DEPARTMENT OF CHEMISTRY FACULTY OF NATURAL SCIENCES



JAMIA MILLIA ISLAMIA

(A Central University)

B.Sc. Hons CHEMISTRY Effective from Academic Year 2022-2023

Syllabus of Courses Offered

Core courses, Elective Courses, Skill and Ability Enhancement courses

Р	roposed Se	emester-wise		Papers & Ci	, U		oice Base C	Credit Systen	n (CBCS
Semester	Qualifying Papers	Compulsory Papers	Core Courses (Hons.)	Core Courses (Subsidiary)	Choice based Courses Elective	Skill Enhance- ment Courses (SEC)	Ability Enhance- ment Compuls- ory Course (AECC)	Total Papers	Credit
I	1* (General Urdu & Islamiat/ IRC/ HRC)	1ª English**	2	1	1	-	-	1+2+1+1=5	20
П	1* (General Urdu & Islamiat/ IRC/ HRC)	1 * English**	2	1	1	-	-	1+2+1+1=5	20
III	-	-	3	1	-		1 ⁰	3+1=1=5	20
IV	-	-	3	1	1			3+1=1=5	20
V	-	-	3	1	1			3+1=1=5	20
VI	-	-	3	1	-	1 ⁰		3+1=1=5	20
No. of Papers	4	2	16	6	4	1	1	30	-
Total Credits	-	4x2 = 8	16x4= 64***	4x6= 24	4x4= 16	4x1= 4 or 2x2= 4	4x1= 4 or 2x2= 4	-	120

B.A/B.Sc. (Hons.) Programme ber of Paners & Credits under the Choice Base Credit System (CBCS)

Note: *Not to be counted in the Credit/ Merit;

** Those students who have secured > 75% marks in English in the qualifying exam can opt one language other than English; *** Includes a Project/ General Viva-Voce of 4 Credit in the VI Sem. If the department is willing to do so;

^a Each English paper/ Other language paper shall be of 4 credits ^o It can be split into two papers of 2 credit each

Ability Enhancement Courses: Environmental Science, English, MIL Communication, Disaster Management etc.

COURSE OUTLINE

SEMESTER-I

Paper/	Paper		Total	Ma	arks	
Practical	No	code	Title	Credits	UE	IA
Theory (Core)	I-H	BCH-101	Inorganic Chemistry-I	03	60	40
Practical (Core)		BCH-101L	Inorganic Chemistry Practical-I	01	25	25
Theory (Core)	II-H	BCH-103	Physical Chemistry-I	03	60	40
Practical (Core)		BCH-103L	Physical Chemistry Practical-I	01	25	25
Theory (Elective)	III-H	BCH-104	Industrial Chemicals & Environment	03	60	40
Practical (Elective)		BCH-104L	Industrial Chemicals & Environment Practical	01	25	25
TOTAL CREDITS				12		

SEMESTER-II

Theory (Core)	IV-H	BCH-202	Organic Chemistry-I	03	60	40
Practical(Core)		BCH-202L	Organic Chemistry Practical-I	01	25	25
Theory (Core)	V-H	BCH-203	Physical Chemistry-II	03	60	40
Practical (Core)		BCH-203L	Physical Chemistry Practical-II	01	25	25
Theory (Elective)	VI-H	BCH-204	Polymer Chemistry	03	60	40
Practical(Elective)		BCH-204L	Polymer Chemistry Practical	01	25	25
TOTAL CREDITS				12		

SEMESTER-III

Theory (Core)	VII-	BCH-301	Inorganic Chemistry-II	03	60	40
Practical (Core)	Н	BCH-301L	Inorganic Chemistry Practical-	01	25	25
			II			
Theory (Core)	VIII-	BCH-302	Organic Chemistry-II	03	60	40
Practical (Core)	Н	BCH-302L	Organic Chemistry Practical-II	01	25	25
Theory (Core)	IX-H	BCH-303	Physical Chemistry-III	03	60	40
Practical (Core)		BCH-303L	Physical Chemistry Practical-	01	25	25
			III			
Theory	Х-Н	BCH-305	Inorganic Materials of	04	60	40
(Ability			Industrial Importance			
Enhancement)			_			
TOTAL CREDITS				16		
				10		

SEMESTER-IV

Theory (Core)	XI-H	BCH-401	Inorganic Chemistry-III	03	60	40
Practical (Core)		BCH-401L	Inorganic Chemistry Practical-III	01	25	25
Theory (Core)	XII-H	BCH-402	Organic Chemistry-III	03	60	40
Practical(Core)		BCH-402L	Organic Chemistry Practical-III	01	25	25
Theory (Core)	XIII-H	BCH-403	Physical Chemistry-IV	03	60	40
Practical (Core)		BCH-403L	Physical Chemistry Practical-IV	01	25	25
Theory (Elective)	XIV-H	BCH-404	Green Chemistry	03	60	40
Practical		BCH-404L	Green Chemistry Practical	01	25	25
TOTAL CREDIT	S			16		

SEMESTER-V

Theory (Core)	XV-H	BCH-501	Inorganic Chemistry-IV	03	60	40
Practical (Core)		BCH-501L	Inorganic Chemistry Practical-IV	01	25	25
Theory (Core)	XVI-H	BCH-502	Organic Chemistry-IV	03	60	40
Practical (Core)		BCH-502L	Organic Chemistry Practical-IV	01	25	25
Theory (Core)	XVII-H	BCH-503	Physical Chemistry-V	03	60	40
Practical (Core)		BCH-503L	Physical Chemistry Practical-V	01	25	25
Theory (Elective)	XVIII-H	BCH-504	Molecular Modeling and Drug Design	03	60	40
Educational Tour (A report]	Approved by	7 AC & EC) [2	5 Marks of visit + 25 Educational tour	01	5	50
TOTAL CREDITS	S			16		

SEMESTER-VI

Theory (Core)	XIX-H	BCH-601	Inorganic Chemistry-V	03	60	40
Practical		BCH- 601L	Inorganic Chemistry Practical-V	01	25	25
(Core)						
Theory (Core)	XX-H	BCH-602	Organic Chemistry-V	03	60	40
Practical		BCH- 602L	Organic Chemistry Practical-V	01	25	25
(Core)						
Theory (Core)	XXI-	BCH-603	Physical Chemistry-VI	03	60	40
Practical	Н	BCH- 603L	Physical Chemistry Practical-VI	01	25	25
(Core)						
Skill	XXII-	BCH-604	Chemistry of Pesticides and	03	60	40
Enhancement	H		Cosmetics			
		BCH- 604L	Chemistry of Pesticides	01	25	25
			and Cosmetics practical			
Total Credits				16		
				10		

BCH-101 Paper No: I-H	INORGANIC CHEMISTRY-I	Theory	y(Marks)	Total Credits
		U.E (60)	I.A (40)	03 (100)

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.

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; Kapustinskii expression; Madelung constant, Born-Haber cycle and its application, *Covalent bond:* Lewis structure, Valence Bond theory, Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, concept of resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules; VSEPR theory, covalent character in ionic compounds, polarizing power and polarizability. Ionic character in covalent compounds: Bond moment and dipole moment. *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.

- 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.

BCH-101L	INORGANIC PRACTICAL -	Practica	al (Marks)	Total Credits	
		U.E (25)	I.A(25)	01 (50)	

1. Titrimetric Analysis

- 1.1 Calibration and use of apparatus
- 1.2 Preparation of solutions of different Molarity/Normality of titrants

2. Acid-Base Titrations

- 2.1 Estimation of carbonate and hydroxide present together in mixture
- 2.2 Estimation of carbonate and bicarbonate present together in a mixture.
- 2.3 Estimation of free alkali present in different soaps/detergents

3. Oxidation-Reduction Titrimetry

- 3.1 Estimation of Fe(II) and oxalic acid using standardized KMnO₄ solution.
- 3.2 Estimation of oxalic acid and sodium oxalate in a given mixture.
- 3.3 Estimation of Fe(II) with K₂Cr₂O₇ using internal (diphenylamine, anthranilic acid) and external indicator.

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

BCH-103 Bonon Not II II	PHYSICAL CHEMISTRY-I	Theory	y (Marks)	Total Credits
Paper No: II-H		U.E (60)	I.A(40)	03 (100)

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 Walls 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 Cholestric 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 of indices, Inter-planer 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 – Applications of solubility product principle and Common ioneffect.

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).

BCH-103L	PHYSICAL CHEMISTRY PRACTICAL -I	Practica	al (Marks)	Total Credits
		U.E (25)	I.A(25)	01 (50)

1. Surface tension measurements.

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

2. Viscosity measurement using Ostwald's viscometer.

- 2.1 Determination of viscosity of (i) ethanol (ii) amyl alcohol and (iii) aqueous solution of sugar at room temperature.
- 2.2 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

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

- 1. O.P. Pandey, D.N. Bajpai& S. Giri, Practical Chemistry, S. Chand & CompanyLtd.
- 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. A.M. Halpern & G.C. McBane, *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York(2003).

BCH-104 Paper No: III-H	INDUSTRIAL CHEMICALS AND ENVIRONMENT	Theory	y(Marks)	Total Credits
		U.E (60)	I.A(40)	03 (100)

Unit I Industrial Gases and Inorganic Chemicals

Industrial Gases: Large scale production and hazards in handling of the following gases: hydrogen. nitrogen, helium, argon, acetylene and phosgene.

Inorganic Chemicals: Manufacture, application and hazards in handling the following chemicals: sulphuric acid, caustic soda, bleaching powder, hydrogen peroxide, potassium dichromate and potassium permanganate.

Industrial Metallurgy: Preparation of metals for semiconductor technology.

Unit II: Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur. Air Pollution: Major regions of atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, 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.

Unit III Water Pollution

Hydrological cycle, water resources, sources and nature of water pollutants, Techniques for measuring water pollution, Industrial effluents and their treatment; Sludge disposal; Industrial waste management, 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. Introduction to biocatalysis: Importance in "Green Chemistry" and Chemical Industry.

- 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, NewDelhi.
- 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. A. Mishra, Environmental Studies. Selective and Scientific Books, New Delhi (2005).

BCH-104L	INDUSTRIAL CHEMICALS AND ENVIRONMENT	Practical (Marks)		Total Credits
	PRACTICAL	U.E (25)	I.A (25)	01 (50)

- 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 (AgNO₃ and potassium chromate).
- 6. Estimation of total alkalinity of water samples $(CO_3^{2^-}, HCO_3^-)$ using doublet itration method.
- 7. Measurement of dissolved CO₂.
- 8. Study of some of the common bio-indicators of pollution.
- 9. Estimation of SPM in air samples.
- 10. Preparation of borax/ boric acid.

- 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, NewDelhi.
- 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.

BCH-202	ORGANIC CHEMISTRY-I	Theory (Marks)		Total Credits	
Paper No: IV-H		U.E (60)	I.A (40)	03 (100)	

Unit I: Basics of Organic Chemistry

Organic Compounds: Classification, and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties. Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications; Dipole moment; Organic acids and bases; their relative strength. Homolytic and Heterolytic fission with suitable examples. Electrophiles and Nucleophiles; Nucleophilcity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals.

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. Baeyer strain theory, Conformation analysis of alkanes: Relative stability with energy diagrams: cyclohexane: Chair, Boat and Twist boat forms.

Unit III: Chemistry of Aliphatic Hydrocarbons

Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity. 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, hydroboration-oxidation, 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 benzylicbromination 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: Aromatic Hydrocarbons

Aromaticity: 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.

- 1. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (PearsonEducation).
- 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. (PearsonEducation).
- 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, 2013.

BCH-202L	ORGANIC CHEMISTRY PRACTICAL -I	Practical (Marks)		Total Credits
		U.E (25)	I.A(25)	01(50)

- 1. Purification of organic compounds by crystallization using the following solvents:
 - 1.1 Water
 - 1.2 Alcohol
 - 1.3 Alcohol-Water
- 2. Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
- 3. Effect of impurities on the melting point, mixed melting point of two unknown organic compounds.
- 4. Determination of boiling point of liquid compounds. (Boiling point lower than and more than 100 °C by capillary method).
- 5. Separation of a mixture of two amino acids by ascending paper chromatography. a. Separation of a mixture of two sugars by ascending paper chromatography.
- 6. Preliminary examination of some organic compounds.

- 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. PracticalOrganic Chemistry, 5th Ed., Pearson(2012)

BCH-203 Paper No: V-H	PHYSICAL CHEMISTRY-II	Theory (Marks)		Total Credits
		U.E (60)	I.A (40)	03 (100)

Unit I. Thermochemistry

Exothermic and endothermic reactions, Heats of reactions, standard states, relation between heat of reaction at contant volume (q_v) and at contant pressure (q_p) , Heat capacity, relation between Cp and Cv, 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 Kp and Kc and Kx. 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, Raoults 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

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

BCH-203L	PHYSICAL CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		U.E (25)	I.A(25)	01(50)

- a. Determination of the heat capacity of a calorimeter.
- b. Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) of solution of salts.
- c. To determine the enthalpy of neutralization of a weak acid / weal base versus strong base/ strong acid and determine the enthalpy of ionization of the weak acid / weak base.
- d. To determine the enthalpy of hydration of CuSO₄.
- e. To study of the solubility of benzoic acid in water and determination of ΔH .
- f. 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.
- g. Verification of Hess's law by utilizing the enthalpy of neutralization of (i) HCl(aq),
 (ii) NaOH(s) + HCl(aq), and (iii) enthalpy of solution of NaOH(s) in water.
- h. 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.
- i. Determination of the molar mass of the given solute by using Rast method.

- 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.: NewDelhi(2011).
- 3. C. W. Garland, J.W. Nibler, & D.P. Shoemaker, *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York(2003).
- 4. A.M. Halpern & G.C. McBane, *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

BCH-204	POLYMER CHEMISTRY	Theory (Marks)		Total Credits
Paper No: VI-H		U.E (60)	I.A (40)	04 (100)

Unit-I Introduction and History of Polymeric Materials

Introduction to concepts and classification of polymers; a brief history of polymers, definitions and terms used in polymer literature; polymers nomenclature; importance of synthetic polymers; classification of polymers on the basis of molecular structure; thermal properties; chain configuration; methods of polymerization and applications

Unit-II Synthesis of Polymers

Characteristics of step growth and chain growth polymerization; mechanism of free radical polymerization ionic and step growth polymerizations; copolymers; types of copolymers; copolymer structure and monomer reactivity ratios; copolymer equation and its significance.

Unit-III Molecular weights and mechanical properties of polymers

Basic principles of polymer molecular weight- number average molecular weight; weight average molecular weight; viscosity average molecular weight; molecular weight distribution curve; technique for measurements of molecular weights

Thermal transition in polymers; crystallization of polymers; degree of crystallinity; amorphous polymers; glass transition temperature (tg); measurements of tg.

Unit-IV Commercial polymers

Preparation, properties and application of thermoplastic polymers and thermoset polymers; polyethylene; polypropylene, polystyrene; poly(vinyl chloride); polyacrylamide; polyurethane; polyesters; alkyd resins; phenol-formaldehyde; polyamides and polysiloxanes; Additives used in plastic manufacture.

- 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.

BCH-204L	POLYMER CHEMISTRY	Practical	l (Marks)	Total Credits	
	PRACTICAL	U.E (25)	I.A (25)	01 50)	

1. Polymer synthesis

- 1.1 To prepare polystyrene by bulk polymerization and report the yield and solubility of theprepared polymer
- 1.2 To prepare polyvinyl acetate by solution polymerization and convert polyvinyl acetate to polyvinyl alcohol by alkaline hydrolysis.
- 1.3 To prepare copolymers of styrene and methyl methacrylate. Report the yield and solubility.
- 1.4 To synthesize Novolac and resole resins

2. Polymer analysis

- 2.1 To determine the viscosity average molecular weight of the polymers prepared in experiments 1.1 and 1.2 by using ubbehlode viscometer.
- 2.2 To determine the hydroxyl number of polyvinyl alcohol by colorimetric method.

3. Polymer characterization

- 3.1 To determine the tensile strength of the polymers prepared.
- 3.2 To study the IR spectra of the polymers

- 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)

BCH-301 Paper No: VII-H	INORGANIC	CHEMISTRY-II	Theory (Marks)		Total Credits
			U.E (60)	I.A(40)	03 (100)

Unit I Group I Elements

Hydrogen: Isotopes (separation method not needed). Ortho and para hydrogen, Hydrides and their classification. *Alkali metals:* Chemical properties of the metals: reaction with water, air, nitrogen; uses of s-block metals and their compounds, Compounds of s-block metals: oxides, hydroxides, peroxides, superoxides - preparation and properties; oxo salts-carbonates, bicarbonates, nitrates; halides and polyhalides; anomalous behavior of Li.

Unit II Group II Elements

Alkaline earth metals: Comparative study of these elements with special reference to their hydrides, oxides, hydroxide and halides. Diagonal relationship, solvation and Complexes of *s*-block metals including their applications in biosystems.

Unit III Group III Elements

Comparative study of physical and chemical properties of these elements with special reference to their oxides, hydrides, halides and nitirides. Preparation and properties of boric acids (ortho & meta boric acids) and borax, borax bead test. Study of hydrides formed by boron, structure and bonding in diboranes, an idea of three center-two electron bond in the light of molecular orbital theory, borazine, borohydrides

Unit IV Group IV Elements

Comparative study of physical and chemicals 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 nonmetallic character, catenation and hetero catenation.

- 1. J.D. Lee, Concise Inorganic Chemistry, 5th edn., Blackwell Science, London
- 2. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley, VCH, 1999.
- 3. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3rd edn., Oxford University Press.
- 4. Inorganic Chemistry by G.L. Miessler and D.A. Tarr.
- 5. Inorganic Chemistry by A. G. Sharp.

BCH-301L	INORGANIC CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		U.E (25)	I.A(25)	01 (50)

1. Iodo/Iodimetric Titrations

- 1.1 Estimation of Cu(II) and K₂Cr₂O₇ using sodium thiosulphate solution (Iodimetrically).
- 1.2 Estimation of (i) arsenite and (ii) antimony iodimetrically.
- 1.3 Estimation of available chlorine in bleaching powder iodometrically.

2. Inorganic Preparations

- 2.1 Cuprous chloride, Cu₂Cl₂
- 2.2 Preparation of Manganese(III) phosphate, MnPO₄.H₂O.
- 2.3 Preparation of Aluminium potassium sulphate K_2SO_4 . Al(SO_4)₂.12H₂O (Potash alum) or Chrome alum.

Reference Books

1. Vogel's Quantitative Chemical Analysis 6thEd., Pearson, 2009.

BCH-302 Paper No: VIII-H	ORGANIC CHEMISTRY-II	Theory (Marks)		Total Credits
		U.E (60) I.A(40) 03 (100)	03 (100)	

Unit-I Chemistry of Halogenated Hydrocarbons

Alkyl halides: Methods of preparation, nucleophilic substitution reactions $-SN^1$, SN^2 and SNi mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination. *Aryl halides:* Preparation, including preparation from diazonium salts. Nucleophilic aromatic substitution; SNAr, 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's– Schmidt Reactions, Fries and Claisen rearrangements with mechanism. *Ethers and Epoxides:* Preparation and reactions with acids. Reactions of epoxides with alcohols, ammoniaderivatives and LiAlH₄.

Unit-III Carbonyl Compounds

Structure, reactivity and preparation; Nucleophilic additions, Nucleophilic addition- elimination reactions with ammonia 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, LiAlH₄, NaBH₄, 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.

- 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. CengageLearning India Edition, 2013.

BCH-302L	ORGANIC CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		U.E (25)	I.A(25)	01 (50)

- 1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
- 2. Acetylation of aniline.
- 3. Benzolyation of β -naphthol, by Schotten- Baumann reaction.
- 4. Bromination of acetanilide by conventional methods.
- 5. Bromination of acetanilide green approach (Bromate-bromide method).
- 6. Nitration of acetanilide by conventional method.
- 7. Salicylic acid by green approach (using ceric ammonium nitrate).
- 8. Selective reduction of *meta* dinitrobenzene to*m*-nitroaniline.
- 9. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
- 10. Hydrolysis of amides and esters.
- 11. Semicarbazone of any one of the following compounds: acetone, ethyl methylketone, cyclohexanone, benzaldehyde.
- 12. Aldol condensation using either conventional or green method.

- 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).

BCH-303 Paper No: IX- H	PHYSICAL CHEMISTRY- III	Theory	y (Marks)	Total Credits
raper ivo: ix- n		U.E (60)	I.A(40)	03 (100)

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 solidliquid, 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-I

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.

Unit-III Chemical Kinetics-II

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, Lindermann mechanism, qualitative treatment of the theory of absolute reaction rates.

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.

- 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.

BCH-303L

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

- 1. O.P. Pandey, D.N. Bajpai& S. Giri, Practical Chemistry, S. Chand & CompanyLtd.
- 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 McGrawHill.

BCH-305 Paper No: X-H	INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE	Theory (Marks)		Total Credits
		U.E (60)	I.A(40)	04 (100)

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, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass. *Ceramics:* Important clays and feldspar, ceramic, their types and manufacture. High technology 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.

- 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*HandbookofIndustrialChemistry*,CBSPublishers,NewDelhi.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).

BCH-401 Paper No: XI- H	INORGANIC CHEMISTRY-III	Theory (Marks)		Total Credits	
		U.E (60)	I.A(40)	03 (100)	

Unit I Group V Elements

Comparative study of the physical and chemical properties of these elements with special reference to their hydrides, oxides, halodes, 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 tetra polyphosphoric acids.

Unit II 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 oxyacids, peroxyacids and thio-oxyacids of sulphur (with special emphasis on their structure).

Unit III Organometallic Compounds

Definition and classification of 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 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, synergic effect and extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Unit IV: 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

- 1. Cotton, F.A.G.; Wilkinson & Gaus, P.L. Basic Inorganic Chemistry 3rd Ed.; Wiley India,
- 2. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
- 3. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005.
- 4. Greenwood, N.N. & Earnshaw, A. Chemistry of the Elements, Elsevier 2nd Ed,1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- 5. Basolo, F. & Pearson, R. Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed., John Wiley & Sons Inc; NY.

	BCH-401L	INORGANIC CHEMISTRY PRACTICAL - III	Practical (Marks)		Total Credits	
	FRACTICAL - III	U.E (25)	I.A(25)	01 50)		

1. Gravimetric Analysis:

- 1.1 Estimation of nickel(II) using Dimethylglyoxime(DMG).
- 1.2 Estimation of copper as CuSCN
- 1.3 Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃.
- 1.4 Estimation of Al(III) by precipitating with oxine.

2. Inorganic Preparations

- 2.1 *Cis* and *trans* K[Cr(C₂O₄)₂(H₂O)₂] Potassium dioxalato diaquachromate(III)
- 2.2 Tetra ammine carbonato cobalt(III) ion iii. Potassiumtris (oxalato) ferrate(III)
- **3. Chromatography of metal ions:** Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions: 3.1 Ni(II) and Co(II)

3.2 Fe(III) and Al(III)

Reference Book

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

BCH-402 Paper No: XII-H	ORGANIC CHEMISTRY- III	Theory (Marks)		Total Credits
		U.E (60)	I.A(40)	03 (100)

Unit-I Nitrogen Containing Functional Groups

Preparation and important reactions of nitro compounds, nitriles and isonitriles Amines: Effect of substituent and solvent on basicity; Preparation and properties of 1° , 2° and 3° amines Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hofmannelimination reaction; Distinction between 1° , 2° and 3° amines with Hinsberg reagent and nitrous acid. Diazonium Salts: Preparation and their synthetic applications.

Unit-II Heterocyclic Compounds

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Derivatives of furan: Furfural and furoic acid

Unit-III: Dyes

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

Unit IV: Polynuclear Hydrocarbons

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons.

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

BCH-402L	L ORGANIC CHEMISTRY PRACTICAL - III		al (Marks)	Total Credits	
		U.E (25)	I.A(25)	01 (50)	

- 1. Detection of extra elements. (Presence of N, S and halogens X=Cl, Br,I).
- 2. Functional group test
 - 2.1 Nitro
 - 2.2 Amine (Presence of primary, secondary, tertiary or aliphatic/aromatic)
 - 2.3 Amide & Anilide
- 3. Qualitative analysis of unknown organic compounds containing simple functional groups
 - 3.1 Alcohols,
 - 3.2 Carboxylic acids,
 - 3.3 Phenols and
 - 3.4 Carbonyl compounds (Aldehydes and ketones)
 - 3.5 Thiourea
 - Preparation of dyes
 - 4.1 Malachite Green
 - 4.2 1-2 coupling reaction
 - 4.3 1-4 coupling reaction

Reference Books

4.

- 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 OrganicChemistry*, *5thEd.*, 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).

BCH-403 Paper No: XIII-H	PHYSICAL CHEMISTRY- IV	Theory (Marks)		Total Credits
raper No: AIII-H		U.E (60)	I.A(40)	03 (100)

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 spraringly 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.

- 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, NewYork (1970)
- 6. Rastogi, R. P. & Mishra, R. R. An Introduction to Chemical Thermodynamics.

BCH-403L	PHYSICAL CHEMISTRY PRACTICAL- IV	Practical (Marks)		Total Credits
	I KACHCAL-IV	U.E (25)	I.A(25)	01 (50)

1. Conductometry

- **1.1** Determination of cell constant
- **1.2** Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- **1.3** Perform the following conductometric titrations:
 - **1.3.1** Strong acid vs. strong base
 - **1.3.2** Weak acid vs. strong base
 - **1.3.3** Mixture of strong acid and weak acid vs. strong base
 - **1.3.4** Strong acid vs. weak base

2. Potentiometry

2.1 Perform the following potentiometric titrations:

- 2.1.1 Strong acid vs. strong base
- **2.1.2** Weak acid vs. strong base
- 2.1.3 Dibasic acid vs. strong base
- **2.1.4** 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).
- Halpern, A. M. &McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York(2003).

6

BCH-404 Paper No: XIV-H	GREEN CHEMISTRY	Theory (Marks)		Total Credits
		U.E (60)	I.A(40)	03 (100)

Unit- I Introduction to Green Chemistry

Twelve principles of Green Chemistry: Designing a Green Synthesis using these principles 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

Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products, Green solvents- supercritical fluids, water as a solvent for organic reactions, ionic liquids, Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy. careful use of blocking/ protecting groups. catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis. Strengthening/ development of analytical techniques to prevent generation of hazardous substances in chemical processes.

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

Green Synthesis of 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. Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO₂. 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(C Green chemistry in sustainabledevelopment.

- 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.

BCH-404L	GREEN CHEMISTRY PRACTICAL	Practical (Marks)		Total Credits
	I MICHE	U.E (25)	I.A(25)	01 (50)

1. Using renewable resources

1.1 Preparation of biodiesel from vegetable/ waste cooking oil.

- Use of enzymes as catalyst
 2.1 Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.
- Alternative Green solvents
 3.1 Extraction of D-limonene from orange peel using liquid CO2 prepared form dryice.
 3.2 Mechanochemical solvent free synthesis of azomethines
- 4. Alternative sources of energy4.1 Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
- 5. Avoiding waste 5.1 Synthesis of Tris(acetylacetonato) manganese(III) without the use of any buffer.

- 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 CISBN978-93-81141-55-7 (2013).
- 4. Cann, M.C. & Connelly, M. E., Real world cases in Green Chemistry, American Chemical Society(2008).

BCH-501	INORGANIC CHEMISTRY-IV	Theory (Marks)		Total Credits
Paper No: XV-H		U.E. (60)	I.A. (40)	03 (100)

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 filed 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 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 oxyacids, peroxyacids, strength of oxoacids, Interhalogens, polyhalides (with special emphasis on their structures), pseudo-halogens -structure and properties.

- 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 sons2008.
- 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.

BCH-501L	INORGANIC CHEMISTRY PRACTICAL - IV	Practical (Marks)		Total Credits
		U.E (25)	I.A. (25)	01 (50)

1. Gravimetric Analysis:

- 1.1 Determination of aluminium as aluminum oxide.
- 1.2 Determination of sulphate ions as barium sulphate.
- 1.3 Determination of copper and nickel involving volumetric and gravimetric methods.
- 1.4 Determination of copper and barium involving volumetric and gravimetric methods.

2. Inorganic Preparation

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

3. Spectrophotometric Determination:

- 3.1 Determination of copper in brass sample by spectrophotometric method.
- 3.2 Determination of the composition of the iron-salicylic acid complex by Job'smethod.

- 1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6thEd., Pearson, 2009.
- 2. Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons1972.

BCH-502	ORGANIC CHEMISTRY- IV	Theory (Marks)		Total Credits
Paper No: XVI- H		U.E. (60)	I.A. (40)	03 (100)

Unit-I Amino Acids, Peptides and Proteins Amino acids

Peptides and their classification: α-Amino Acids – 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 – 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; Killiani Fischer synthesis and Ruff degradation; Disaccharides – Structure elucidation of maltose, lactose and sucrose.; Polysaccharides – 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 1 & ll), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

BCH-502L	ORGANIC CHEMISTRY PRACTICAL - IV	Practical	(Marks)	Total Credits	
		U.E. (25)	I.A. (25)	01 (50)	

- 1. To determine the saponification value of an oil or a fat.
- 2. To determination of iodine number of an oil/ fat.
- 3. To determination of acid value of an oil/ fat.
- 4. Preparation of benzoic acid from toluene using KMnO₄.
- 5. Preparation of *p*-benzoquinone from hydroquinone using KBrO₃.
- 6. Preparation of acetylsalicylic acid (aspirin).
- 7. Preparation of 2,4,6-tribromoaniline from aniline.
- 8. Synthesis of hydrazones.
- 9. Synthesis of Dibenzylideneacetone.
- 10. Oxidation of ethanol/ isopropanol (Iodoform reaction).
- 11. *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid,oxalic acid, phenyl acetic acid and phthalic acid).

Reference Book:

Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of

Delhi. Arthur, I. V. Quantitative Organic Analysis, Pearson.

BCH-503	PHYSICAL CHEMISTRY- V	Theory (Marks)		Total Credits
Paper No: XVII-H				
		U.E. (60)	I.A. (40)	03 (100)

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 Uncertainity 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 anti-bonding 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.

- 1. Verify Lambert-Beer's law and determine the concentration of CuSO₄/KMnO₄/K₂Cr₂O₇ in a solution of unknown concentration
- 2. Determine the concentrations of KMnO₄ and K₂Cr₂O₇ in a mixture.
- 3. 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:

- 1. Roots of equations (iteration and Newton Raphson methods, binary bisection and Regula Falsi) e.g. volume of van der Waals gas and comparison with ideal gas, pH of aweak acid.
- 2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
- 3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
- 4. Matrix operations. Application of Gauss-Siedel method in colourimetry. Calculation of electron Huckel Molecular orbitals of conjugated molecules (Linear, Cyclic, effect of Hetero atom),
- 5. Monte Carlo methods –random numbers; (a) Simulate coin toss, dice roll etc.; (b) Estimating the value of "pi" 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).
- 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).

BCH-504	BCH-504MOLECULAR MODELING ANDTheory (Marks)		arks)	Total Credits
Paper No: XVIII- H	DRUG DESIGN	U.E (60)	I.A. (40)	03 (100)

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 – Chemoinformatics – QSAR.

- 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.

BCH-601	INORGANIC CHEMISTRY-V	Theory (Marks)	Total Credits
Paper No: XIX-H		U.E. (60) I.A. (40)	03 (100)

Unit-I 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)

Unit-II Lanthanoids and Actinoids

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

Unit-III Noble Gases

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2 , XeF_4 and XeF_6 ; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2). Molecular shapes of noble gas compounds (VSEPR theory).

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. Na / K-pump, carbonic anhydrase and carboxypeptidase A. 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.

- 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. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- 4. Shriver, D.D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford UniversityPress,1994.
- 5. Purcell, K.F. &Kotz, J.C., Inorganic Chemistry, W.B. Saunders Co.1977.
- 6. Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
- 7. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books.

BCH-601L	L INORGANIC CHEMISTRY PRACTICAL -V	Practical (Marks)		Total Credits
	TRACTICAL - V	U.E. (25)	I.A. (25)	01 (50)

1. 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^-} , $SO_3^{2^-}$, $S_2O_3^{2^-}$, CH_3COO^- , F^- , CI^- , Br^- , I^- , NO_3^- , $BO_3^{3^-}$, $C_2O_4^{2^-}$, $PO_4^{3^-}$, 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 (BaSO₄, SrSO₄, PbSO₄, CaF₂ or Al₂O₃) or combination of anions e.g. CO₃²⁻ and SO₃⁻²⁻, NO₂⁻ and NO₃⁻, Cl⁻ and Br⁻, Cl⁻ and I⁻, Br⁻ and I⁻, NO₃⁻ and Br⁻, NO₃⁻ and I⁻. Spot tests should be done whenever possible.
- 3. Measurement of 10 Dq by spectrophotometric method
- 4. Verification of spectrochemical series.
- 5. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.

- 1. Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla. Pearson Education, 2002.
- 2. Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons1972.

BCH-602 Paper No: XX-H	ORGANIC CHEMISTRY-V	Theory (Marks)		Total Credits
		U.E. (60) I.A. (40)		03 (100)

Unit-I UV-Visible and IR 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: α,β 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. 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-II 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 III: Natural Products

Natural occurrence, General structural features, Isolation and their physiological action Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine. Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral, Neral and α -terpineol.

Unit-IV Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type. The Grignard reagents: formation, structure and chemical reactions; Organozinc compounds: formation, structure and chemical reactions; Organolithium compounds: formation, structure and chemical reactions; Concept of hapticity of organic ligands. 18 electron rule, Ziegler-Natta Catalyst and Zeise's salt.

- 1. Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley(India) Pvt. Ltd. (Pearson Education).
- Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.Gowariker, V. R.; Viswanathan, N. V. &Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.\
- 3. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (PearsonEducation).
- 4. Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition,2013.
- 5. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford UniversityPress.
- 6. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Prakashan(2010).
- 7. Kemp, W. Organic Spectroscopy, Palgrave.
- 8. Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning India Ed.(2015).

BCH-602L	ORGANIC CHEMISTRY PRACTICAL -V	Practical (Marks)		Total Credits
		U.E. (25)	I.A. (25)	01 (50)

- 1. Extraction of caffeine from tealeaves.
- Preparation
 2.1 phenol formaldehyde resins
 2.2 Urea-formaldehyde.
- 3. Analysis of Carbohydrate:
 - 3.1 Carbohydrate and a non-carbohydrate
 - 3.2 Aldoses and ketoses
 - 3.3 Reducing and non-reducing sugars
- 4 Qualitative analysis
 - 4.1 Unknown organic compounds containing mono-functional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines andamides)
 - 4.2 Simple bi-functional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols etc.
- 5 Identification of simple organic compounds by IR spectroscopy (Spectra to be provided).

- 1. Vogel, A.I. Quantitative Organic Analysis, Part 3, Pearson(2012).
- 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

CH-603 Paper No: XXI- H	PHYSICAL CHEMISTRY-VI	Theory (Marks)		Total Credits
		U.E. (60) I.A. (40)		03 (100)

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 (δ 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 IndiaLtd.

2. Fundamentals of Molecular Spectroscopy by CN Banwell and EM McCash, Tata McGraw Hill.

BCH-603L	PHYSICAL CHEMISTRY PRACTICAL -VI	Practical (Marks)		Total Credits	
		U.E. (25)	I.A. (25)	01 (50)	

1. UV/Visible spectroscopy

- 1.1 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 (Jmolecule⁻¹, kJ mol⁻¹, cm⁻¹, eV).
- 1.2 Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K₂Cr₂O₇
- 1.3 Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

2. Colorimetry

- 2.1 Study the kinetics of iodination of propanone in acidic medium.
- 2.2 Determine the amount of iron present in a sample using 1,10-phenathroline.
- 2.3 Determine the dissociation constant of an indicator (phenolphthalein).
- 2.4 Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
- 2.5 Analysis of the given vibration-rotation spectrum of HCl(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).

BCH-604 Paper No: XXII-H	CHEMISTRY OF PESTICIDES AND	Theory (Marks)				Total Credits
	COSMETICS	U.E. (60)	I.A. (40)	03 (100)		

Unit I: Introduction to pesticides

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship.

Unit II: Synthesis and Uses of pesticides

Synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Unit III: Synthesis of Cosmetics

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours.

Unit IV: Essential oils and applications

Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

- 1. Cremlyn, R. *Pesticides. Preparation and Modes of Action*, John Wiley & Sons, New York, 1978.
- 2. Stocchi, E. Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK (1990).
- 3. Engineering Chemistry Dhanpat Rai & Sons, Delhi.
- 4. Industrial Chemistry, Goel Publishing House, Meerut (1996).

BCH-604L	CHEMISTRY OF PESTICIDES AND COSMETICS PRACTICAL	Practical (Marks)		Total Credits
		U.E. (25)	I.A. (25)	01 (50)

- 1. To determine acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
- 2. Preparation of simple organophosphates, phosphonates and thiophosphates.
- 3. Preparation of talcum powder.
- 4. Preparation of shampoo.
- 5. Preparation of enamels.
- 6. Preparation of face cream.
- 7. Preparation of nail polish and nail polish remover.

Reference Books

1. Cremlyn, R. *Pesticides. Preparation and Modes of Action*, John Wiley & Sons, New York, 1978.

2. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).