

DEPARTMENT OF CHEMISTRY

FACULTY OF NATURAL SCIENCES



JAMIA MILLIA ISLAMIA
(A Central University)

B.Sc.Hons CHEMISTRY
Effective from Academic Year 2017-2018

Syllabus of Courses Offered
Core courses, Elective Courses and Ability Enhancement courses

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COURSE OUTLINE

Semester	Paper/ Practical	Paper No	Paper Code	Paper Title	Total Credits
Semester-I	Theory (Core)	I-H	BCH-101	Inorganic Chemistry-I	03
	Practical (Core)		BCH-101L	Inorganic Chemistry Practical-I	01
	Theory (Core)	II-H	BCH-103	Physical Chemistry-I	03
	Practical (Core)		BCH-103L	Physical Chemistry Practical-I	01
	Theory (Elective)	III-H	BCH-104	Industrial Chemicals & Environment	03
	Practical (Elective)		BCH-104L	Industrial Chemicals & Environment Practical	01
Semester-II	Theory (Core)	IV-H	BCH-202	Organic Chemistry-I	03
	Practical (Core)		BCH-202L	Organic Chemistry Practical-I	01
	Theory (Core)	V-H	BCH-203	Physical Chemistry-II	03
	Practical (Core)		BCH-203L	Physical Chemistry Practical-II	01
	Theory (Elective)	VI-H	BCH-204	Polymer Chemistry	03
	Practical (Elective)		BCH-204L	Polymer Chemistry Practical	01
Semester-III	Theory (Core)	VII-H	BCH-301	Inorganic Chemistry-II	03
	Practical (Core)		BCH-301L	Inorganic Chemistry Practical-II	01
	Theory (Core)	VIII-H	BCH-302	Organic Chemistry-II	03
	Practical (Core)		BCH-302L	Organic Chemistry Practical-II	01
	Theory (Core)	IX-H	BCH-303	Physical Chemistry-III	03
	Practical (Core)		BCH-303L	Physical Chemistry Practical-III	01
	Theory (Ability Enhancement)	X-H	BCH-305	Inorganic Materials of Industrial Importance	03
Semester-IV	Theory (Core)	XI-H	BCH-401	Inorganic Chemistry-III	03
	Practical (Core)		BCH-401L	Inorganic Chemistry Practical-III	01
	Theory (Core)	XII-H	BCH-402	Organic Chemistry-III	03
	Practical (Core)		BCH-402L	Organic Chemistry Practical-III	01
	Theory (Core)	XIII-H	BCH-403	Physical Chemistry-IV	03
	Practical (Core)		BCH-403L	Physical Chemistry Practical-IV	01
	Theory (Elective)	XIV-H	BCH-404	Green Chemistry	03
	Practical		BCH-404L	Green Chemistry Practical	01
Semester-V	Theory (Core)	XV-H	BCH-501	Inorganic Chemistry-IV	03
	Practical (Core)		BCH-501L	Inorganic Chemistry Practical-IV	01
	Theory (Core)	XVI-H	BCH-502	Organic Chemistry-IV	03
	Practical (Core)		BCH-502L	Organic Chemistry Practical-IV	01
	Theory (Core)	XVII-H	BCH-503	Physical Chemistry-V	03
	Practical (Core)		BCH-503L	Physical Chemistry Practical-V	01
	Theory (Elective)	XVIII-H	BCH-504	Molecular Modeling and Drug Design	03
	Practical (Elective)		BCH-504L	Molecular Modeling and Drug Design Practical	01
Semester-VI	Theory (Core)	XIX-H	BCH-601	Inorganic Chemistry-V	03
	Practical (Core)		BCH-601L	Inorganic Chemistry Practical-V	01
	Theory (Core)	XX-H	BCH-602	Organic Chemistry-V	03
	Practical (Core)		BCH-602L	Organic Chemistry Practical-V	01
	Theory (Core)	XXI-H	BCH-603	Physical Chemistry-VI	03
	Practical (Core)		BCH-603L	Physical Chemistry Practical-VI	01
	General Viva				04
Total Credits					88

Paper code – 1st letter for semester, 2nd and 3rd for subject as mentioned below:-

01- Inorganic Chemistry, 02- Organic Chemistry, 03- Physical Chemistry, 04- Elective, 05- Ability Enhancement

Inorganic Chemistry-I

Unit I Atomic Structure

Bohr's theory; its limitations and atomic spectrum of hydrogen atom; Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2 . Quantum numbers and their significance. Sign of wave functions. Radial and angular wave functions for hydrogen atom; Radial and angular distribution curves; Shapes of *s*, *p*, *d* and *f* orbitals. Contour boundary and probability diagrams; Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Unit II Periodicity of Elements

s, *p*, *d*, *f* block elements, the long form of periodic table; Discussion of following properties with reference to *s* and *p*-block elements: Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.; Atomic radii (van der Waals) Ionic and crystal radii; Covalent radii (octahedral and tetrahedral; Ionization enthalpy; Successive ionization enthalpies and factors affecting ionization energy; Applications of ionization enthalpy; Electron gain enthalpy; trends of electron gain enthalpy. Electronegativity, Pauling's/Mulliken's/Allred-Rachow's and Mulliken-Jaffé's electronegativity scales; Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity; Sanderson's electron density ratio.

Unit III Chemical Bonding and Molecular Structure

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy. *Covalent bond*: Lewis structure, 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 diatomic and simple polyatomic molecules N_2 , O_2 , C_2 , B_2 , F_2 , CO , NO , and their ions; HCl , BeF_2 , CO_2 , (idea of *s-p* mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths. Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference. *Metallic Bond*: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

Unit IV Oxidation-Reduction

Redox reactions, Standard Electrode Potential and its application to inorganic reactions, Oxidation state, rules for the determination of oxidation states, electrochemical series, applications of electrochemical series.

Reference Books

1. Lee, J.D., Concise Inorganic Chemistry, 5th edn., Blackwell Science, London.
2. Douglas, B.E. and McDaniel, D.H., *Concepts & Models of Inorganic Chemistry*, Oxford, 1970
3. Atkins, P.W. & Paula, J. *Physical Chemistry*, 10th Ed., Oxford University Press, 2014.
4. Day, M.C. and Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications, 1962.
5. Rodger, G.E., *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.

Inorganic Chemistry Practical -I

A. Titrimetric Analysis

- i. Calibration and use of apparatus
- ii. Preparation of solutions of different Molarity/Normality of titrants

B. Acid-Base Titrations

- i. Estimation of carbonate and hydroxide present together in mixture.
- ii. Estimation of carbonate and bicarbonate present together in a mixture.
- iii. Estimation of free alkali present in different soaps/detergents

C. Oxidation-Reduction Titrimetry

- i. Estimation of Fe(II) and oxalic acid using standardized KMnO_4 solution.
- ii. Estimation of oxalic acid and sodium oxalate in a given mixture.
- iii. Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

Reference Books

1. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis 6th Ed.*, Pearson, 2009.
2. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.

Physical Chemistry-I

Unit I. Gaseous State

Gas laws, Ideal gas equation, Dalton's law of partial pressure, Graham's law of diffusion, Postulates of kinetic theory of gases, Kinetic gas equation. Deviation from ideal behavior: Effect of temperature and pressure. Maxwell's distribution of molecular velocities: Root mean square, Average and Most probable velocities. Collision properties: Collision number, Mean free path, Collision diameter and Collision frequency. Liquefaction of gases. Critical Phenomena: PV isotherms of real gases, Continuity of states, van der Waals equation, Isotherms of van der Waals equation, Relationship between critical constants and van der Waals constants, Law of corresponding states, Reduced equation of state.

Unit II. Liquid State

Description of liquids, Structural differences between solids, liquids and gases, Intermolecular forces. Variation of vapour pressure of liquids with temperature and Trouton's rule. Liquid Crystals, Vapour pressure-Temperature diagram, Classification of liquid crystals, Difference between liquid crystals. Structure of Smectic, Nematic and Cholesteric liquid crystals.

Unit III. Solid State

Crystalline and Amorphous solid, Symmetry of crystal systems, Space lattice and Unit cell, Summary of crystal systems, Applications of crystallographic studies; Packing fraction, Density of crystalline solid, Coordination number, Number of atoms in unit cell. Law of rational indices, Inter-planar spacing. X-ray diffraction, Bragg's equation. Powder method, Determination of Grain size using X-ray line broadening studies (Scherrer's formula), The Rotating crystal method. Determination of crystal structure of NaCl using powder method.

Unit IV. Ionic Equilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization. Acid-base concept. Dissociation constants of weak acids and weak bases. Ionization constant and Ionic product of water. The pH scale, Buffer solutions, Calculations of pH values of buffer mixtures, Derivation of Henderson equation and its applications, buffer capacity and buffer action. Salt hydrolysis, Determination of hydrolysis constant, degree of hydrolysis and pH for different salts. Relation between K_h , K_a and K_b . Solubility and solubility product of sparingly soluble salts ó Applications of solubility product principle and Common ion effect.

Books Recommended:

1. Essentials of Physical Chemistry, B.S. Bahl, G.D.Tuli and Arun Bahl, S. Chand & Company Ltd.
2. A Text Book of Physical Chemistry, A.S. Negi and S.C. Anand, New Age International Publishers.
3. Physical Chemistry, G. M. Barrow, International Student Edition, McGraw Hill.
4. Physical Chemistry through Problems, S. K. Dogra and S. Dogra Wiley Eastern Ltd.
5. Physical Chemistry, P. W. Atkins, & J. de Paula, 10th Ed., Oxford University Press (2014).

Physical Chemistry Practical -I

1. Surface tension measurements.

- Determine the surface tension of given solution using drop number method.
- Study the variation of surface tension of detergent solutions with concentration.

2. Viscosity measurement using Ostwald's viscometer.

- Determination of viscosity of (i) ethanol (ii) amyl alcohol and (iii) aqueous solution of sugar at room temperature.
- Study the variation of viscosity of sucrose solution with the concentration of solute.

3. Indexing of a given powder diffraction pattern of a cubic crystalline system.

4. pH metry

- Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
- Preparation of buffer solutions of different pH
 - Sodium acetate-acetic acid
 - Ammonium chloride-ammonium hydroxide
- pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
- Determination of dissociation constant of a weak acid.

5. Any other experiment carried out in the class.

Reference Books

- O.P. Pandey, D.N. Bajpai & S. Giri, Practical Chemistry, S. Chand & Company Ltd.
- B. D. Khosla, V. C. Garg & A. Gulati, *Senior Practical Physical Chemistry*, S. Chand & Co.: New Delhi (2011).
- C. W. Garland, J.W. Nibler, & D.P. Shoemaker, *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- A.M. Halpern & G.C. McBane, *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

Industrial Chemicals and Environment

Unit I Industrial Gases and Inorganic Chemicals

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

Industrial Metallurgy: Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

Unit II: Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur. Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution. Pollution by SO₂, CO₂, CO, NO_x, H₂S, and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures. Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Unit III Water Pollution

Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

Unit IV Energy & Environment

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion/Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc. Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management. Biocatalysis: Introduction to biocatalysis: Importance in Green Chemistry and Chemical Industry.

Reference Books

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. J.A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
4. S.S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
5. K. De, Environmental Chemistry: New Age International Pvt., Ltd, New Delhi.
6. S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi.
7. S.E. Manahan, Environmental Chemistry, CRC Press (2005).
8. A. Mishra, Environmental Studies. Selective and Scientific Books, New Delhi (2005).

Industrial Chemicals & Environment Practical

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO_3 and potassium chromate).
6. Estimation of total alkalinity of water samples (CO_3^{2-} , HCO_3^-) using double titration method.
7. Measurement of dissolved CO_2 .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

Reference Books

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. J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
5. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
6. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.

Organic Chemistry-I

Unit-I Basic Concepts of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values.

Unit-II Stereochemistry

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis/trans and, syn-anti isomerism E/Z notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

Unit-III Chemistry of Aliphatic Hydrocarbons

Carbon-Carbon sigma bonds: Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity. Carbon-Carbon pi bonds: Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations. Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroborationoxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation (oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene. Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

Unit-IV Cycloalkanes and Aromatic Hydrocarbons

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane: Chair, Boat and Twist boat forms; Relative stability with energy diagrams.

Hückel's rule; aromatic character of arenes; cyclic carbocations/carbanions and heterocyclic compounds with suitable examples; Electrophilic aromatic substitution: halogenation; nitration; sulphonation and Friedel-Craft's alkylation/acylation with their mechanism; Directing effects of the groups.

Reference Books

1. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
3. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.
5. Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.
6. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition,

Organic Chemistry Practical-I

1. Purification of organic compounds by crystallization using the following solvents:
 - a. Benzoic acid from Water
 - b. *m*-Dinitrobenzene from Alcohol
 - c. Phenylbenzoate from Alcohol-Water
2. Determination of the melting points of above compounds and unknown organic compounds.
3. Determination of boiling point of liquid compounds by capillary method.
4. Preliminary examination and determination of the functional groups:
 - (A) Carboxylic acid: Formic acid, acetic acid,
 - (B) Phenols: Phenol, *o*-cresol, *m*-cresol, *p*-cresol, α -naphthol, β -naphthol
 - (C) Aldehydes: Formaldehyde, Acetaldehyde, Benzaldehyde
 - (D) Ketones: Acetone, Acetophenone, Benzophenone
 - (E) Hydrocarbons: toluene, naphthalene, benzene, diphenyls

Reference Books

1. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

Physical Chemistry-II

Unit I. Thermochemistry

Exothermic and endothermic reactions, Heats of reactions, standard states, relation between heat of reaction at constant volume (q_v) and at constant pressure (q_p), Heat capacity, relation between C_p and C_v , laws of thermochemistry, enthalpy of formation, heat of solution and dilution, heat of neutralization, bond dissociation energy, bond energy and its calculation, concept of lattice energy, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions.

Unit II. Thermodynamics

Introduction: System, surroundings, intensive and extensive properties, isolated, closed and open systems; thermodynamic processes, state and path functions. First law of thermodynamics: Concept of heat (q), work (w), internal energy (U), and statement of first law; concept of Carnot cycle, calculations of q , w , U and H for reversible, irreversible and free expansion of gases under isothermal and adiabatic conditions. Second Law: Spontaneous process, Criteria of spontaneity, concept of entropy and statements of second law of thermodynamics, Calculation of entropy change for reversible and irreversible processes. Entropy change for isolated systems and entropy change in phase transitions. Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy from heat capacity data. Gibbs free energy and spontaneity; free energy and work function, variation of free energy with temperature and pressure. Gibbs-Helmholtz equation, Clausius-Clapeyron equation and Maxwell relations.

Unit III. Chemical Equilibrium

Reversible and irreversible reactions, Characteristics of chemical equilibrium, Formulation of equilibrium law, equilibrium law for ideal gases, relation between K_p and K_c and K_x . Reaction quotient, factors affecting the equilibrium constant. Equilibrium between gases and solids, equilibrium constant for a system of real gases, equilibrium constant of reactions in solution. Thermodynamic treatment of equilibrium constant. Variation of equilibrium constant with temperature, pressure and concentration, effect of inert gas on reaction equilibrium, Le Chatelier's principle.

Unit IV. Solutions and Colligative Properties

Methods of expressing concentrations of solutions, Dilute solution, colligative properties, Raoult's law, relative lowering of vapour pressure, Experimental method for measuring the lowering of vapour pressure, molecular weight determination. Osmosis, Law of osmotic pressure, determination of molecular weight from osmotic pressure. Elevation of boiling point and depression of freezing point, Thermodynamic derivation of relation between molecular weight and elevation in boiling point and depression in freezing point. Abnormal molar mass, degree of dissociation and association of solutes.

Books Recommended

2. Essentials of Physical Chemistry, B.S. Bahl, G.D. Tuli and Arun Bahl, S. Chand & Company Ltd.
6. A Text Book of Physical Chemistry, A.S. Negi and S.C. Anand, New Age International Publishers.
7. Physical Chemistry, G. M. Barrow, International Student Edition, McGraw Hill.
8. Physical Chemistry through Problems, S. K. Dogra and S. Dogra Wiley Eastern Ltd.
9. Physical Chemistry, P. W. Atkins, & J. de Paula, 10th Ed., Oxford University Press (2014).

Physical Chemistry Practical-II

1. Determination of the heat capacity of a calorimeter.
2. Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) of solution of salts.
3. To determine the enthalpy of neutralization of a weak acid / weak base versus strong base/ strong acid and determine the enthalpy of ionisation of the weak acid / weak base.
4. To determine the enthalpy of hydration of CuSO_4 .
5. To study of the solubility of benzoic acid in water and determination of H .
6. To determine the enthalpy of solution of solid calcium chloride and calculate the lattice energy of calcium chloride from its enthalpy data using Born Haber Cycle.
7. Verification of Hess's law by utilizing the enthalpy of neutralization of (i) $\text{HCl}(\text{aq})$, (ii) $\text{NaOH}(\text{s}) + \text{HCl}(\text{aq})$, and (iii) enthalpy of solution of $\text{NaOH}(\text{s})$ in water.
8. Determination of basicity 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.
9. Determination of the molar mass of the given solute by using Rast method.
10. **Any other experiment carried out in the class.**

Reference Books

1. O.P. Pandey, D.N. Bajpai & S. Giri, Practical Chemistry, S. Chand & Company Ltd.
2. B. D. Khosla, V. C. Garg & A. Gulati, *Senior Practical Physical Chemistry*, S. Chand & Co.: New Delhi (2011).
1. C. W. Garland, J.W. Nibler, & D.P. Shoemaker, *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
2. A.M. Halpern & G.C. McBane, *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

Polymer Chemistry

Unit-I Introduction and History of Polymeric Materials

History of polymers, polymers nomenclature: Based on sources and structure, Trade name and no names, classifications of polymers, linear, branched and cross linked polymers, molecular interactions, chemical bonding in polymers, texture of polymers,.

Unit-II Synthesis of Polymers

Polycondensation (step reaction polymerization), comparison between polymer type, mechanism of polycondensation. Ionic chain reaction (both cationic and anionic) and coordination polymerization, Free radical polymerization (addition).

Unit-III Characterization Polymers

Measurement of molecular weight of polymers (M_n, M_w , etc) by end group analysis, colligative property, light scattering technique, ultra centrifugation, gel permeation chromatography, Glass transition temperature (T_g) and determination of T_g , Factors affecting glass transition temperature (T_g).

Unit-IV Individual Polymers (Physical, Thermal and Mechanical Properties)

Brief introduction, preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride), poly(vinyl acetate), acrylic polymers, polyamides. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Platinum containing polymers, Ferrocene.

Reference Books

1. R.B. Seymour & C.E. Carraher: *Polymer Chemistry: An Introduction*, Marcel Dekker, Inc. New York, 1981.
2. G. Odian: *Principles of Polymerization*, 4th Ed. Wiley, 2004.
3. F.W. Billmeyer: *Textbook of Polymer Science*, 2nd Ed. Wiley Interscience, 1971.
4. P. Ghosh: *Polymer Science & Technology*, Tata McGraw-Hill Education, 1991.
5. R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*. Interscience Publishers, New York, 1967.

Polymer Chemistry Practical

A. Polymer synthesis

- i. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) Methyl Acrylate (MA) / Acrylic acid (AA).
- ii. Purification of monomer
- iii. Polymerization using benzoyl peroxide (BPO) / 2,2'-azobis-isobutyronitrile (AIBN)
- iv. Redox polymerization of acrylamide
- v. Precipitation polymerization of acrylonitrile
- vi. Preparation of urea-formaldehyde resin
- vii. Preparations of novalac resin/ resold resin.
- viii. Microscale Emulsion Polymerization of Poly(methylacrylate).

B. Polymer characterization

1. Determination of molecular weight by viscometry: Polyacrylamide-aq. NaNO₂ solution (Poly vinyl propylidene (PVP) in water.
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of head-to-head monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

C. Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. IR studies of polymers
4. DSC analysis of polymers
5. Preparation of polyacrylamide and its electrophoresis

Reference Books

1. M.P. Stevens, *Polymer Chemistry: An Introduction*, 3rd Ed., Oxford University Press, 1999.
2. H.R. Allcock, F.W. Lampe & J.E. Mark, *Contemporary Polymer Chemistry*, 3rd ed. Prentice-Hall (2003)
3. F.W. Billmeyer, *Textbook of Polymer Science*, 3rd ed. Wiley-Interscience (1984)
4. J.R. Fried, *Polymer Science and Technology*, 2nd ed. Prentice-Hall (2003)

Semester-II
Paper No: VII-H
Paper Code: BCH-301

UE = 75 marks
IA = 25 marks

Inorganic Chemistry- II

Unit I Group IV Elements

Comparative study of physical and chemical properties of these elements with special references to their oxides, hydrides, nitrides, sulphides and carbides, fluorocarbons, study of silicates (structural aspects only), silicones, allotropy, inert pair effect, metallic and non-metallic character, catenation and heterocatenation.

Unit II Group V Elements

Comparative study of the physical and chemical properties of these elements with special reference to their hydrides, oxides, halides, oxyhalides and sulphides, Oxoacids of nitrogen: nitrous acid, nitric acid, hyponitrous acid, hydrazoic acid, pernitric acid; oxoacids of phosphorus: orthophosphorous acid, metaphosphorous acid, hypophosphorous acid; orthophosphoric acid, di-, tri-, and tetrapolyphosphoric acids.

Unit III Group VI Elements

Comparative study of physical and chemical properties of these elements with special reference to their hydrides, oxides, halides and oxyhalides. Detailed study of oxoacids, peroxyacids and thio-oxoacids of sulphur (with special emphasis on their structure).

Unit IV General Principles of 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 agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.

Reference Books

1. F.A. Cotton, G. Wilkinson and P.L. Gaus, Basic Inorganic Chemistry,
2. J.D. Lee, Concise Inorganic Chemistry, 5th edn., Blackwell Science, London.
3. W.W. Porterfield, Inorganic Chemistry,
4. D.E. Shriver, P.W. Atkins and C.H. Longford, Inorganic Chemistry by
5. Inorganic Chemistry by A.G. Sharpe.

Inorganic Chemistry Practical-II

A. Iodo/Iodimetric Titrations

- i. Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
- ii. Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically.
- i. Estimation of available chlorine in bleaching powder iodometrically.

B. Inorganic preparations

- i. Cuprous chloride, Cu_2Cl_2
- ii. Preparation of Manganese(III) phosphate, $MnPO_4 \cdot H_2O$.
- iii. Preparation of Aluminium potassium sulphate $K_2SO_4 \cdot Al(SO_4)_2 \cdot 12H_2O$ (Potash alum) or Chrome alum.

Reference Books

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.*, Pearson, 2009.

Organic Chemistry-II

Unit-I Chemistry of Halogenated Hydrocarbons

Alkyl halides: Methods of preparation, nucleophilic substitution reactions S_{N}^1 , S_{N}^2 and $\text{S}_{\text{N}}^{\text{i}}$ mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination. *Aryl halides:* Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; $\text{S}_{\text{N}}\text{Ar}$, Benzyne mechanism. Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Unit-II Alcohols, Phenols, Ethers and Epoxides

Alcohols: preparation, properties and relative reactivity of 1° , 2° , 3° alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement. *Phenols:* Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer-Tiemann and Kolbe-Schmidt Reactions, Fries and Claisen rearrangements with mechanism. *Ethers and Epoxides:* Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and LiAlH_4 .

Unit-III Carbonyl Compounds

Structure, reactivity and preparation; Nucleophilic additions, Nucleophilic addition-elimination reactions with amine derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α -substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, LiAlH_4 , NaBH_4 , MPV, PDC and PGC); Addition reactions of unsaturated carbonyl compounds: Michael addition. Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

Unit-IV 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; Comparative study of nucleophilic substitution at acyl group - Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann bromamide degradation and Curtius rearrangement.

Reference Books

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. Pearson Education).
3. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
4. McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

Organic Chemistry Practical -II

1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
2. Organic preparations:
 - a. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and phenols (*o*-naphthol, vanillin, salicylic acid) by any one method:
 - b. Using conventional method.
 - c. Using green approach
3. Benzoylation of one of the following amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols (*o*-naphthol, resorcinol, *p*-cresol) by Schotten-Baumann reaction.
- iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
- iv. Bromination of any one of the following:
 - a. Acetanilide by conventional methods
 - b. Acetanilide using green approach (Bromate-bromide method)
- v. Nitration of any one of the following:
 - a. Acetanilide/nitrobenzene by conventional method
 - b. Salicylic acid by green approach (using ceric ammonium nitrate).
- vi. Selective reduction of *meta*-nitrobenzene to *m*-nitroaniline.
- vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
- viii. Hydrolysis of amides and esters.
- ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
- x. *S*-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
- xi. Aldol condensation using either conventional or green method.
- xii. Benzil-Benzilic acid rearrangement.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

Reference Books

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
- Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.* Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).

Semester-III
Paper No: IX-H
Paper Code: BCH-303

UE = 75 marks
IA = 25 marks

Physical Chemistry-III

Unit-I Phase Equilibria

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapor and solid-vapor equilibria, phase diagram for one component systems, with application. Phase diagram for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points. Three component systems, water-chloroform-acetic acid system, triangular plots.

Unit-II Chemical Kinetics

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws. Factors affecting the rates of reactions, Reaction of zero order, Half-life time. Opposing reactions, Parallel reactions, and Consecutive reactions and their differential rate equations, temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

Unit-III Surface Chemistry

Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). nature of adsorbed state. Qualitative discussion of BET.

Unit-IV Catalysis

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis- Menten mechanism, acid-base catalysis.

Reference Books

1. Peter Atkins & Julio De Paula, Physical chemistry 10th Ed., Oxford University Press (2014)
2. Castellan, G. W. Physical chemistry, 4th Ed., Narosa (2004)
3. McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
4. Engel, T. & Reid, P. Physical chemistry, 3th Ed., Prentice-Hall (2012)
5. Maron, Samuel H., Principles of Physical chemistry, 4th Ed., Macmillan company, New York (1970)
6. Rastogi, R. P. & Mishra, R. R. An Introduction to chemical Thermodynamics.

Physical Chemistry Practical -III

Chemical Kinetics

1. To determine the order of the reaction between thiosulphate and HCl w.r.t. thiosulphate.
2. To determine the order of the reaction between thiosulphate and HCl w.r.t. HCl.
3. To study the kinetics of the reaction between thiosulphate and HCl at moderate concentration of $[H^+]$ by using initial rate method.
4. To determine the order of reaction for acid hydrolysis of methyl acetate at room temperature.
5. To determine the kinetics of the hydrolysis of ethyl acetate catalyzed by hydrogen ions at room temperature.
6. To study the effect of acid strength on the hydrolysis of an ester.
7. To study the kinetics of alkaline hydrolysis of M/40 methyl acetate by providing M/40 HCl and M/40 NaOH.
8. To study the kinetics of the saponification of ethyl acetate by integrated rate method.

Ionic Equilibria

9. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
10. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
11. Determination of dissociation constant of a weak acid.
12. Preparation of buffer solutions of different pH
 - (i) Sodium acetate-acetic acid
 - (ii) Ammonium chloride-ammonium hydroxide

Any other experiment carried out in the class.

Reference Books

1. O.P. Pandey, D.N. Bajpai & S. Giri, Practical Chemistry, S. Chand & Company Ltd.
2. B. D. Khosla, V. C. Garg & A. Gulati, *Senior Practical Physical Chemistry*, S. Chand & Co.: New Delhi (2011).
3. C. W. Garland, J.W. Nibler, & D.P. Shoemaker, *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
4. R.C. Das and B. Behra, *Experiments in Physical Chemistry*,; Tata McGraw Hill.

Inorganic Materials of Industrial Importance

Unit-I Industrial Chemicals

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, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. Hightechnology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Unit II 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.

Unit III 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.

Unit IV Alloys

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

Chemical explosives: Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Reference Books

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. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
5. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
6. Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).

Inorganic Chemistry- III

Unit I Group VII Elements

Comparative study of physical and chemical properties with special reference to their electron affinity, electronegativity, bond dissociation energy, oxidation number, oxidizing power, reactivity, hydrides, oxides and oxoacids, peroxyacids, strength of oxoacids.. Interhalogens, polyhalides (with special emphasis on their structures), pseudo-halogens -structure and properties.

Unit II Noble Gases

Occurrence and uses, rationalization 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).

Unit III Inorganic Polymers

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes, and polysulphates.

Unit IV Transition Elements

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer and Bsworth diagrams). Difference between the first, second and third transition series. Chemistry of first transition series elements (Ti, V, Cr, Mn, Fe and Co in various oxidation states, excluding their metallurgy). Chemistry of Second and third transition series elements (Zr, Nb, Mo, W, Re, Ru, and Rh in various oxidation states, excluding their metallurgy)

Reference Books

1. J.D. Lee, Concise Inorganic Chemistry.
2. Cotton F. A., Wilkinson G., Murillo C. A., Bochmann M., Advanced Inorg. Chemistry, 6th edn., Pubs: John Wiley India. (2003).
3. Basolo, F, and Pearson, R.C. *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.
4. Greenwood, N.N. & Earnshaw A. *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
5. W.W. Porterfield, Inorganic Chemistry.

Inorganic Chemistry Practical- III

A. Gravimetric Analysis:

- i. Estimation of nickel(II) using Dimethylglyoxime (DMG).
- ii. Estimation of copper as CuSCN
- iii. Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃.
- iv. Estimation of Al(III) by precipitating with oxine.

B. Inorganic Preparations

- i. *Cis and trans* K[Cr(C₂O₄)₂(H₂O)₂] Potassium dioxalato diaquachromate(III)
- ii. Tetraamminecarbonatocobalt(III) ion
- iii. Potassium tris(oxalato)ferrate(III)

C. Chromatography of metal ions

Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

- i. Ni(II) and Co(II)
- ii. Fe(III) and Al(III)

Reference Book

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.*, Pearson, 2009.

Organic Chemistry- III

Unit-I Nitrogen Containing Functional Groups

Preparation and important reactions of nitro compounds, nitriles and isonitriles.

Unit-II Amines: Effect of substituent and solvent on basicity; Preparation and properties of 1°, 2° and 3° amines 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.

Unit-III Polynuclear Hydrocarbons

Reactions of naphthalene and anthracene Structure, Preparation and reactions.

Unit-IV Heterocyclic Compounds

Classification and nomenclature, Structure, aromaticity in 5-numbered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of Furan, Pyrrole and Thiophene,

Reference Books

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume I)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Acheson, R.M. *Introduction to the Chemistry of Heterocyclic compounds*, John Wiley & Sons (1976).
4. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.

Organic Chemistry Practical-III

1. Detection of extra elements.
2. Functional group test for nitro, amine and amide groups.
3. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)

Reference Books

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000)
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000)

Physical Chemistry-IV

Unit-I Conductance

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Huckel-Onsager equation. Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Unit-II Electrochemistry

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) p^H values, using hydrogen, quinone-hydroquinone, glass electrodes.

Unit-III Concentration cells

Difference between chemical cells and concentration cells, liquid junction potential, its derivation, Electrode concentration cells without liquid junction potential, electrolyte concentration cells without liquid junction potential, concentration cells with liquid junction potential.

Unit-IV Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mosotti equation, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements.

Reference Books

1. Peter Atkins & Julio De Paula, Physical chemistry 10th Ed., Oxford University Press (2014)
2. Castellan, G. W. Physical chemistry, 4th Ed., Narosa (2004)
3. McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
4. Engel, T. & Reid, P. Physical chemistry, 3th Ed., Prentice-Hall (2012)
5. Maron, Samuel H., Principles of Physical chemistry, 4th Ed., Macmillan company, New York (1970)
6. Rastogi, R. P. & Mishra, R. R. An Introduction to chemical Thermodynamics.

Practical Code: BCH-403L

UE = 25 marks
IA = 25 marks

B.Sc. (Hons.) Chemistry: Semester – IV
Physical Chemistry Practical Lab –IV

Conductometry

- I. Determination of cell constant
- II. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- III. Perform the following conductometric titrations:
 - i) Strong acid vs. strong base
 - ii) Weak acid vs. strong base
 - iii) Mixture of strong acid and weak acid vs. strong base
 - iv) Strong acid vs. weak base

Potentiometry

- I. Perform the following potentiometric titrations:
 - 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

Books Recommended:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

Semester-IV
Paper No: XIV-H
Paper Code: BCH-404

UE = 75 marks
IA = 25 marks

Green Chemistry

Unit- I Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit-II Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following: Designing a Green Synthesis using these principles; Prevention of Waste/byproducts; maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions. Prevention/ minimization of hazardous/ toxic products reducing toxicity. risk = (function) hazard \times exposure; waste or pollution prevention hierarchy. Green solvents \acute{o} supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorinated biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents. Energy requirements for reactions \acute{o} alternative sources of energy: use of microwaves and ultrasonic energy. Selection of starting materials; avoidance of unnecessary derivatization \acute{o} careful use of blocking/protecting groups. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis. Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD \acute{o} What you don't have cannot harm you \acute{o} , greener alternative to Bhopal Gas Tragedy (safer route to carbaryl) and Flixborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation, Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit-III Examples of Green Synthesis/ Reactions and some real world cases

Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis). Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine). Surfactants for carbon dioxide \acute{o} replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments. Designing of Environmentally safe marine antifoulant. Rightfit pigment: synthetic azo pigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn. Healthier Fats and oil by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils, Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.

Unit- IV Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C²S³); Green chemistry in sustainable development.

Reference Books

1. Ahluwalia, V.K. & Kidwai, M.R. *New Trends in Green Chemistry*, Anamalaya Publishers (2005).
2. Anastas, P.T. & Warner, J.K.: *Green Chemistry - Theory and Practical*, Oxford University Press (1998).
3. Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
4. Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
5. Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
6. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition, 2010.

Practical Code: BCH-404L

UE = 25 marks
IA = 25 marks

Green Chemistry Practical

1. Using renewable resources
 - a. Preparation of biodiesel from vegetable/ waste cooking oil.
2. Use of enzymes as catalysts
 - a. Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.
3. Alternative Green solvents
 - a. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
 - b. Mechanochemical solvent free synthesis of azomethines
4. Alternative sources of energy
 - a. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
5. Avoiding wast
 - a. Synthesis of Tris(acetylacetonato)manganese(III) without the use of any buffer.

Reference Books

1. Anastas, P.T & Warner, J.C. Green Chemistry: Theory and Practice, Oxford University Press (1998).
2. Kirchoff, M. & Ryan, M.A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
3. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore ISBN 978-93-81141-55-7 (2013).
4. Cann, M.C. & Connelly, M. E., Real world cases in Green Chemistry, American Chemical Society (2008).

Inorganic Chemistry -IV

Unit-I Coordination Compounds and Structure

The coordination compounds, The Alfred Werner's theory of coordination compounds, Conductivities of salts and complexes, Sidgwick theory - EAN rule, Ligands, Chelating agents, and chelates, Nomenclature of coordination compounds, Isomerism of coordination compounds, Geometrical arrangement and coordination numbers.

Unit-II Bonding in Transition Metal Complexes

Valence bond theory, Limitations of Valence Bond Theory, The electro neutrality principle and back bonding, Crystal field theory, Behavior of d-orbitals in electrostatic fields, Octahedral, tetrahedral and square-pyramidal, Crystal field stabilizing energy (CFSE) and its measurement by spectrophotometry, Factors affecting the magnitude of crystal field splitting, Spectrochemical series, Crystal field splitting and magnetic properties of the complexes, Factors which favour tetrahedral complexes.

Unit-III Structural and Thermodynamic Effects of Crystal Field Splitting

Ionic radii, Jahn-Teller effect, Effects of crystal field splitting, Hydration, ligation and lattice energies, Evidences for covalence and adjusted crystal field theory (ACFT), Experimental evidence for metal- ligand orbital overlap, Intensities of d-d transitions, The nephelauxetic effect.

Unit-IV Lanthanoids and Actinoids

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only).

Reference Books

1. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
2. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005.
3. Lee, J.D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
4. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
5. Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
6. Crabtree, R. H., The Organometallic Chemistry of the Transition Metals, New York, NY: John Wiley, 2000.

Inorganic Chemistry Practical-IV

A. Gravimetric Analysis:

- i. Determination of aluminium as aluminum oxide.
- ii. Determination of sulphate ions as barium sulphate.
- iii. Determination of copper and nickel involving volumetric and gravimetric methods.
- iv. Determination of copper and barium involving volumetric and gravimetric methods.

B. Inorganic Preparation

- i. Preparation of acetylacetonato complexes of $\text{Cu}^{2+}/\text{Fe}^{3+}$. Find the λ_{max} of the complex.
- ii. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

C. Spectrophotometric Determination:

- i. Determination of copper in brass sample by spectrophotometric method.
- ii. Determination of the composition of the iron-salicylic acid complex by Job's method.

Reference Books

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.*, Pearson, 2009.
2. Marr & Rockett *Practical Inorganic Chemistry*. John Wiley & Sons 1972.

Organic Chemistry-IV

Unit-I Amino Acids, Peptides and Proteins Amino acids

Peptides and their classification: -Amino Acids ó stereochemistry, Synthesis, chromatographic separation, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis. Resolution of racemic aminoacids, Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups -Solid-phase synthesis. Primary Secondary and tertiary structure of proteins.

Unit-II Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides; Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine; Structure of polynucleotides. DNA and RNA ó Base pair formation and double helical structure. Comparison of structural stability.

Unit-III Carbohydrates

Occurrence, classification and their biological importance; Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; KillianiFischer synthesis and Ruff degradation; Disaccharides ó Structure elucidation of maltose, lactose and sucrose.; Polysaccharides ó Elementary treatment of starch, cellulose and glycogen.

Unit-IV Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Saturated and unsaturated fatty acids. Classification of unsaturated fatty acids. Melting and boiling point of fatty acids. Hydrogenation and Free radical reactions of fats and oils; Saponification value, acid value, iodine number; Reversion and rancidity.

Reference Books

1. Finar, I. L. *Organic Chemistry (Volume I & II)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Practical Code: BCH-502L

UE = 25 marks
IA = 25 marks

Organic Chemistry Practical-IV

1. Estimation of glycine by Sorenson's formalin method.
2. Study of the titration curve of glycine.
3. Estimation of proteins by Lowry's method.
4. Study of the action of salivary amylase on starch at optimum conditions.
5. Effect of temperature on the action of salivary amylase.
6. Saponification value of an oil or a fat.
7. Determination of Iodine number of an oil/ fat.
8. Isolation and characterization of DNA from onion/ cauliflower/peas.

Reference Books

1. Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
2. Arthur, I. V. *Quantitative Organic Analysis*, Pearson.

Semester-V
Paper No: XVI-H
Paper Code: BCH-503

B.Sc. (Hons.) Chemistry: Semester – V
Physical Chemistry – IV
(Quantum Chemistry)
Paper No. – XIII

UE = 75 marks
IA = 25 marks

Unit-I: Elementary Quantum Mechanics

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and *particle in a box* (rigorous treatment), quantization of energy levels, zero point energy and Heisenberg Uncertainty principle, wave functions, probability, extension to three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion. Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero point energy.

Unit II: Angular momentum:

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar coordinates (derivation not required). Separation of variables. Spherical harmonics. Qualitative discussion of solution.

Unit III: Atomic structure

Qualitative treatment of hydrogen atom and hydrogen like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from the nucleus. Setting up of Schrödinger equation for many electron atoms (He, Li). Need for approximate methods.

Unit IV: Chemical bonding

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+ . Bonding and antibonding orbitals. Qualitative extension to H_2 . Comparison of LCAO-MO and VB treatments of H_2 (only wave functions, detailed solution not required) and their limitations. Refinements of the two approaches (configuration interaction for MO, ionic terms in VB). Qualitative treatment of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH).

Books Recommended:

1. Physical Chemistry by KL Kapoor, Vol. 4, MacMillan India Ltd.
2. Introductory Quantum Chemistry by AK Chandra, Tata McGraw Hill.
3. Physical chemistry, 8th Edition, Peter Atkins, Julio de Paula, Oxford University Press.

Practical Code: BCH-503L

UE = 25 marks
IA = 25 marks

B.Sc. (Hons.) Chemistry: Semester – V
Physical Chemistry Practical Lab – XII

- I. Verify Lambert-Beer's law and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration
- II. Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture.
- III. Determine the standard enthalpy of combustion of naphthalene, using oxygen bomb calorimeter and compare it with the literature value. Also calculate the resonance stabilization energy of Naphthalene.

Numerical methods using Electronic Spreadsheets:

- I. Roots of equations (iteration and Newton ó Raphson methods, binary bisection and Regula Falsi) e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid.
- II. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
- III. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
- IV. Matrix operations. Application of Gauss-Siedel method in colourimetry. Calculation of π -electron Huckel Molecular orbitals of conjugated molecules (Linear, Cyclic, effect of Hetero atom),
- V. Monte Carlo methods ó random numbers; (a) Simulate coin toss, dice roll etc.; (b) Estimating the value of π using random numbers on a circle & sphere ; (c) Monte Carlo Integration.

Books Recommended:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).
4. Jurs, Peter C., Isenhour, Thomas L. and Wilkins, Charles L. *BASIC Programming for Chemists: An Introduction*, Wiley-Blackwell (1987).
5. Balagurusamy, E. *Numerical Methods*, Tata McGraw Hill (2000).
6. Rajaraman, V. *Computer oriented numerical methods* , 3rd Ed., Prentice-Hall (1998).

Semester-V
Paper No: XVII-H
Paper Code: BCH-504

**B.Sc. (H) Chemistry V Semester
Molecular Modeling and Drug Design (CBCS -IV)
Paper XVIII**

IA = 25, UE = 75

Unit I: Introduction to Molecular Modeling

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

Unit II: Force Fields

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

Unit III: Molecular Dynamics and Monte Carlo Simulation

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

Unit IV: Structure Prediction and Drug Design

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by Threading. Molecular docking. Structure based de novo ligand design.

Drug Discovery ó Chemoinformatics ó QSAR.

Reference Books:

1. A.R. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
2. J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
3. Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008.

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane bonds and ethene, ethyne, benzene and pyridine bonds.
- ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software.

Reference Books:

1. A.R. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
2. J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
3. Gupta, S.P. *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008.

Inorganic Chemistry-V

Unit-I Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π -acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Unit-II Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism: Alkene hydrogenation (Wilkinson's Catalyst), Hydroformylation (Co salts), Wacker Process, Synthetic gasoline (Fischer Tropsch reaction), Synthesis gas by metal carbonyl complexes.

Unit-III Reaction Kinetics and Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics Aspects of Metal Complexes, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

Unit-IV Bioinorganic Chemistry

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine. Iron and its application in bio-systems, Haemoglobin; Storage and transfer of iron.

Reference Books

1. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity, 4th Ed., Harper Collins 1993, Pearson, 2006.
2. Sharpe, A.G., Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005.
3. Lee, J.D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
4. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
5. Shriver, D.D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford University Press, 1994.
6. Purcell, K.F. & Kotz, J.C., Inorganic Chemistry, W.B. Saunders Co. 1977.
7. Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
8. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books.

Inorganic Chemistry Practical-V

- A. Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different 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+}
- B. 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 e.g. 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.
- C. Measurement of 10 Dq by spectrophotometric method
- D. Verification of spectrochemical series.
- E. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.

Reference Books

1. Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla. Pearson Education, 2002.
2. Marr & Rockett *Practical Inorganic Chemistry*. John Wiley & Sons 1972.

Organic Chemistry-V

Unit-I UV-Visible Spectroscopy

General principles Introduction to absorption and emission spectroscopy. UV Spectroscopy: Types of electronic transitions, λ_{max} , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{max} for the following systems: , unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers.

Unit-II IR Spectroscopy

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

Unit-III NMR Spectroscopy

Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin-spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds; Applications of IR, UV and NMR for identification of simple organic molecules.

Unit-IV Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing; Synthesis and applications of: Azo dyes δ Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes -Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes δ Phenolphthalein and Fluorescein; Natural dyes δ structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

Reference Books

1. Kemp, W. *Organic Spectroscopy*, Palgrave.
2. Pavia, D. L. *et al. Introduction to Spectroscopy* 5th Ed. Cengage Learning India Ed. (2015).
3. Kalsi, P. S., *Spectroscopy of Organic Compounds.*, New Age International (P) Ltd. Pub.
4. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
5. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Organic Chemistry Practical -V

1. Extraction of caffeine from tea leaves.
2. Extraction of piperine from pepper.
3. Preparation of urea formaldehyde resin.
4. Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.
5. Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols, etc.
6. Identification of simple organic compounds by IR spectroscopy
7. Preparation of methyl orange.

Reference Books:

1. Vogel, A.I. *Quantitative Organic Analysis*, Part 3, Pearson (2012).
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
3. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012)
4. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
5. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).

Semester-VI
Paper No: XX-H
Paper Code: BCH-603

UE = 75 marks
IA = 25 marks

B.Sc. (Hons.) Chemistry: Semester – VI
Physical Chemistry – VI
(Spectroscopy)
Paper No. – XX-H

Unit I: Introduction

Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer Approximation.

Unit II: Rotational, Vibrational and Raman spectroscopy

Rotational spectroscopy: Selection rules, Intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibration, Anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degree of freedom for polyatomic molecules, Normal modes of vibration, concept of group frequencies.

Vibration–rotation spectroscopy: Diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of rotational Raman effect; effect of nuclear spin, vibrational Raman spectra, Stokes and Anti Stokes lines; their intensity difference, rule of mutual exclusion.

Unit III: Electronic Spectroscopy

Frank-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation.

Unit IV: Nuclear Magnetic Resonance (NMR) Spectroscopy and Electron Spin Resonance (ESR) Spectroscopy

Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales (τ and T), spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals

Books Recommended:

1. Physical chemistry by KL Kapoor, Macmillan India Ltd.
2. Fundamentals of Molecular Spectroscopy by CN Banwell and EM McCash, Tata Mc Graw Hill.

Practical Code: BCH-603L

UE = 25 marks

IA = 25 marks

B.Sc. (Hons.) Chemistry: Semester –VI
Physical Chemistry Practical Lab –VI

UV/Visible spectroscopy

- I. Study the 200-500 nm absorbance spectra of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ (in 0.1 M H_2SO_4) 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).
- II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $\text{K}_2\text{Cr}_2\text{O}_7$.
- III. 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.

Colourimetry

- I. Study the kinetics of iodination of propanone in acidic medium.
- II. Determine the amount of iron present in a sample using 1,10-phenanthroline.
- III. Determine the dissociation constant of an indicator (phenolphthalein).
- IV. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
- V. Analysis of the given vibration-rotation spectrum of $\text{HCl}(\text{g})$.

Books Recommended:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).