests of functional groups including their solubility / miscibility behavior: -NH₂ (aliphatic & aromatic); -NO₂ (aromatic); -CONH₂; -CN (nitrile); -OH (alcoholic, phenolic & enolic); -CO₂H; =CO; -CO₂R.

Preparation based on the reaction of the following functional groups: Bezoylation of amines; nitration of nitro compounds; hydrolysis of amides / anilides / imides / esters; bromination of anilides; acetylation of phenols; preparation of amides through acid chloride by SOCl₂ / DMF; semicarbazone / oxime formation of carbonyl compounds.

Separation of Dyes by chromatography.

SECOND SEMESTER
Course No. CHEM0202 (FM=50; C=4)

Organic Chemistry (M=17)

Stereochemistry and conformations:

Stereochemistry: Symmetry, chirality, optical activity, optical purity. Stereogenic units i) stereocentres: systems involving 1, 2, 3 centres, stereogenicity, chirotopicity. pseudo asymmetric (D/ L and R/S descriptor, threo / erythro and syn / anti nomenclatures (for aldols) ii) stereoaxis: chiral axis in allenes & biphenyls, R / S descriptor; cis / trans, syn / anti, E / Z descriptors (for C=C, C=N). Topicity of ligands and faces (elementary idea) and descriptors.

Conformation: Conformational nomenclature; factors affecting stability of conformations, conformational analysis of ethane, propane, butane, haloethane, 1,2-haloethane, 1,2-glycol, 1,2-halohydrin; invertomerism of trialkylamines. Conformational analysis: 4, 5, 6-membered rings; substituted cyclohexane.

Inorganic Chemistry (M=17)

Chemical Periodicity (I) (M = 10)

Periodic table, group trends and periodic trends in physical properties. Classification of elements on the basis of electronic configuration. Modern IUPAC Periodic table. General characteristic of s, p, d and f block elements. Position of hydrogen and noble gases in the periodic table. Effective nuclear charges, screening effects, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii. Ionization potential, electron affinity and electronegativity (Pauling's, Mulliken's and Allred-Rochow's scales) and factors influencing these properties. Inert pair effect. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements.

Ionic Bonding (M = 7)

Size effects, radius ratio rules and their limitations. Packing of ions in crystals, lattice energy, Born- lande equation and its applications, Born-Haber cycle and its applications. Solvation energy, polarizing power and polarizability, ionic potential, Fajan's rules. Defects in solids (elementary idea).

Physical Chemistry (M=16)

Thermodynamics-I (M = 9)

Importance and scope, definition of system and surroundings: type of systems (isolated, closed and open); extensive and intensive properties; steady state versus equilibrium state; concept of thermal equilibrium and the zeroth law of thermodynamics; thermodynamic coordinates, state of a system, equation of state, state functions and path functions; partial derivatives and cyclic rule; concept of heat and work (IUPAC convention); graphical explanation of work done during expansion and compression of a ideal gas; reversible and

irreversible processes and work done; first law of thermodynamics, internal energy (U) as a state function; enthalpy as a state function; energy conservation in the living organism; heat changes at constant volume and constant pressure; relation between C_p and C_v using ideal gas and van der Waals equations; joule's experiment and its consequence; explanation of term $(\delta U/\delta V)_T$; isothermal and adiabatic processes; thermochemistry: heat changes during physicochemical processes at constant pressure/volume; Kirchoff's relations; bond dissociation energies; changes of thermodynamic properties in different chemical changes.

Chemical Kinetics-I (M = 7)

Phenomenological kinetics: degree of advancement of a reaction, reaction rate, rate constant, order and molecularity of a reaction, determination of order of a reaction by half life and differential method: zero, first, second and fractional order reactions, pseudo first order reaction; solutions of elementary differential equations, complex reaction: opposing, parallel and consecutive reactions (all step of first order), kinetic and thermodynamic control of reaction; idea of rate determining step; steady-state approximation; temperature dependence of rate constant, Arrhenius equation, energy of activation.

Course No. CHEM0291 (FM=50; C=4) **PRACTICAL**

Inorganic Chemistry Practical

Qualitative analysis of Inorganic mixtures

Cation radicals derived from:

Na, K, NH_3 , Mg, Ca, Sr, Ba, Al, Pb, Bi, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd

Anion radicals:

F^- , Cl^- , Br^- , I^- , NO_3^- , NO_2^- , SCN^- , S^{2-} , SO_4^{2-} , $\text{S}_2\text{O}_3^{2-}$, PO_4^{3-} , BO_3^{3-} , CrO_4^{2-} , BrO_3^- , IO_3^- , $[\text{Fe}(\text{CN})_6]^{4-}$, $[\text{Fe}(\text{CN})_6]^{3-}$

Detection and confirmation of four radicals by macro, semi- micro tests and assignment of probable composition of the mixtures.

THIRD SEMESTER
Course No. CHEM0301 (FM=50; C=4)

Organic Chemistry (M=17)

General treatment and investigation of reaction mechanism (Part-I)

Mechanistic classification: ionic, radical and pericyclic; representation of mechanistic steps using arrow formalism. Reactive intermediates: carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes - structure using orbital picture, electrophilic / nucleophilic reactivity, stability, generation and fate. Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factor, intermolecular & intramolecular reactions. Application of thermodynamic principles in tautomeric equilibria (keto-enol tautomerism). Composition of the equilibrium in different systems (simple carbonyl, 1,3- and 1,2-dicarbonyl systems, phenols and related system; substituent and solvent effect).

Reaction kinetics: rate const and free energy of activation, free energy profiles for one step and multi step reactions, catalyzed reactions, kinetic control and thermodynamic control, kinetic isotopic effect, principle of microscopic reversibility, Hammond postulate.

Nucleophilic substitution at sp^3 centre: Mechanism: S_N1 , S_N2 , S_{Ni} mechanisms, effect of solvent, substrate structure, leaving group, nucleophiles including ambident nucleophiles, substitution involving NGP; relative rate & stereochemical features [systems: alkyl halides, allyl halides, alcohols, ethers, epoxides].

Inorganic Chemistry (M=16)

Covalent and Chemical Bonding

Lewis structures, formal charge. Valence Bond Theory, directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, VSEPR theory, shapes of molecules and ions containing lone pairs and bond pairs (examples from main group chemistry), Partial ionic character of covalent bonds, bond moment, dipole moment and electronegativity differences. Concept of resonance, resonance energy, resonance structures, Heitler-London theory for H_2 molecule (elementary idea), Molecular Orbital (MO) concept of bonding (elementary pictorial approach): sigma and pi- bonds, multiple bonding, MO diagrams H_2 , F_2 , C_2 , B_2 , N_2 , CO, NO, CN^- , HF, bond orders and bond lengths, Multicentre bonding in electrondeficient molecules, bond strength and bond energy.

Weak chemical forces: van der Waal's forces, ion-dipole, dipole-dipole, dipole-induced dipole interactions and hydrogen bonding and effect of these weak chemical forces on the physical properties of compounds of the main group elements.

Metallic bonding: Qualitative idea of band theory, conducting, semi-conducting and insulating properties with example from main group elements.

Physical Chemistry (M=17)

Thermodynamics-II (M = 17)

Second law of thermodynamics: need for a second law, Clausius and Kelvin-Planck statements and their equivalence; Carnot's theorem, thermodynamic scale of temperature, concept of heat engine, Carnot cycle and refrigerator; Clausius inequality, entropy as a state function, second law in terms of entropy, calculation of entropy change for various transformation; auxiliary state function (G and A) and their variation with temperature, pressure and volume; criteria of spontaneity and equilibrium; Gibbs-Helmholtz equation; Maxwell's relation, thermodynamic equation of state, C_p - C_v values, Joule-Thomson coefficient for van der Waal's gases.

Open system, chemical potential and activity, partial molar quantities, chemical potential in terms of Gibbs free energy and other thermodynamic state functions and its variation with temperature and pressure, Gibbs-Duhem equation; Eulers theorem; expression for ideal gas. Non-ideal system: idea of fugacity and activity; standard states.

Course No. CHEM 0302 (FM=50; C=4)

Organic Chemistry (M=17)

Reaction mechanism (part-II)

Substitution at sp^2 carbon (carbonyl system): Mechanism: B_{AC2} , A_{AC2} , A_{AC1} , A_{AL1} . Systems: acids, esters, amides, anhydrides & acyl halides.

Nucleophilic aromatic substitution: Addition-elimination mechanism, S_N1 mechanism, benzyne mechanism.

Electrophilic aromatic substitution: Mechanisms, orientation and reactivity. Reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reactions, one carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Hoesch, Vilsmeier-Haack reaction, Reimer-Tiemann, Kolbe - Schmidt).

Radical substitution: Aliphatic and aromatic system.

Addition reaction [reaction of carbon-carbon multiple bonds]:

Addition to $C=C$: Mechanism, reactivity, regioselectivity and stereoselectivity. Reactions: halogenations, hydrohalogenation, hydration, hydrogenation, epoxidation, hydroxylation, ozonolysis, addition to dienes, Diels-Alder reaction

Radical addition: Dissolving metal reduction of alkynes and benzenoid aromatics (Birch).

Inorganic Chemistry (M=16)

Acid -Base and Non-aqueous Solvents

Bronsted and Lowry's concept, solvent system concept, Lewis concept, Lux-Flood concept, relative strength of acids, hydracids and oxyacids, Pauling's rules, amphotericism, and super acids, HSAB principle, acid-base equilibria in aqueous solution, pH, buffer solutions and

buffer actions, acid-base neutralization curves, acid-base indicators, choice of indicators, Acid-base titrations.

Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents.

Physical Chemistry (M=17)

Thermodynamics-III (M=7)

Thermodynamics and equilibrium, degree of advancement, van't Hoff's reaction isotherm (deduction from chemical potential), equilibrium constant and standard Gibbs free energy change; definition of K_p , K_c , K_x ; van't Hoff's reaction isobar and isochore from different standard states; shifting of equilibrium due to change of external parameters like temperature and pressure and influence of inert gas; Le Chatelier principle of dynamic equilibrium (thermodynamics approach) and its application to homogeneous chemical equilibria.

Ionic equilibrium: concept of pH, hydrolysis of salts, buffer solution, elementary idea of biological buffers, acid-base indicators; solubility equilibria and influence of common and indifferent ions there on.

Distribution equilibria and Nernst distribution law, solvent extraction.

Electrochemistry (M=10)

Types of electrochemical cells and examples, cell reactions, EMF and changes in free energy, ΔH and ΔS of cell reactions from EMF measurements; thermodynamic derivation of Nernst equation, standard cells, half cells/electrodes, different types of electrode (with examples), standard electrode potential (IUPAC convention) and principle of its determination; types of concentration cells, liquid junction potential and its minimization, determination of transport number by EMF method, glass electrode and determination of pH, applications of EMF measurement: potentiometric titrations: acid-base, redox and precipitation. Activity coefficient of electrolytes/ions in solution, Debye-Hückel model: limiting law, applications.

Molecular motions in liquids including electrolytic conduction: Electronic versus electrolytic conduction, measurement of conductance, cell constant; specific, equivalent and molar conductance; variation of specific and equivalent conductances with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions, ion conductance and ionic mobility; Walden's rule; equivalent conductance at infinite dilution and its determination for strong and weak electrolytes; Ostwald dilution law and determination of ionization constants for weak electrolytes from conductance measurements; applications of conductance measurement: determination of solubility product and ionic product of water, conductometric titration; transport number, Hittorf's rule, determination of transport number by the moving boundary method.

Course No. CHEM 0391 (FM=50; C=4)
PRACTICAL

Physical Chemistry Practical

Title of the experiment:

1. Determination of the equilibrium constant of the reaction $KI + I_2 = KI_3$ by partition method as a prerequisite to this, determine the partition coefficient of I_2 between CCl_4 and H_2O .
2. Determination of the rate constant of the first order acid catalysed hydrolysis of an ester (preferably methyl acetate) titrimetrically **OR** Determination of the rate constant of decomposition of H_2O_2 by acidified KI solution using the clock reaction **OR** Determination of the rate constant(s) for the acid catalysed inversion of sucrose using the supplied catalysed solution(s) polarimetrically
3. Determination of the coefficient of viscosity (η) of a series of solutions having known concentrations using an Ostwald viscometer and hence to determine the concentration of an unknown solution from a calibration curve.
4. Determination of the surface tension of a series of solutions having known concentrations using a stalagmometer and hence to determine the concentration of an unknown solution from a calibration curve.
5. Determination of solubility and the thermodynamic solubility product of sparingly soluble salts in water and various (common and indifferent) electrolytes by titrimetric method and study of temperature dependence
6. Determination of the specific rotation of a given optically active compound and percent composition of its aqueous solution polarimetrically and determination of optical rotation of a mixture to determine the concentration of one component of the mixture.
7. Calorimetric experiment: Temperature sensor to measure the heat of reaction and related instrumentation.

FOURTH SEMESTER
Course No. CHEM0401 (FM=50; C=4)

Organic Chemistry (M=17)

Spectroscopy:

NMR Spectra: Nuclear spin, NMR active nuclei, principle of nuclear magnetic resonance, equivalent and non equivalent carbons and protons, chemical shift δ , shielding / deshielding, upfield and downfield shifts. NMR peak area (integration for PMR), diamagnetic anisotropy, relative peak positions of different kinds of carbons and protons

IR Spectra: Modes of molecular vibrations, application of Hooke's law, characteristic stretching frequencies and factors effecting stretching frequencies.

UV Spectra: Electronic transition, relative positions of λ -max, Woodward's empirical rule.

Mass spectra: Elementary idea.

Reaction of carbon-heteroatom multiple bonds:

Addition to C=O: Mechanism, reactivity, equilibrium and kinetic control. Reactions with alcohols, amines, thiols, HCN, bisulfite, Wittig reaction.

Carbonyl Reduction: hydride addition, Wolff-Kishner reduction, dissolving metal (Bouveault-Blanc reduction, Clemmensen Reduction), Cannizzaro reaction, Tischenko reaction, aldol condensation, benzoin condensation. Hydrolysis of nitriles and isonitriles. Nucleophilic addition to α,β -unsaturated carbonyl system (general principles).

Inorganic Chemistry (M=17)

Chemical Periodicity (II) (M = 17)

General trends of variation of electronic configuration, elemental forms, metallic nature, magnetic properties (if any), catenation and catalytic properties (if any), oxidation states, inert pair effect (if any), aqueous and redox chemistry in common oxidation states, properties and reactions of important compounds such hydrides, halides, oxides, oxyacids (if any), complex chemistry (if any) in respect of the following elements: s- and p- block elements (except Po, At and Rn).

(i) Structure, bonding and reactivity of B_2H_6 ; $(SN)_x$ with $x = 2, 4$; phosphazines; interhalogens. (ii) Structure of borates, silicates, polyphosphates, borazole, boron nitride, silicones, thionic acids, polythionic acids. (iii) Reactivity of poly halides, pseudo halides, interhalogens, fluorocarbons, freons and NO_x with environmental effects. (iv) Chemistry of hydrazine, hydroxylamine, sodium azide, hydrazoic acid, thio- and per-sulphates. Potassium biiodate, potassium bromate, potassium iodate, potassium periodate, Noble gases from air; oxides, fluorides and oxofluorides of xenon; chemical and photochemical reactions of ozone. Extraction/properties/uses of ultrapure silicon germanium, selenium, lithium tin and lead.

Physical Chemistry (M=16)

Chemical Kinetics-II (M=6)

Activation energy profile for one step and two step reactions; enthalpy of activation and free energy of activation; kinetics and mechanism of reaction; kinetics of chain reaction; catalysed reactions: homogeneous catalysis, mechanism of catalytic action, acid-base catalysis, auto catalysis, enzyme catalysis - kinetics and various kinds of inhibition: Michaelis-Menten equation, turnover number, Lineweaver-Burk plot; influence of temperature and pH.

Quantum Chemistry-I (M=10)

Breakdown of classical ideas – Line Spectra, black body (or cavity) radiation, Planck's quantization, photoelectric effect, Elementary idea of Bohr Theory, Compton scattering for relativistic (preliminary idea only); wave properties of particles: de Broglie hypothesis and the concept of matter waves, Davisson-Germer experiment, nature of matter waves: group and phase velocities and the idea of a wave packet; Heisenberg uncertainty principle and its relation to the measurement process, Differentiation of small and large particles on the basis of Uncertainty Principle, necessity of more general theory.

Time-independent form of the Schrödinger equation; probabilistic interpretation of the wave function; conditions for acceptability of wave functions; elementary idea of operator, operator algebra, eigen value equation, expectation value; time dependent Schrödinger equation, concept of stationary states, study of a simple (model) system: Free particle, particle in a box problem: setting up of the Schrödinger equation, its solution, interpretation of the solutions (in the light of energies and wave functions) – normalization, orthogonality and probability eigenfunctions and eigenvalues, energy quantization (and its connection to the boundary conditions), evaluation of expectation values of x , x^2 , p_x , p_x^2 , their significance in the light of uncertainty principle, extension of the particle in one-dimensional box to two- and three-dimensional cases, idea of degenerate energy states and relationship of symmetry and degeneracy.

Course No. CHEM 0402 (FM=50; C=4)

Organic Chemistry (M=16)

Elimination reaction: Acyclic and cyclic system

Elimination - Mechanisms: E1, E2 and E1cB; reactivity, orientation (Saytzeff / Hofmann) and stereoselectivity; substitution vs elimination.

Rearrangements

1,2-shifts: Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol-pinacolone and related rearrangements, dienone-phenol; benzil-benzilic acid rearrangement. Rearrangement to electron-deficient oxygen: Baeyer-Villiger oxidation, hydroperoxide rearrangement cumene hydroperoxide-phenol rearrangement, Dakin reaction. Aromatic rearrangements: migration from oxygen to ring carbon (Fries rearrangement, Claisen rearrangement); migration from nitrogen to ring carbon (Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger

rearrangement, Orton rearrangement, Benzidine rearrangement.

Transformation: Radical coupling (pinacol, acyloin, McMurry), epoxides, phenols and quinones.

Inorganic Chemistry (M=17)

Redox Chemistry

Elementary idea on standard redox potentials with sign convention, Nernst equation. Influence of complex formation, precipitation and change of pH on redox potentials, formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators, redox potential diagram (Latimer and Frost) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples).

Physical Chemistry (M=17)

Transport Phenomena (M=9)

Flows under the influence of mechanical, chemical and electrical forces: General features of fluid flow (streamline and turbulent flows, Reynold's number); nature of viscous drag for streamline motion, Newton's equation, viscosity coefficient, Poisuille equation (with derivation), Viscosity of gas, temperature dependence of viscosity coefficient of liquid and comparison with that for gases; Stokes' law and terminal velocity; experimental determination of viscosity of liquids.

Chemical Instrumentation (M=8)

Instrumentation and Basic electronics: Electronic components, transistors and multimeter; Basic concept of signal, noise and signal amplification; Elementary idea about the instruments used in Chemistry.

Course No. CHEM 0491 (FM=50; C=4)

PRACTICAL

Instrument based Physical Practical (M=30)

1. Determination of the E^0 (reduction potential) of $\text{Fe}^{3+}/\text{Fe}^{2+}$ system and the concentration of an unknown sample (KMnO_4 or $\text{K}_2\text{Cr}_2\text{O}_7$) solution using a potentiometer by titrating a supplied Mohr salt solution against a standard solution of KMnO_4 or $\text{K}_2\text{Cr}_2\text{O}_7$.
2. Determination of the concentration and pK value(s) of the supplied solutions (a weak monobasic/dibasic acid) pH-metrically, comparison with titration using indicator.
3. Determination of the concentration of the strong and weak acids in a supplied mixture conductometrically, comparison with titration using indicator.
4. Determination of the ionization constant (K_a) and the equivalent conductance at infinite dilution (Λ_0) of a weak acid conductometrically, study of Debye-Hückel-Onsagar equation and the use of extended form.

5. Familiarization with electronic components, transistors and usage of multimeter.
6. Basic instrumentation of Spectrophotometer and its applications: (i) Determination of the rate constant and the order of the reaction between KI and $K_2S_2O_8$ and Determination of the molar extinction coefficient and concentration of a coloured solution ($KMnO_4$ / $K_2Cr_2O_7$ / I_2 in $KI/CuSO_4$, etc.).

Computer Applications (M=20):

Algorithms and flow charts, Introduction of Languages and elementary programming: basic numerical analysis – iterative method for solving polynomial equation, simple integration, linear list square fit. Use of softwares for curve / equation / evolution of area under a curve, use of commercially available software – CHEM Draw, CHEM – 3D for the understanding of stereochemistry.

FIFTH SEMESTER

Course No. CHEM 0501 (FM = 50; C = 4) Organic Chemistry

Unit I: Synthesis (M = 30)

Enolate chemistry: Enolates and enamines: formation; alkylation and acylation, reactions with carbonyls, conjugate addition. Chemistry of acetacetic ester and malonic ester

Synthetic strategy: Retrosynthetic analysis- disconnections, synthons, donor and acceptor synthons, functional group interconversion, C-C disconnections and synthesis [one group and two group (1,2 to 1,6-dioxygenated)], reconnection (1,6-di carbonyl), natural reactivity and umpolung, protection-deprotection strategy [alcohol, amine, carbonyl, acid]

Asymmetric synthesis: Stereoselective and stereospecific reactions, diastereoselectivity, and enantioselectivity (only definition), diastereoselectivity: addition of nucleophiles to C=O, adjacent to a stereogenic centre (Felkin-Anh model); addition of electrophiles to C=C (Houk model).

Carbocycles: *Synthesis and reactions:* Thermodynamic and kinetic factors, Baldwin rules. Synthesis of carbocycles through alkylation, condensation, cycloaddition, rearrangement and their reactions. Synthesis of polycyclic aromatics.

Heterocycles: Synthesis and reactions of heterocycles (monocyclic and bicyclic) with one heteroatom.

Green Chemistry:

Need for green chemistry – goals of green chemistry – limitations, examples of green synthesis/reactions in organic chemistry.

Unit II: Reagents and Reactions (M = 20)

Organometallic Chemistry: Preparation of Grignard and organo lithium reagents; addition of Grignard and organo lithium to carbonyl compounds, substitution on -COX; conjugate addition by cuprates, Reformatsky reaction.

Nitrogen compounds: *amines:* Electron-deficient nitrogen (Beckmann rearrangement, Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement), nitrile and isonitrile. diazomethane, diazoacetic ester, aromatic nitro compounds, aromatic diazonium salts.

Course No. CHEM0502 (FM = 50; C = 4) Inorganic Chemistry

Chemistry of coordination compounds (M = 8)

Coordinate bonding, reactivity and stability: double salts and complex salts, Werner's theory of coordination compounds. Ambidentate and polydentate ligands, chelate complexes. IUPAC nomenclature of coordination compounds (upto two metal centres).

Coordination number and geometry, constitutional and stereoisomerism, determination of configuration of *cis*- and *trans*- isomers by physical/chemical methods. Labile and inert complexes, substitution reaction on square planar complexes, trans effect. Stability constants of coordination compounds and their importance in inorganic analysis.

Structure and bonding (M = 10)

Valence bond theory of transition metal complexes and its limitations, elementary crystal field theory: splitting of d^n configurations in octahedral, square planar and tetrahedral fields, crystal field stabilization energy in weak and strong fields; pairing energy. Jahn-Teller distortion. Metal-ligand bonding (MO concept, elementary idea), sigma- and pi-bonding in octahedral complexes (qualitative pictorial approach) and their effects on the oxidation states of transitional metals (examples). Stabilization of unusual oxidation states of transition metals.

Magnetism and Spectra (M=10)

Orbital and spin magnetic moments, spin only moments of d^n ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and ferromagnetic/antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling; qualitative Orgel diagrams for $3d^1$ - $3d^9$ ions and their spectroscopic ground states; selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

Chemistry of d- and f-block elements (M = 10)

General comparison of 3d, 4d and 5d elements in terms of electronic configuration, elemental forms, metallic nature, atomization energy, oxidation states, redox properties, coordination chemistry, spectral and magnetic properties. f-block elements: electronic configuration, ionization energies, oxidation states, variation in atomic and ionic ($3+$) radii, separation of lanthanides by ion-exchange methods.

Gravimetric and titrimetric methods of analysis (M = 12)

Requirements of gravimetry: properties of precipitates and precipitating reagents, particle size and filterability of precipitates; colloidal and crystalline precipitates coprecipitation and post precipitation, peptization, drying and ignition of precipitates.

Primary and secondary standard substances in acid-base, redox, complexometric (EDTA) and argentometric titrations. Principle and application of redox titrimetric estimation based on the use of the following reagents: $KMnO_4$, $K_2Cr_2O_7$, I_2 , $Na_2S_2O_3 \cdot 5H_2O$. Principle of argentometric titration, adsorption indicators, estimation of chloride using adsorption indicators. Principle of complexometric EDTA titration, metal ion indicators (examples), masking and demasking reactions.

Course No. CHEM0503 (FM = 50; C = 4)
Physical Chemistry

Quantum Chemistry-II (M = 10)

Simple harmonic oscillator (SHO): setting up of the Schrödinger equation, connection with the uncertainty principle, classical turning points, expressions for energy and wave functions for the ground and the first excited states (quantitative treatment), series solutions of differential equation: Hermite equation, recursion relation, their characteristics features, the zero-point energy and its importance, limitations thereof and the idea of the anharmonic oscillator.

Central force problem: setting of the Schrödinger equation in Cartesian coordinates, Transformation of coordinate systems, transforming the Schrödinger equation to spherical polar coordinates, Rigid rotor and Hydrogen atom: separation of variables into radial (r) and angular (Θ and ϕ) parts, solution of the ϕ dependent equation and the idea of the magnetic quantum number (m_l), energy expression (no derivation required), idea of degeneracy, the principal (n) and the azimuthal (l) quantum numbers, hydrogen wave functions (up to $n=3$), the concept of an orbital, real orbitals (suitable linear combinations), radial density distributions, radial and angular nodes, shapes of s, p and d orbitals.

Molecular Spectroscopy - I (M = 10)

Rotational spectroscopy of diatomic molecules: the rigid rotor model, selection rules, spectrum, characteristic features of spectral lines (spacing and intensity); determination of bond length, effect of isotopic substitution; vibrational spectroscopy of diatomic molecules: selection rules stemming out of the SHO model, spectra, anharmonicity and its consequence on energy levels, overtones, hot bands; preliminary ideas of magnetic resonance: NMR and ESR spectroscopies.

Chemical Dynamics (M = 10)

Collision of gas molecules: collision diameter, collision number and mean free path; frequency of binary collision (similar and dissimilar molecules); wall collision and rate of effusion. Collision theory, transition state theory, Lindmann theory of unimolecular reaction; primary and secondary kinetic salt effect, kinetic isotope effect. Photochemical Reactions: kinetics of HI decomposition, H_2-Br_2 reaction, dimerization of anthracene, photostationary state.

Chemistry of surfaces (M = 7)

Surface tension, surface energy (thermodynamic treatment), excess pressure, capillary rise and measurement of surface tension, work of cohesion and adhesion, spreading of liquid over other surface, vapour pressure over curved surface, temperature dependence of surface tension; special features of interfaces compared to bulk, surface dynamics: physical and chemical adsorption, Freundlich and Langmuir adsorption isotherm,

multilayer and BET isotherm (without derivation) and applications, Gibbs adsorption isotherm and surface excess, effect of addition of substances on surface tension, surfactants and micelles and reverse micelles: applications, size and solubility; Microencapsulation for personal care; Nanoencapsulation. Heterogeneous catalysis (single reactant).

Statistical thermodynamics and the third law (M = 13)

Concept of probability. Micro- and macrostates, thermodynamic probability, entropy and probability, the Boltzmann-Planck entropy formula, the Maxwell-Boltzmann distribution law for the distribution of molecular energies, partition function: molecular and molar, the transitional partition function, thermodynamic quantities from partition function, vibrational partition functions, Einstein's theory of heat capacity of solids, the characteristics temperature, its limitations and Debye's modification thereof; Nernst heat theorem, approach to zero Kelvin, adiabatic demagnetization, Planck's formulation of third law and the concept of absolute entropies.

Course No. CHEM0591 (FM=50; C=4)

PRACTICAL

Synthesis-based Practical (Organic)

Two-step preparations based on organic reactions and interpretation of Spectra (IR, NMR). Experiment related to green chemistry (at least one).

Course No. CHEM0592 (FM=50; C=4)

PRACTICAL

Inorganic Quantitative analysis

Experiments-1: Gravimetric Estimations (any one)

- i) Estimation of Ni as $[\text{Ni}(\text{DMG})_2]$,
- ii) Estimation of Ba as BaSO_4 .

Experiments-2: Redox Titrimetric Estimations Based on Permanganometry (any two)

- i) Estimation of Fe(III) and Fe(II) mixture.
- ii) Estimation of Fe and Ca in a mixture.
- iii) Estimation of total Mn in pyrolusite.

Experiments-3: Redox Titrimetric Estimations with standard $\text{K}_2\text{Cr}_2\text{O}_7$ solution (any two)

- i) Estimation of Fe(III) and Fe(II) mixture.
- ii) Estimation of Fe and Cu in a mixture.
- iv) Estimation of Fe(III) and Cr_2O_7 in mixture.
- v) Estimation of Cu in brass.

Experiments-4: Titrimetric Estimations Based on complexometric EDTA Titrations. (any two)

- i) Estimation of Ca and Mg in a mixture.
 - ii) Determination of the amount of calcium in milk powder
 - iii) Estimation of permanent and temporary hardness of water.
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SIXTH SEMESTER
Course No. CHEM0601 (FM = 50; C = 4)
Organic Chemistry

Unit I: Pericyclic reactions, Advanced spectroscopy and polymers (M = 25)

Pericyclic Reactions

Electrocyclic reactions: 4e and 6e neutral systems; cycloaddition reactions: [4 + 2] and [2 + 2] reactions, cheletropic addition of carbene; sigmatropic rearrangements: [1,3] and [1,5] H shifts, [3,3] Cope and Claisen rearrangements. FMO analysis and Woodward-Hoffmann selection rules.

Advanced spectroscopy

Spin coupling and coupling constant, interpretation of IHNMR spectra for some simple systems. Structural elucidation using MS, UV, IR and NMR.

Polymers and nanomaterials

Addition and condensation polymers; carbon polymers: fullerenes, nanotubes, graphene; conducting polymers.

Unit II: Biomolecules [Introduction, structure and function of selected biomolecules] (M = 25)

Carbohydrates

Monosaccharides: Aldoses upto 6 carbons, structure of D- glucose & D-fructose (configuration & conformation), anomeric effect, mutarotation. Important reactions and conversions including protection / deprotection protocol. Disaccharides and polysaccharide: nature of glycosidic linkages.

Aminoacids and peptides

Amino acids: Synthesis: (Strecker, Gabriel, acetamido malonic ester, azlactone); isoelectric point, ninhydrin reaction. Peptides: peptide linkage, synthesis of peptides using N-protection & C-protection, solid phase synthesis; peptide sequence: C-terminal and N-terminal amino acid determination.

Problems based on chemical reactions and structure covering the above topics.

Proteins and Nucleic acids

Primary, secondary, tertiary and quaternary structure of proteins and protein folding. Nucleic acids: Structure of nucleosides and nucleotides, RNA and DNA.

Course No. CHEM 0602 (FM = 50; C = 4)
Inorganic Chemistry

Bioinorganic Chemistry (M = 12)

Elements of life: essential, major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na⁺, K⁺, Mg²⁺, Ca²⁺, Fe^{3+/2+}, Cu^{2+/+}, and Zn²⁺). Metal ion transport across biological membrane Na⁺, K⁺-ion pump, ionophores. Biological functions of hemoglobin and myoglobin, cytochromes and ferredoxins, carbonate bicarbonate buffering system and carbonic anhydrase. Biological nitrogen fixation, Photosynthesis: Photo system-I and Photosystem-II. Toxic metal ions

and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases.

Organometallics (M = 14)

18-electron rule and its applications to carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, and nature of bonding involved therein. Simple examples of metal-metal bonded compounds and metal clusters. Metal-olefin complexes: Zeise's salt (preparation, structure and bonding), Ferrocene (preparation, structure and reactions). Hapticity (η) of organometallic ligands, examples of mono, tri- and penta-hapto cyclopentadienyl complexes. Simple examples of fluxional molecules, coordinative unsaturation, oxidative addition, reductive elimination, insertion reactions.

Environmental analysis (M = 14)

Principles for determination of BOD, COD, DO, TDS, suspended solid in water samples. Detection and estimation of As, Fe, Hg, Cd, Pb, NH_4^+ , and F^- , NO_3^- , NO_2^- , PO_4^{3-} , in water sample. Sampling, detection, and principles of estimation of CO, NO_x , SO_2 , H_2S and SPM in air samples. Basic principles and instrumentation of atomic absorption and atomic emission spectrometry, estimation of sodium and potassium in water samples.

Metals and special compounds of transition metals (M= 10)

Preparation, properties, reactions and uses of some selected metallic compounds in respect of the following: $(\text{h}^5\text{-C}_5\text{H}_5)_2\text{TiCl}_2$, NH_4VO_3 , V_2O_5 , $\text{K}_2\text{Cr}_2\text{O}_7$, KMnO_4 , $\text{K}_3[\text{Fe}(\text{CN})_6]$, $\text{K}_4[\text{Fe}(\text{CN})_6]$, Prussian blue, $(\text{NH}_4)_2[\text{PtCl}_6]$, *cis*- $[\text{Pt}(\text{NH}_3)_2\text{Cl}_2]$, *trans*- $[\text{Pt}(\text{NH}_3)_2\text{Cl}_2]$, AgNO_3 ; gold chloride, fulminating gold, auric acid, uranyl acetate.

Course No. CHEM0603 (FM = 50; C = 4)

Physical Chemistry

Molecular Spectroscopy - II (M = 10)

Brief history of Photochemistry, Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer's law; quantum yield and its measurement for a photochemical process, Photosensitized reaction. Actinometry, Raman effect, characteristic features and conditions of Raman activity with suitable illustrations, rotational and vibrational Raman spectra, the rule of mutual exclusion with examples. Potential energy curve (diatomic molecules), Electronic transitions and Quantum theory, Theory of Electronic Spectra, Intensities of Electronic transitions, The Franck Condon principle, vibrational structure of electronic spectra, Franck-Condon factor, bond dissociation and principle of determination of dissociation energy (ground state). Molecular electronic absorption spectra, Molecular electronic emission spectra, Radiationless transitions, Jablonski diagram, non-radiative transitions, Kasha's rule, fluorescence and phosphorescence.

Chemistry of solid state (M = 10)

Forms of solids, preliminary idea of symmetry elements, Crystal structure of solids: Fundamental of lattices, unit cell, atomic coordinates, crystal system, crystal direction and

planes, Bravais lattice type and its identification of lattice planes, laws of crystallography: law of constancy of interfacial angle and law of rational indices, Weiss and Miller indices, packing in solids and the radius ratio rule, and their implications; Crystal diffraction by X-rays, idea of a simple diffraction grating, Bragg's law and its applications for the determination of crystal structure for cubic systems, crystal structure of NaCl and KCl, single crystal and powder diffraction methods (preliminary ideas), Structure determination by X-ray diffraction, packing in solids and corresponding efficiency.

Colloids and macromolecules (M = 12)

Lyophobic and lyophilic sols, origin of charge and stability of lyophobic colloids, coagulation and Schultz-Hardy rule, zeta potential and Stern double layer (qualitative idea); Tyndall effect, electrokinetic phenomenon (qualitative idea only);

Macromolecules, degree of polymerization, different average molar masses in a poly disperse system, determination of molar mass by osmometry and viscometry; Donnan equilibrium, transport across membranes, elementary idea about Biomolecules: biopolymers – peptide linkage, enzyme substrate interaction. Microporous materials, microgels, bioconjugate polymers, gels, ointments and creams, biodegradable polymers.

Fundamentals of nano science: definition, nano versus bulk, quantum confinement: nano-scale in 1D, 2D and 3D with examples, synthesis of nano materials: top-down and bottom-up approaches, size dependent properties; nanoclusters and nanowires, semiconductor nanoparticles, applications of nano materials.

Colligative properties and Phase rule (M = 12)

ΔG , ΔS , ΔH and ΔV of mixing for binary solutions, vapour pressure of solution, ideal solutions, ideally dilute solutions and colligative properties, Raoult's law, thermodynamic derivation (using chemical potentials) of colligative properties of solution and their inter-relationships, abnormal colligative properties, van't Hoff factor; biomedical application: osmosis and dialysis.

Definition of phase, number of component and degrees of freedom, Gibbs phase rule and its derivation, definition of phase diagram, phase equilibria for one component system, first order phase transition and Clapeyron equation, Clausius-Clapeyron equation: derivation and its use; liquid vapour equilibrium for two component systems; ideal solution at a fixed temperature and pressure, principle of fractional distillation, Duhem-Margules equation, Henry's law, Konowaloff's rule; positive and negative deviations from ideal behaviour, azeotropic solutions, liquid-liquid phase diagram using phenol-water system, solid-liquid phase diagram, simple eutectic diagram.

Magnetic and electrical properties of matter (M = 6)

Magnetic permeability, specific and molar magnetic susceptibility, determination of magnetic susceptibilities: Curie law, paramagnetism and unpaired electrons; polarizability

of atoms and molecules, dielectric constant and polarization, molar polarization for polar and non-polar molecules, Clausius-Mosotti, Debye and Lorentz-Lorenz equation (derivation not required) and their application; determination of dipole moment.

Course No. CHEM 0691 (FM=50; C=4)

PRACTICAL

Combined Practical

- (i) Chromatographic separation
- (ii) Estimation of organic compounds, e.g. ascorbic acid, sucrose, aniline
- (iii) Identification of insoluble radicals
- (iv) Colorimetric estimation of Metal ion (Fe^{2+} , Mn^{2+})
- (v) Determination of indicator constant of methyl orange/bromocresol green by colorimetric method
- (vi) Study of the phase diagram
- (vii) Study of the Freundlich adsorption isotherm for acetic acid on activated charcoal
- (viii) Determination of critical micellar concentration (CMC) of SDS conductometrically.

Course No. CHEM0692 (FM = 50; C = 4)

- 1. Project Work / Seminar / Review: dissertation and presentation (M= 30).**
- 2. Grand Viva and Lab Quiz (M = 20).**
