DEPARTMENT OF CHEMISTRY

FACULTY OF NATURAL SCIENCES

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(A Central University)

Syllabus for MSc Chemistry Entrance Test 2021

BCH-101	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.

Unit II Periodicity of Elements

s, p, d, f block elements, the long form of periodic table; Discussion of followingproperties 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 andinsulators, 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.

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.

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 phosphorusorthophosphorous acid, metaphosphorous acid, hypophosphorous acid; orthophosphoric acid, di-, tri-, and tetrapolyphosphoric 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 (ZieglerNatta 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.

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 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.

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 invarious 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 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-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.

- 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.

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; Nucleophilicity 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.

Unit-I Chemistry of Halogenated Hydrocarbons

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – SN¹, SN² 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 leadtetraacetate, 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, ammonia derivatives and LiAlH4.

Unit-III Carbonyl Compounds

Structure, reactivity and preparation; Nucleophilic additions, Nucleophilic additionelimination 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-enoltautomerism. 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. Cengage Learning India Edition, 2013.

Unit-I Nitrogen Containing Functional Groups

Preparation and important reactions of nitro compounds, nitriles and isonitrilesAmines: 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-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.

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; KillianiFischer 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. Hydrogenntion and Freeradical reactions of fats and oils; Saponification value, acid value, iodine number; Reversion and rancidity.

- 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).
- 2. 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. (Pearson Education).
- 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, OxfordUniversityPress.
- 6. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Prakashan (2010).

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; Organozinccompounds: 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.

- 7. 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).
- 8. 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.\
- 9. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (PcarsonEducation).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc. McMurry, J.E.Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition.2013.
- 11. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, OxfordUniversityPress.
- 12. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiPrakashan(2010).
- 13. Kemp, W. Organic Spectroscopy, Palgrave.
- 14. Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning IndiaEd.(2015).

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 ion effect.

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 International Publishers.
- 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).

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 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 Equillibrium

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 International Publishers.
- 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-303	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-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.

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 Hitt orf 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) pH 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, Clauius-Mosotti equation, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements.

- 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 chemicalThermodynamics.

BCH-503	PHYSICAL CHEMISTRY- IV

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 sphericalpolar 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 IndiaLtd.
- 2. Introductory Quantum Chemistry by AK Chandra, Tata McGrawHill.
- 3. Physical chemistry, 8th Edition, Peter Atkins, Julio de Paula, Oxford UniversityPress.

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.