

Semester –I: Chemistry I (45 h)

Unit	Content	Contact Hours
Unit I: Atomic structure	Historical development on structure of atom; Bohr's model, H-atom Spectrum; Black Body Radiation; Photoelectric effect (qualitative treatment only); The dual behaviour and uncertainty Quantum mechanical approach to atomic structure: Concept of Wave function, well behaved function, operator, Normalised and Orthogonal wave function, Schrodinger Wave equation, eigenfunction, Significance of Ψ and Ψ^2 , Particle in a 1D box; Schrodinger equation of hydrogen atom (no derivation), radial and angular wave functions for hydrogen atom, probability distribution, Quantum numbers, Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations.	8
Unit II: Periodicity and Chemical behaviour	Effective Nuclear Charge; Slater's Rule; Covalent and ionic Radii, Ionization energies, Electronegativity (Various scales), Electron affinities	3
Unit III: Chemical Bonding I (Ionic interaction)	General characteristics of Ionic compounds; Lattice and Solvation energy; Born Lande equation; Kapustinski equation, Madelung constant, Born Haber Cycle for lattice energy calculation	4
Unit IV: Structure of organic molecules	Nature of Bonding: Hybridisation of atomic orbitals (qualitative VB and MO approach); Effect of hybridization on bond properties.	4
Unit V: Stereochemistry of organic molecules	Representation of organic molecules in 2D and 3D (Fischer, Newman and Sawhorse Projection formulae and their interconversions); Geometrical isomerism (cis-trans, syn-anti, E/Z notations); Concept of chirality (enantiomers and diastereomers); Configuration and Conformation, Barriers to rotation, Conformational Analysis (ethane, butane, cyclohexane)	8
Unit VI: Electronic effects in organic molecules	Concept of Electrophiles and Nucleophiles; Inductive effects; Resonance, Conjugation and Delocalisation.	3

Unit VII: Gaseous state	Causes of deviation from ideal gas behaviour, compressibility factor, Z , and its variation with pressure and temperature for different gases. State variables and equation of states for real gases; van der Waals equation of state, its derivation and application in explaining real gas behaviour. Reasons and examples of failure of van der Waal equation of state and interpretation of van der Waals pressure-volume isotherm. Critical state and phenomena, mathematical definition and interpretation of critical point, relation between critical constants and van der Waals constants: along with their thermodynamic interpretation. Introduction to virial equation and virial coefficients, derivation of Boyle temperature.	8
Unit VIII: Liquid state	Qualitative treatment of the structure of the liquid state. Physical properties of liquids, vapour pressure, surface tension coefficient of viscosity, and their determination. Temperature variation of viscosity of liquids and comparison with that of gases. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents (micelle formation and critical micelle concentration).	7

<p>Lab Course I</p>	<ol style="list-style-type: none"> 1. Introduction to laboratory apparatus and safety measures in laboratory, 2. Calibration of apparatus (volumetric flask, thermometer, melting point apparatus etc.) <p>Group A</p> <ul style="list-style-type: none"> • Preparation of normal and molar solution, for example KCl, Na₂C₂O₄, HCl, H₂SO₄ etc. (Verification by conductometric measurement). • Determination of solubility of a given salt at different temperature and plot solubility curve. • Determination of water of crystallisation of hydrated salt by ignition and weighing. <p>Group B</p> <ul style="list-style-type: none"> • Determination of the melting points of above compounds and unknown organic Compounds (Here, the student is required to learn about thermometer calibration before performing the experiment). • Effect of impurities on the melting point – mixed melting point of two unknown organic compounds. • Purification of organic compounds by crystallization using the following solvents: (a) Water, (b) Alcohol, (c) Alcohol-Water. <p>Group C</p> <ul style="list-style-type: none"> • Evaluating the compressibility factor using standard package such as Excel/Origin/Python/Fortran. • Simulating an ideal gas using programming. • Simulation of a real gas using programming. • To determine the partial molar volume of ethanol-water mixture at a given composition. • Determine the surface tension of a given liquid at room temp using stalagmometer by drop number method. • Determine the surface tension of a given liquid by means of stalagmometer using drop weight method. • Determine the composition of a given mixture by surface tension method. • Study the variation of surface tension of detergent solutions with concentration. <p>(Students are required to perform Expt. 1, 2 and a minimum of two experiments from each group)</p>	<p>30</p>
---------------------	--	-----------

Text Book /Reference Book	<ol style="list-style-type: none"> 1. University Chemistry, P. Siska, O. K. Medhi, 2nd edition, Pearson Education 2. General and Inorganic Chemistry, R.P. Sarkar (part 1) 3rd edition, NCBA 3. Concise Inorganic Chemistry, J. D. Lee, 5th Edition, Pearson Education 4. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5th edition, Pearson Education 5. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48th Edition, Vishal Publishing Com. 6. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11th Edition, Oxford University Press. 7. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7th Edition (Wiley) 8. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2nd Edition (Oxford) 9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji, S. P. Singh 3rd Edition (Macmillan) 10. Organic Reactions and their Mechanisms, P. S. Kalsi 11. Organic Chemistry, Maitland Jones, Jr., Steven A. Fleming 5th Edition (Norton)
---------------------------	---

Semester –II, Chemistry-II (45 h)

Unit I: Chemical Bonding II (Covalent Bond and Chemical forces)	<p>Valence Bond theory (Heitler-London approach), Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of homonuclear (N₂, O₂) and heteronuclear diatomic (CO, NO, CN⁻), Bonding in BeF₂ and HCl (idea of s-p mixing and orbital interaction). Valence shell electron pair repulsion theory (VSEPR). Covalent character in ionic compounds, polarising power and polarizability. Fajan's rules and consequences of polarisation. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.</p> <p>Weak Chemical Forces (van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions and hydrogen bonding) and their effects on melting and boiling points, solubility and hydration energy.</p>	10
---	---	----

Unit II: Coordination Chemistry-I (structure and Isomerism)	Introduction to coordination complexes (Werner theory, types of ligands) IUPAC nomenclature, Isomerism in coordination complexes, Stereochemistry of complexes with coordination numbers 4, 5, and 6. Berry pseudorotation.	5
Unit III: Reactive Intermediates in Organic Reactions	Formation, structure and stability of reactive intermediates: Carbocations, Carbanions, Radicals, Carbenes, Nitrenes, Benzyne (Brief mechanistic perspective using concepts of Substitution, Addition, Elimination and Rearrangements reactions).	12
Unit IV: Acidity, basicity, and pK _a	The definition of pK _a ; Lewis acids and bases; Organic acids and bases (Factors affecting relative strength); Substituents affect the pK _a (carbon acids).	3
Unit V: Thermodynamics	<p>Mathematical treatment: Exact and inexact differentials, partial derivatives, Euler's reciprocity, cyclic rules.</p> <p>Intensive and extensive variables, isolated, closed and open systems. Cyclic, reversible and irreversible processes. Zeroth law of thermodynamics. First law of thermodynamics, concept of heat (q) and work (w), internal energy (U) and enthalpy (H) in differential forms: their molecular interpretation. Calculation of w, q, ΔU and ΔH for expansion of ideal gas under isothermal and adiabatic conditions for reversible and irreversible processes. Derivation of Joule-Thomson Coefficient and inversion temperature.</p> <p>Application of First law of thermodynamics: standard state, standard enthalpy changes of physical and chemical transformations: fusion, sublimation, vaporization, solution, dilution, neutralization, ionization. Bond-dissociation energy Kirchhoff's equation, relation between ΔH and ΔU of a reaction. Difference between enthalpy and standard enthalpy.</p> <p>Second law of thermodynamics, entropy (S) as a state function, molecular interpretation of entropy. Residual Entropy. Free energy: Gibbs function (G) and Helmholtz function (A) and their molecular interpretation. Difference between free energy and standard free energy. Gibbs-Helmholtz equation, criteria for thermodynamic equilibrium and spontaneity of a process. Maxwell's Relations and their physical significance.</p>	15

Lab Course II	<p>a) Determination of total hardness of water by titration against standardised EDTA solution.</p> <p>b) Synthesis of coordination compounds i) Potassium tris(oxalato)chromate(III), ii) [Ni(DMG)₂]</p> <p>c) Qualitative organic analysis for N, S, halogen and functional group test</p> <p>d) Preparation of Buffer solution and measurement of pH using pH-meter (acetic acid-sodium acetate buffer)</p> <p>e) Determination of heat capacity of the calorimeter and enthalpy of neutralisation of hydrochloric acid with sodium hydroxide.</p> <p>f) Detect the presence of nitrogen, sulphur and halogens in a given organic compounds.</p> <p>g) Detection of presence of unsaturation and aromaticity in an organic sample.</p> <p>h) Identify acidic functional groups of a given organic sample (Acetic acid, Lactic acid, Tartaric acid and Phthalic acid) and determine the pK_a by titrametric methods.</p> <p>i) Determine the enthalpy of solution of oxalic acid from solubility measurements.</p> <p>j) Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.</p> <p>k) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).</p> <p>l) Calculation of the enthalpy of ionization of ethanoic acid.</p> <p>Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.</p> <p>m) Determination of enthalpy of hydration of copper sulphate.</p>	30
Text Book /Reference Book	<ol style="list-style-type: none"> General and Inorganic Chemistry, R.P. Sarkar (part 1) 3rd edition, NCBA Concise Coordination Chemistry, R. Gopalan, V. Ramalingam, 1st Edition, Vikash Publishing House Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5th edition, Pearson Education Principles of Physical Chemistry, Puri, Sharma, Pathania, 48th Edition, Vishal Publishing Com. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11th Edition, Oxford University Press. 	

Semester III, Chemistry –III (3 L-0 T-1 P)

Unit	Content	Contact Hrs
Unit I: Acid and Bases	Acid-base concepts, Measure of acid and base strength, proton affinity, acidity and basicity of binary hydrogen compounds, inductive effect and strength of oxyacids, acidity of aqua ions, steric effect, proton sponge, solvation and acid base strength, non-aqueous solvents and acid base strength, levelling effect, superacids and superbases. Hard and Soft Acids and Bases (HSAB), Application of HSAB principle and symbiosis	7
Unit II: Oxidation and reduction -I	Reduction potentials: Redox half-reactions, standard potentials and spontaneity, trends in standard potentials, the electrochemical series, Nernst equation (Influence of pH and concentration on electrode potential). Principles of redox titration and choice of redox indicators.	4
Unit III: Coordination Chemistry-II	Valence bond theory, inner and outer orbital complexes, electroneutrality principle and back bonding, effects of hybridization in metal ligand bond strength and stability of complexes, choice of metal d-orbital(s) in hybridization in different coordination geometries, magnetic properties of complexes, Drawback of VBT	4
Unit IV: Aromaticity	Concepts of aromatic, anti-aromatic and non-aromatic compounds (including examples of cyclic carbocations, carbanions and heterocyclic compounds); Hückel's rule.	3
Unit V: Hydrocarbons and halogenated compounds	Methods of preparation, properties and relative reactivity of alkyl and aryl halides; Selectivity in electrophilic and nucleophilic substitution reactions (S_NAr), Preparation and reactions of diazonium salts; Benzyne mechanism.	4
Unit VI: Alcohols, Phenols, Thiols and related compounds:	Preparation, properties and relative reactivity of 1° , 2° , and 3° -alcohols, Ethers, Epoxides (Preparation and reactions with alcohols, ammonia derivatives and $LiAlH_4$). Thiols and Sulfides; Phenols (Preparation, properties and reactivity; Reimer–Tiemann and Kolbe's–Schmidt Reactions)	4
Unit VII: Carbonyl Compounds	Structure, reactivity and preparation; Oxidations and Reductions (Jones reagent, PCC and PDC, Oppenauer, Clemmensen, Wolff-Kishner, $NaBH_4$, $LiAlH_4$, MPV), Baeyer Villiger oxidation.	4

Unit VIII: Solution	Vapour pressure of solution. Ideal solutions, ideally diluted solutions and colligative properties. Raoult's law & Henry's Law. Thermodynamic derivation of colligative properties of solution (using chemical potentials) and their inter-relationships. Abnormal colligative properties.	7
Unit IX: Partial Molar quantities	Fugacity, activity coefficients and Concept of chemical potential: Gibbs Duhem Equation and Duhem-Margules Equation: their use and application, Enthalpy, free energy and entropy of mixing, excess thermodynamic functions.	8
Lab course III (at least three experiments from each group)	<p>Group A</p> <ul style="list-style-type: none"> • Acid-base titration: Estimation of carbonate, bicarbonate and hydroxide. • Redox titration: Estimation of Fe(II) using standardised KMnO_4 solution. • Determination of water of crystallisation of Mohr Salt using standardised KMnO_4 solution. • Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicators (diphenylamine). <p>Group B</p> <ul style="list-style-type: none"> • Determine the surface tension of a given solution at room temp using a stalagmometer. • Prepare derivatives of a given organic sample containing a single functional group (i.e. alcohols, phenols, carbonyl and carboxylic acid group). • Identification of functional groups in a given organic sample: Simple functional groups such as alcohols, phenols, amines, carbonyl and carboxylic acid groups. • Prepare derivatives of a given organic sample containing single functional group (i.e. alcohols, phenols, amines, nitro, carbonyl and carboxylic acid group). <p>Group C</p> <ul style="list-style-type: none"> • Determine the viscosity of a liquid at a given concentration at laboratory temperature, by viscometer. • Determine the composition of a given liquid mixture by viscosity method. • Study the variation of viscosity of sucrose solution with the concentration of the solute. • Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate. 	30

Books:

1. General and Inorganic Chemistry, R.P. Sarkar (part 1), 3rd edition, NCBA
2. Concise Coordination Chemistry, R. Gopalan, V. Ramalingam, 1st Edition, Vikash Publishing House
3. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5th edition, Pearson Education
4. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48th Edition, Vishal Publishing Com.
5. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11th Edition, Oxford University Press.
6. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7th Edition (Wiley).
7. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2nd Edition (Oxford)
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji, S. P. Singh 3rd Edition (Macmillan).
9. Organic Reactions and their Mechanisms, P. S. Kalsi.
10. Organic Chemistry, Maitland Jones, Jr., Steven A. Fleming 5th Edition (Norton).

Semester –IV, Inorganic Chemistry-I (45 h)

Unit	Content	Contact Hrs
Unit I Introduction to molecular symmetry	Symmetry elements and operations, molecular point groups, symmetry elements present in C_{2v} , C_{3v} , T_d and O_h point group (pictorial representation), Introductory idea of character tables, Mulliken symbols.	6
Unit II: D-block Chemistry	Chemistry of first row transition elements (Ti-Cu) in various oxidation states as halides and oxides, Comparison of the first, second and third transition series elements.	8

Unit III Coordination chemistry III	Crystal Field Theory (qualitative treatment): d-Orbital splitting in tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral geometries, Calculation of CFSE, Thermodynamic and structural aspect of orbital splitting, pairing energies (contribution of exchange and coulomb energy), factors affecting the magnitude of $10 Dq$ (Δ_o , Δ_t), Spectrochemical series, tetragonal distortions from octahedral geometry and Jahn-Teller theorem. Limitations of CFT (nephelauxetic effect and EPR evidences), Elementary idea on Ligand field theory, MOT with special reference to sigma bonded octahedral and tetrahedral complexes (qualitative treatment only), Pi bonding in octahedral complexes. Metal-metal quadruple bond in $[\text{Re}_2\text{Cl}_8]^{2-}$	10
Unit IV: Metallurgy	Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agents. Electrolytic Reduction, Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.	5
Unit V: Oxidation and reduction - II	Redox stability: Reaction with water, oxidation by atmospheric oxygen, disproportionation and comproportionation, the influence of complexation, relation between solubility and standard potential Diagrammatic representation of potential data (Latimer diagram, Frost diagram, Pourbaix diagram)	6
Unit VI Lanthanoids and Actinoids:	Lanthanoids: Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only). Coordination chemistry of lanthanides Actinoids: electronic configuration, oxidation states, magnetic properties, Comparison with lanthanides	6
Unit VII Nuclear Chemistry	Stability of nucleus and radioactive decay processes, Fermi theory, half-lives, auger effect, Mass defect, Nuclear reactions – notations, comparison with chemical reaction: Types of nuclear reactions. Applications of radioisotopes in age determination.	4

Lab: Inorganic Qualitative analysis	Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of reactions. The following radicals are suggested: CO_3^{2-} , NO_2^- , S^{2-} , SO_3^{2-} , $\text{S}_2\text{O}_3^{2-}$, CH_3COO^- , F^- , Cl^- , Br^- , I^- , NO_3^- , BO_3^{3-} , $\text{C}_2\text{O}_4^{2-}$, PO_4^{3-} , NH_4^+ , K^+ , Pb^{2+} , Cu^{2+} , Cd^{2+} , Bi^{3+} , Sn^{2+} , Sb^{3+} , Fe^{3+} , Al^{3+} , Cr^{3+} , Zn^{2+} , Mn^{2+} , Co^{2+} , Ni^{2+} , Ba^{2+} , Sr^{2+} , Ca^{2+} , Mg^{2+} Mixtures should preferably contain one interfering anion, or insoluble component (BaSO_4 , SrSO_4 , PbSO_4 , CaF_2 or Al_2O_3) or combination of anions such as CO_3^{2-} and SO_3^{2-} , NO_2^- and NO_3^- , Cl^- and Br^- , Cl^- and I^- , Br^- and I^- , NO_3^- and Br^- , NO_3^- and I^- . Spot tests should be done whenever possible.	30
Text Book/ Ref. Book	1. Inorganic Chemistry, G.L. Meissler and D. A. Tarr, 5 th Edition, Pearson 2. Inorganic Chemistry, P. Atkins, Overtone Rourke, Weller and Armstrong 5 th Edition, Oxford	

Semester IV - (Organic Chemistry-I) – 45 h

Unit	Content	Contact Hrs
Unit I: Carboxylic Acids and their Derivatives:	Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids. Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparison of nucleophilic substitution at acyl group: Mechanism of acidic and alkaline hydrolysis of esters; Claisen condensation, Dieckmann and Reformatsky reactions.	10
Unit II: Nitrogen Containing Functional Groups	Amines: Effect of substituent and solvent on basicity; Preparation and properties: Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid. Diazonium Salts: Preparation and their synthetic applications. General methods for preparation of nitro compounds, nitriles and isonitriles and important reactions.	10
Unit III: Heterocyclic Compounds	Classification and nomenclature (5-numbered and 6-membered rings containing one heteroatom); Synthesis and reactions of Furan, Pyrrole, Thiophene, Pyridine, Pyrimidine, and Indoles: Selected name reactions (Paal-Knorr synthesis, Knorr synthesis, Hantzsch synthesis, Fischer indole synthesis, Skraup synthesis, Knorr quinolone synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction)	9
Unit IV: Alkaloids	Natural occurrence, General structural features, Isolation and their physiological action; Hoffmann's exhaustive methylation,	6

	Emde's modification, Structure elucidation of Nicotine; Medicinal importance of Nicotine, Hygrine, Quinine, Morphine and Cocaine.	
Unit V: Organic Spectroscopy	Introduction to UV-visible and infrared spectroscopy in structure elucidation of organic compounds; Relation between absorption spectroscopy and molecules containing conjugated C=C and C=O groups Analysis of compounds containing alkenes, alkynes and carbonyl compounds using infrared spectroscopy (conceptual aspects).	10
Laboratory experiments	<ol style="list-style-type: none"> Organic preparations (any two from each): Benzoylation of organic compounds: amines (aniline, toluidines, anisidine) and phenols (phenol, β-naphthol, salicylic acid) by the following methods: <ol style="list-style-type: none"> Using conventional method. Using green chemical approach. Organic preparations (any three): <ol style="list-style-type: none"> Bromination of acetanilide by conventional methods. Nitration of salicylic acid using ceric ammonium (green chemistry approach). Selective reduction of meta dinitrobenzene to m-nitroaniline Oxidation of ethanol/ isopropanol (Iodoform reaction). Aldol condensation using either conventional or green method. Benzil-Benzilic acid rearrangement. Chromatography : (a) Separation of a mixture of two amino acids by ascending and horizontal paper chromatography; (b) Separation of a mixture of o-and p-nitrophenol or o-and p-nitro-aniline by thin layer chromatography (TLC) 	30

Semester IV - (Theoretical Chemistry) – 45 h

Learning objectives: Students will be exposed to the fundamental aspects of atomic structure through mathematical point of view. The students may be demonstrated the following lab activities using open-source programs such as GAMESS, MacMolPlt, Avogadro, etc or commercial software such as Gaussian, GaussView, etc Building and manipulating a small molecular model using a molecular builder such as MacMolPlt, Avogadro, GaussView etc.

Unit	Content	Contact Hrs
Unit I: Quantum Theory	Plancks' Quantization of energy and Hydrogen Line spectrum. Postulates of quantum mechanics and their physical interpretation, wavefunctions and quantum mechanical operators. Born interpretation. Well behaved wavefunctions	37

	<p>and commutation relations. Orthonormality and physical meaning of expanding a wavefunction in orthonormal basis. Hermitian Operators and Real Eigenvalues, Eigenvectors: their physical significance.</p> <p>Particle in a 1-D box (complete solution with orthonormalization) and relation to conjugated polyenes. Heisenberg Uncertainty Principle from expectation values of 1 D box, extension to two and three-dimensional boxes. Rotational Motion and Energy: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.</p> <p>Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Interpretation of zero-point energy.</p> <p>Hamiltonian for 1 electron H-atom, its wavefunctions (only explanation, no derivation) and its relation to atomic orbitals. Constructing Radial and Angular Distribution Curves from H-like wave functions. Quantum mechanical idea of chemical bond formation: Heitler-London's Valence bond theory. Atomic Units. Good quantum numbers for multi-electron systems and Atomic Term Symbols. LS and j-j coupling schemes. Qualitative idea of tunneling.</p>	
Unit II: Molecular Properties	Intermolecular forces and potentials, Polarizability of atoms and molecules, dielectric constant and polarisation, molar polarisation for polar and non-polar molecules. Clausius- Mosotti equation (with derivation) and Debye equation and their application.	8
Laboratory experiments	<ol style="list-style-type: none"> 4. Writing and plotting basic expressions and graphs (eg. Maxwell-Boltzmann distribution law, radial and angular distribution functions for H-atom etc.) using any spreadsheet software such as MSEXcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc). 5. Putting atoms and fragments, choosing an element, selecting hybridization, changing bond angle/bond length, editing individual atoms, centering, rotation of structure, etc 6. Geometry optimization (energy minimization): Making input file through selection of calculation method (e.g., using Hartree Fock or Density Functional Theory), basis set, specifying charge and multiplicity, etc 7. Frequency calculation: Locating results in output file, displaying calculated properties through molecular viewing software such as Avogadro, MacMolPlt, VMD, GaussView, etc. 8. Calculate the energy of the H-like atoms (H, He+, C+5) using the Hartree-Fock method and the cc-pVnZ basis set series (n=D,T). Tabulate the energy (in Hartree) and 	

	<p>number of basis functions for each calculation. Compare your energy results with the exact value and discuss the effect of the number of basis functions. Discuss the effect of increasing nuclear charge on the energy.</p> <p>9. Perform optimization of malonaldehyde and obtain energy, dipole moment, charge on various atoms and important geometrical parameters such as bond length, bond angle, etc.</p> <p>10. Perform geometry optimizations (energy minimizations) to calculate the energy of various conformations of molecules (e. g. butane, and predict the most stable conformation.</p> <p>11. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.</p>	
<p>Textbooks:</p> <ol style="list-style-type: none"> 1. Molecular Quantum Mechanics, Atkins and Friedman, 5th Edition, Oxford University Press 2. Quantum Chemistry, McQuarrie, Viva Student Edition, Viva Press <p>Reference Books:</p> <ol style="list-style-type: none"> 1. Quantum Chemistry, AK Chandra 2. Introduction to Quantum Chemistry, Eyring, Walter and Kimball 3. Modern Quantum Chemistry, Szabo 		

Semester IV – Magnetic Resonance Spectroscopy and Analytical Techniques – 45 h

Unit	Content	Contact Hrs
Unit I: NMR spectroscopy	Nuclear Spin quantum number, effect of magnetic field on the nuclear spin, Zeeman effect and nuclear agneton, and Larmor Precision. Radiowaves and principles of NMR spectroscopy. Chemical shift and factors affecting it. Factors affecting intensity and spectral width. NMR peak area integration relative peak positions of organic functional groups eg. alkyl halides, olefins, alkynes, aldehyde H, substituted benzenes (toluene, anisole, 15 nitrobenzene, halobenzene, dinitrobenzenes, chloronitrobenzene), first order coupling (splitting of the signals: ordinary ethanol, bromoehane, dibromoehanes), Spin-spin coupling and high resolution spectra, interpretation of PMR spectra of simple organic molecules like methanol, ethanol, acetaldehyde, acetic acid and aromatic protons.	12
Unit II:	Electron Spin Resonance and hyperfine splitting. G value and	5

ESR spectroscopy	hyperfine constant, Bohr magneton Electron Zeeman splitting, electron nuclear hyperfine splitting, illustration using simple examples like H atom, methyl radical etc.	
Unit III: Mass Spectrometry	Ionization techniques (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Interpretation of the mass spectrum, base peak and molecular ion peak. Fragmentation patterns of Common organic molecules along with McLafferty rearrangement. Determination of empirical chemical formula from molecular ion peak and isotopic distribution.	8
Unit IV: Separation techniques	Introduction to Chromatography and its techniques, TLC, Column Chromatography, GC and HPLC.	5
Unit V: Electroanalytical Techniques	Conductance measurements and EMF and Cell Reactions. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Conductometric titrations (only acid-base and acid base mixtures). Types of electrodes, standard electrode potential, cell reactions and salt bridges Glass electrodes and others, concentration cells with transference and without transference, liquid junction potential and salt bridge, pH determination using hydrogen electrode and quinhydrone electrode, Potentiometric titrations-qualitative treatment (acid- base, acid mixture and base and oxidation-reduction only). Zeta potential.	10
Unit VI: Diffraction	Packing of solids and how solids diffract (reflection view and scattering view) Bragg's Law, Miller indices and Reciprocal lattices. Laws of Crystallography. Basics of X-ray diffraction (powder and single crystal).	5
Laboratory experiments	<ol style="list-style-type: none"> 1. Determination of cell constant of a conductivity cell. 2. Determine the equivalent conductance of a strong electrolyte (e.g. NaCl) at various concentrations and verify the Onsager equation. 3. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid. 4. Perform the following conductometric titrations: <ol style="list-style-type: none"> a. Strong acid vs. strong base b. Weak acid vs. strong base c. Mixture of strong acid and weak acid vs. strong base 	

	<p>d. Strong acid vs. weak base</p> <p>2. Perform the following potentiometric titrations:</p> <ul style="list-style-type: none"> i) Strong acid vs. strong base ii) Weak acid vs. strong base iii) Dibasic acid vs. strong base iv) Potassium dichromate vs. Mohr's salt <p>3. Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step</p> <p>4. Structure elucidation from simple proton NMR spectrum, MS.</p> <p>5. Separation of organic compounds using TLC, CC.</p>	
<p>Books</p> <ol style="list-style-type: none"> 1. NMR Spectroscopy by Kemp 2. NMR Spectroscopy by Gunther 3. Physical Methods in Inorganic Chemistry, Drago 4. Electroanalytical methods, Bard and Faulkner 		

Inorganic Chemistry-Semester –V (45 h)

Unit	Content	Contact Hrs
Unit I: Coordination Chemistry IV	<p>Electronic spectra and magnetism of coordination compounds: Microstates, Free Ion term symbols and their splitting in tetrahedral and octahedral field, Racah parameters, Selection rules and relaxation mechanism (vibronic coupling and spin orbit coupling), Orgel Diagrams and prediction of spectral transitions, Jahn-Teller effect on electronic spectra, Charge-Transfer spectra, Calculation of spin only and orbital contribution to magnetic moments. Spin crossover.</p>	12

<p>Unit II: Main Group elements</p>	<p>Relative stability of different oxidation states, Inert pair effect, diagonal relationship, and anomalous behaviour of main group elements.</p> <p>a) Preparation and properties of Ortho and Para hydrogen</p> <p>b) Preparation, structure and properties of borane (bonding in diborane, brief idea of styx number, wade's rule), boric acid, borax, borazine, phosphazine, S₄N₄,</p> <p>c) Preparation and properties of oxides, superoxides, peroxides, hydrides, hydroxides, halides and carbonates of alkali and alkaline earth metals. Reactions of alkali and alkaline earth metals with liquid ammonia.</p> <p>d) Allotropes of carbon, phosphorus, and sulphur.</p> <p>e) Oxides and oxoacids of nitrogen, phosphorus, sulphur, and chlorine.</p> <p>g) Interhalogen compounds, polyhalides, pseudo halogen</p> <p>i) Hydrates, clathrates and inclusion compounds</p> <p>j) Preparation, structure and properties of silicates, aluminosilicates.</p>	<p>15</p>
<p>Unit III: Noble Gases</p>	<p>Occurrence and uses, rationalisation of inertness of noble gases, Clathrates; preparation and properties of XeF₂, XeF₄ and XeF₆; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF₂). Molecular shapes of noble gas compounds (VSEPR theory).</p>	<p>6</p>
<p>Unit IV: Organometallics I</p>	<p>Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands, 18 electron rule.</p> <p>Metal carbonyls: Electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series.</p> <p>General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series.</p> <p>Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni -acceptor behaviour of CO (MO diagram of CO to be discussed), synergic bonding effect and use of IR data to explain the extent of back bonding.</p> <p>Zeise's salt: Preparation and structure, evidence of synergic effect and comparison of synergic effect with that in carbonyls.</p>	<p>12</p>

Lab Inorganic quantitative analysis	<p>Estimation by volumetric method of any one of the following :</p> <p>a. Fe(III)- By standard KMnO_4 solution b. Fe(III) – By standard $\text{K}_2\text{Cr}_2\text{O}_7$ solution c. Cu(II) – By Iodometric method. d. Ni(II) by gravimetric method</p> <p>This should be followed by separation and estimation of individual ions in two-component systems of</p> <p>a. Cu and Fe b. Fe and Ca c. Ca and Mg d. Cu and Ni and e. Cl^- and SO_4^{2-}.</p>	
---	--	--

Semester V - (Organic Chemistry) – 45 h

Unit	Content	Contact Hrs
Unit I: Formation of carbon-carbon and carbon-heteroatom bonds:	Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions; Saytzeff and Hofmann eliminations; Reagents of phosphorus, sulfur and boranes; Stereospecific and stereoselective reactions; Stereoselective reactions of alkenes: Epoxidation reaction using mCPBA.	10
Unit II: Reactions of active methylene compounds	Active methylene compounds (Keto-enol tautomerism): Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.	10
Unit III: Reactions of Enolates and Enamines	Formation and stability of enolates and enamines; Alkylation of enolates and enamines; The Aldol reaction; Aldol and Benzoin condensation, Claisen reaction, Claisen-Schmidt reaction, Knoevenagel condensation, Perkin reaction; Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements; Addition reactions of unsaturated carbonyl compounds; Michael addition.	10
Unit IV: Nucleophilic reactions on the C=O groups	Nucleophilic attack at the carbonyl group (geometrical aspects); Concept of Prochirality; Stereoselective additions to carbonyl groups: Cram's rule, Felkin-Anh model.	6

Unit V: Carbohydrate chemistry	Classification of monosaccharides; Absolute configuration of glucose and fructose, Epimers and Anomers; Mutarotation; Determination of ring size of glucose and fructose; Conformations of glucose (Fischer, Haworth and Stereoscopic projections); Interconversions of aldoses and ketoses; Killiani Fischer synthesis and Ruff degradation; Disaccharides: Structure elucidation of maltose, lactose and sucrose. Polysaccharides – Structures of starch, cellulose and glycogen.	9
Laboratory experiments:	<ol style="list-style-type: none"> 1. Qualitative Analysis of Carbohydrates: Aldoses and ketoses, reducing and non-reducing sugars. 2. (a) Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, phenols, amines, carboxylic acids and carbonyl compounds). (b) Interpretation of infrared (IR) spectra of simple organic compounds: The student is required to learn about Identification of functional groups of simple organic compounds by interpreting the IR spectra. The spectra may be recorded and/or provided to the students from literature. 	30

Semester V – Reaction Dynamics – 45 h

Unit	Content	Contact Hrs
Unit I: Kinetics I	Order and molecularity of reactions. Rate laws and rate equations for zero, first and second order reactions ($2A \rightarrow P$, $A+B \rightarrow P$): their derivations, graphical representations and examples. Expressing the rate laws in terms of volume and pressure of reactants. Experimental determination of order of reactions (half-life method and initial rate method). Temperature dependence of reaction rate, energy of activation (its connection to Gibbs free energy). Arrhenius equation, energy of activation. Pre-exponential Factor and failure of Arrhenius Equation.	9

<p>Unit II: Kinetics II</p>	<p>Difference between equilibrium and steady state. Limiting reagents, rate-determining step and steady-state approximation – explanation with suitable examples (eg. dissociation of HBr and acetaldehyde). Opposing reactions, consecutive reactions and parallel reactions (with examples and explanation of kinetic and thermodynamic control of products; all steps first order). Idea on explosive reactions. Enzyme catalysis: Derivation of Michaelis-Menten equation and interpretation of Lineweaver-Burk Plots. Eadie- Hofstee plot. Turn-over number. Oscillating reactions.</p>	<p>14</p>
<p>Unit III: Reaction Dynamics</p>	<p>Collision theory (detailed treatment). Modeling the Preexponential factor. Sphere of influence and collision cross section, Equivalence between Arrhenius and Collision theory. Failure of Collision theory. Physical interpretation of reaction co-ordinates and potential energy surfaces. Activated complex theory (detailed treatment). Thermodynamic formulation and derivation of Eyring equation. Evaluation of Arrhenius pre-exponential factor from transition state theory. Common examples where transition states have been experimentally identified or predicted.</p> <p>Chemically and Diffusion controlled reactions with examples. Primary and secondary salt effects with examples.</p> <p>Derivation of Bronsted-Bjerrum Equation and its graphical representation. Lindemann and Hinshelwood theory of unimolecular reaction and graphical representation.</p>	<p>22</p>

Lab	<ol style="list-style-type: none"> 1. Determine the rate constant of the acid catalysed hydrolysis of methyl acetate. 2. Determine the rate constant of saponification of ethyl acetate. 3. Determine the activation energy of the hydrolysis of methyl acetate catalyzed by hydrochloric acid. 4. Verify the Freundlich isotherm for the adsorption of oxalic acid on activated charcoal. 5. Verify the Langmuir isotherm for the adsorption of acetic acid on activated charcoal. <p>Determine the critical micelle concentration of a surface-active agent by surface tension measurements.</p> <ol style="list-style-type: none"> 6. Study the kinetics of the Iodide-persulphate reaction by Initial rate method. 7. Theory and computer aided linear curve-fitting techniques (eg. first order kinetics using least squares) and evaluation of errors and standard deviations.
<p>Text Books:</p> <ol style="list-style-type: none"> 1. Atkins' Physical Chemistry, Atkins, de Paula and Keeler 2. Chemical Kinetics and Reaction Dynamics, Paul L. Houston <p>Reference books:</p> <ol style="list-style-type: none"> 1. K. L. Kapoor, Volume V 2. Puri, Sharma, Pathania 3. Physical Chemistry: P C Rakshit 4. Physical Chemistry: A Molecular Approach by McQuarrie and Simon 5. Reference Book: Chemical Kinetics by Laidler. 	

Unit	Content	Contact Hrs
Unit I: Photochemistry:	Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence. Beer-Lambert law (for solids and liquids) and limitations; quantum yield and its measurement for a photochemical process, actinometry. Photostationary state. Photosensitized reactions (with examples). Jablonski Diagram, Internal Conversion, Intersystem Crossing, Fluorescence and Phosphorescence. Primary and secondary processes in photochemical reactions. Frank Condon Principle.	10
Unit II: Spectroscopy	Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Absorption Cross section and Einstein's Coefficients. Difference between atomic and molecular spectra. Born- Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components. Factors affecting intensities and width of spectral lines. Microwave (pure rotational) spectra of diatomic molecules. Selection rules and transition dipole moment. Structural information derived from rotational spectroscopy. IR Spectroscopy: Selection rules, IR spectra of diatomic molecules and organic compounds having functional group. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies. Electronic Spectroscopy: Electronic excited states. Free electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts. Woodward-Fieser Rules, Qualitative treatment of Rotational Raman effect; Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. (35)	35

1. Calculate the rotational constant, B, for N₂, F₂, O₂ via quantum chemistry calculations.
2. Calculate the optimum bond length by hand from the rotational constant via the rigid rotor approximation for a diatomic molecule.
3. Perform a series of single point calculations above and below re to generate a potential energy surface (PES). Perform a frequency calculation on the optimized geometry. Use the resulting fundamental frequency, ν_0 , to calculate the force constant of the bond, k.
4. Study the 200-500 nm absorbance spectra of KMnO₄ and K₂Cr₂O₇ (in 0.1 M H₂SO₄) and determine the λ_{\max} values. Calculate the energies of the two transitions in different units (J molecule⁻¹, kJ mol⁻¹, cm⁻¹, eV).
5. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K₂Cr₂O₇.
6. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
7. Analysis of the given vibration-rotation spectrum of HCl(g).
8. Verify Lambert-Beer's law and determine the concentration of CuSO₄/KMnO₄/K₂Cr₂O₇ in a solution of unknown concentration
9. Determine the concentrations of KMnO₄ and K₂Cr₂O₇ in a mixture.
10. Study the kinetics of iodination of propanone in acidic medium.
11. Determine the amount of iron present in a sample using 1,10-phenanthroline.
12. Determine the dissociation constant of an indicator (phenolphthalein).
13. Study the kinetics of interaction of crystal violet/phenolphthalein with sodium hydroxide.

Books:

1. Spectroscopy, Banwell
2. Introduction to Molecular Spectroscopy: Barrow
3. Quantum Chemistry and Spectroscopy, Engel and Reid
4. Atomic and Molecular Spectroscopy; Rita Kakkar
5. Molecular Spectroscopy, Hollas

Unit	Content	Contact Hrs
Unit I Coordination Chemistry -V	<p>Introduction to inorganic reaction mechanisms. Stepwise and overall formation constants, the chelate effect, Thermodynamic and kinetic stability of complexes, chelate effect and its applications in analytical chemistry and biology.</p> <p>Substitution reactions in octahedral complexes, effect of acid and bases on substitution reaction of octahedral complexes, factor affecting the substitution reaction.</p> <p>Substitution reaction of square planar complexes, Trans-effect, theories of trans effect, Trans effect in synthesis of square planar complexes,</p> <p>Electron transfer reactions (elementary ideas only)</p>	12
Unit II Organometallics II	<p>Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicenter bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.</p> <p>Metal alkenes, alkynes and allyls: Synthesis, Structure and Bonding</p> <p>Metal carbene: Synthesis, Structure and Bonding</p> <p>Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene</p> <p>Fundamentals of organometallic reactions: oxidative addition, reductive elimination, insertion and elimination reaction</p> <p>Transition Metals in Catalysis Study of the following industrial processes and their mechanism: Alkene hydrogenation (Wilkinson's Catalyst), Hydroformylation (Co catalysts), Wacker Process, Synthetic gasoline (Fischer Tropsch reaction)</p>	18
Unit III Bioinorganic Chemistry	<p>Essential and trace metals in biology, Effect of deficiency of some metal ions (). Toxic effect of metal ions (Fe, Cu, Hg, Pb, Cd and As), Chelate therapy, Cisplatin as anticancer drug.</p> <p>Storage and transport of iron, active transport of ions (Sodium - potassium pump)</p> <p>Active site structure and function of Haemoglobin (cooperativity and Bohr effect), Myoglobin, Hemocyanin, Hemerythrin, Rubredoxin, Ferredoxin (Fe₂S₂, Fe₄S₄), Cytochrome P450, Superoxide dismutase, carbonic anhydrase and carboxypeptidase, Nitrogenase enzyme, V-B12</p>	15

Inorganic lab III Inorganic Preparation	<p>Following compounds should be prepared and test the presence of ions qualitatively. IR and UV-Visible spectra of these complexes should be recorded, interpreted and discussed.</p> <p>i) Preparation of Mohr's Salt, chrome alum and potash alum</p> <p>ii) Cis and trans $K[Cr(C_2O_4)_2 \cdot (H_2O)_2]$ Potassium dioxalatodiaquachromate (III)</p> <p>iii) Potassium tris(oxalato)ferrate(III)</p> <p>iv) Vanadyl bis(acetylacetonate)</p> <p>v) Cu(thiourea) complex</p> <p>vi) Acetylation of ferrocene and purification of mono and bis derivatives by column chromatography.</p>	30
--	---	----

Semester VI - (Organic Chemistry) – 45 L

Unit	Content	Contact Hrs
Unit I: Photochemistry	Electron excitation in organic molecules (alkenes and carbonyl compounds); Fate of electronically excited molecules; Singlet and Triplet states; Photoreduction of carbonyl compounds; Photoaddition of alkenes to carbonyl compounds (Paterno-Biichi reaction); Photoaddition of alkenes to aromatic compounds; Photorearrangement (Cis-trans isomerization, Intramolecular cyclization of dienes); Photochemical fragmentation (Photolysis of carbonyl compounds: Norrish Type I and Type II reactions).	10
Unit II: Terpenes	Occurrence of terpenes; Structure and Classification, Isoprene rule; Elucidation of structure; Synthesis of Citral, Neral and α -terpineol; Biosynthesis of limonene, pinene, carvone (via Isopentenyl pyrophosphate).	5
Unit III: Pericyclic reactions	Cycloadditions: General description of the Diels–Alder reaction; Frontier orbital description of (4+2) cycloadditions; Regioselectivity in Diels–Alder reactions; Woodward–Hoffmann description of the Diels–Alder reaction; Photochemical [2 + 2] cycloadditions; Thermal [2 + 2] cycloadditions. Sigmatropic reactions: Conditions for sigmatropic reactions Orbital descriptions of [3,3]-sigmatropic rearrangements; Cope rearrangement Electrocyclic reactions: Conditions for (4n+2) and (4n) electrocyclic reactions; Conrotatory and disrotatory reactions	15
Unit IV:	Overview of structure and reactivity of Organolithium,	15

Organometallic Chemistry	Organomagnesium, Organocopper, Organozinc, and Organoboron reagents; General methods of preparation: Deprotonation, Metal-halogen exchange, Transmetallation; Directed metallation.	
Laboratory experiments:	<ol style="list-style-type: none"> 1. Extraction of D-limonene from orange peel by the conventional method/ using liquid CO₂ prepared from dry ice. 2. Extraction of caffeine from tea leaves. 3. Photoreduction of benzophenone to benzopinacol in the presence of sunlight/UV irradiation. 4. Organic estimations: (any three): <ol style="list-style-type: none"> (i). Estimation of glycine by Sorenson's formalin method. (ii). Study of the titration curve of glycine (by pH metric methods). (iii). Determination of Iodine number of an oil/ fat. (iv). Saponification value of an oil or a fat. 	30
Recommended textbooks:		
<ol style="list-style-type: none"> 1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7th Edition (Wiley) 2. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2nd Edition (Oxford) 3. Reaction Mechanism in Organic Chemistry, S. M. Mukherji, S. P. Singh 3rd Edition (Macmillan) 4. Organic Reactions and their Mechanisms, P. S. Kalsi 5. Organic Chemistry, Maitland Jones, Jr., Steven A. Fleming 5th Edition (Norton) 		

Semester VI - Physical Chemistry – 45 h

Unit	Content	Contact Hrs
Unit I: Chemical Equilibria	Equilibrium of homogeneous and heterogeneous systems. Law of mass action, derivation of expression of equilibrium constants; temperature, pressure and concentration dependence of equilibrium constants (K_p , K_c , K_x), their applications. Le Chatelier's principle of dynamic equilibrium and its applications.	5
Unit II: Ionic equilibria	Introduction to Ionic equilibrium. Ionic Product. Common ion effect: its application. Acid Base Equilibria. Dissociation constants of mono and dibasic acids. pH scale, pH of very dilute and very concentrated solutions. Concept of strengths of	10

	<p>solutions (molarity, normality and molality, difference between mass of a substance and amount of a substance). Calculation of strengths of acid and basic mixtures. pH titration curves of acid mixtures, salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions and derivation of Henderson-Hasselbalch equation (for mono and dibasic acids). Solubility and solubility product of sparingly soluble salts – applications of solubility product principle with special reference to inorganic group separation. Explanation of Inorganic Group Separation Table using Le Chatelier's principle, solubility product and common ion effect.</p>	
<p>Unit III: Phase Equilibria</p>	<p>Definitions of phase, component and degrees of freedom. Gibb's phase rule and its derivations.</p> <p>Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications.</p> <p>Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.</p> <p>Fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation.</p> <p>Nernst distribution law. Solvent extraction.</p>	15
<p>Unit IV: Electrochemistry</p>	<p>Conductivity, equivalent and molar conductivity and their properties; Kohlrausch law; Debye-Huckel Theory, Debye-Huckel Limiting Law, Debye Hückel Onsager equation (no derivation required); Ionic velocities, mobilities, transference numbers and its experimental determination using Hittorf and moving boundary methods; Applications of conductance measurement; Quantitative aspects of Faraday's laws of electrolysis, applications of electrolysis in metallurgy and industry; Electrolytic and galvanic cells, Electromotive force of a cell, Nernst equation; Standard electrode potential, Electrochemical series; Concentration cells with and without transference; Applications of EMF measurements including potentiometric titrations.</p> <p>Electrochemistry behind standard Pb Batteries and Li-ion batteries.</p>	15
<p>Laboratory experiments:</p>	<ol style="list-style-type: none"> pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base. Determination of dissociation constant of a weak acid. <ol style="list-style-type: none"> Determination of critical solution temperature 	30

	<p>and composition of the phenol-water system and to study the effect of impurities on it.</p> <ol style="list-style-type: none"> 2. Determine the transition temperature of a salt hydrate. 3. Construction of phase diagram (freezing point curve) using ignition tube method for two- component simple eutectic system. 4. Construction of phase diagram (freezing point curve) using ignition tube method for two- component congruently melting compound forming system. 5. Study the distribution of iodine between water and kerosene/carbon tetrachloride. 6. Determine the association factor of benzoic acid in benzene by distribution of benzoic acid between water and benzene. 7. Determine the vapour pressure of water at different temperatures and hence evaluate the enthalpy of vaporization of water. 8. Determine the equilibrium constant of the $I_2(aq) + KI \rightarrow KI_3(aq)$ system by the distribution method. Hence determine the concentration of the KI solution. 9. Determine the partition coefficient of ammonia between water and chloroform and also determine the formula of copper-ammonia complex. 10. Study of the solubility of benzoic acid in water and determination of ΔH. 	
<p>Books</p> <ol style="list-style-type: none"> 1. Physical Chemistry: Atkins 2. Puri, Sharma, Pathania 3. Physical Chemistry: Berry Rice and Ross 4. Physical Chemistry: PC Rakshit 5. Reference Book: Bockris and Reddy Volume I (Ionics) 		

Semester VI: Industrial Chemistry (45 h)

Units	Content	Contact Hrs
Unit I: Industrial Gases and Common Inorganic Chemicals	<p>Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, helium, hydrogen, acetylene, chlorine, phosgene.</p> <p>Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, bleaching powder, hydrogen peroxide, potash alum, and potassium permanganate.</p>	9

Unit II: Silicate Industries	<p>Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, coloured glass, photosensitive glass.</p> <p>Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, semiconducting Oxides.</p> <p>Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.</p>	8
Unit III: Fertilizers	Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.	6
Unit IV: Surface Coatings	Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments- formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.	8
Unit V: Alloys	Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture composition and properties of different types of steels (stainless steel, Ni-steel, Cr-steel) Brass, Bronze and Cu-Ni alloy.	6
Unit VI: Catalysis	Catalysts and their industrial applications, Deactivation or regeneration of catalysts. Phase transfer catalysts, application of zeolites as catalysts.	4
Unit VII: Pyrotechn ics and Propellant s	Firecrackers- composition and effect, Fire Extinguishers-types and use, Car Airbag chemistry, Introduction to rocket propellants.	4

Lab	<ol style="list-style-type: none"> 1. Determination of free acidity in ammonium sulphate fertilizer. 2. Estimation of Calcium in Calcium ammonium nitrate fertilizer. 3. Estimation of phosphoric acid in superphosphate fertilizer. 4. Electroless metallic coatings on ceramic and plastic material. 5. Determination of composition of dolomite (by complexometric titration). 6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples. 7. Analysis of Cement. 8. Preparation of pigment (zinc oxide). 	30
Text Books and Reference Books	<ol style="list-style-type: none"> 1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK. 2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi. 3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi. 4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi. 5. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi. 6. R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi B. K. Sharma: Engineering Chemistry, Goel Publishing House, Meerut 	