Syllabus for B.Sc 1st year (Semester-I)
Subject: Chemistry

Effective from Academic Session-2015

Inorganic Chemistry

Unit-I Atomic Structure and Periodic Properties: (16 Contact Hours)

***Atomic Structure*: Wave Mechanical concept of Atomic Structure: de-Broglie's wave equation; derivation and experimental verification. Confirmation of quantization of angular momentum and its significance. Heisenberg's Uncertainty Principle: Illustration and significance.**
Reasons for abnormal electronic configurations of some elements; Shapes of s, p & d orbitals; Effective nuclear charge and its calculation by Slater rules.
***Periodic Properties*: Trends in Atomic, Ionic, Metallic and Vander Waal radii.**
Successive ionization energies and factors affecting ionization energy.
Electronegativity and Electron Affinity: Trends , Methods of determination ; Applications in predicting and explaining the chemical behavior of elements.

Unit-II Chemical Bonding: (16 Contact Hours)

Chemical Bonding-I
***Ionic Bond:* Lattice energy and Born Haber Cycle. Factors affecting the structure of ionic solids; Radius ratio effect; Coordination number and limitations of radius ratio rule. Fajan's rules and its applications.**
Solvation energy and solubility of ionic solids. Factors affecting the solubility of ionic solids. *Metallic bond:* Characteristics, comparison with ionic and covalent bonds .Theories (Free electron, VB and MO).
Chemical Bonding-II
***Valence bond theory*: Directional characteristics of covalent bond and types of hybridizations. Limitations of VB theory. Percent ionic character from dipole moment and electronegativity difference.**
***VSEPR theory*: Assumptions; Shapes of some molecules (BF_3, NH_3, H_2O, SF_4, ClF_3 and XeF_2)**
***Molecular Orbital Theory*: Energy level diagrams, Bond order with its significance and Magnetic properties of homo & hetero nuclear diatomic molecules (N_2, O_2, F_2, HCl, CO & NO). Multicenter bonding in electron deficient molecules.**

Unit-III s & p Block Elements: (16 Contact Hours)

***s-Block Elements*: Chemical Reactivity towards Water, Oxygen, Hydrogen, Nitrogen and Halogens. Anomalous behaviour and diagonal relationships (Lithium, Beryllium, Magnesium and Aluminum). Chemical characteristics of the compounds of alkali and alkaline earth metals (Oxides and Hydroxides).**
Hydrides: Classification and general properties.
Some commercially important compounds:- Sodium carbonate, Calcium carbonate and Calcium sulphate(Preparation,properties and Uses)
p–Block Elements - Groups (13-15).
***Boranes*: Nomenclature, Classification, Preparation, Properties, Structure and Bonding with special reference to Diborane.**
***Bonding in higher boranes*: Types of bonds, Introductory concept about carboranes and metallocarboranes.**

***Carbides*: Classification, Preparation, Properties and Uses. Intercalation compounds of graphite.**
***Nitrogen Compounds*: Preparation, properties and uses of Hydrazine, Hydroxylamine and Oxides and Oxoacids of nitrogen. Ammonia as a non-aqueous solvent.**

Unit-IV Inorganic Qualitative Analyses: (16 Contact Hours)
General Safety rules: Maintenance of Equipments; Storage of chemicals & solvents ; Prevention and protection from explosions and hazards. Electrical Safety and UV– radiations. Safe disposal of hazardous / radioactive chemicals . First aid.
Qualitative Analysis: Underlying principles – Common -ion effect and Solubility product. Effect of acids/bases, temperature and solvent upon the solubility of precipitate. Salt effect. Relation between solubility and solubility product.
***Scales of Qualitative Analysis*: Macro, Semi –micro, Micro and Ultramicro Analysis. Spot test analysis.**
***Analysis of Inorganic Mixtures*: Analytical groups and group reagents; Selective precipitation of cations; Reactions involved in separation and identification of cations from different analytical groups . Identification of anions.**

Books Recommended

1. **Basic Inorganic Chemistry; F.A. Cotton, G Wilkinson & P.L. Gauss; 3rd ed.; Wiley; 2002.**
2. **Inorganic Chemistry ; A.G. Sharpe; 3rd ed.; ELBS, 1992.**
3. **Concise Inorganic Chemistry; J.D . Lee; 5th ed.; ELBS; 2003.**
4. **Inorganic Chemistry . G.L. Miessler, T. A Tarr; 3rd ed.; Prentice Hall; 2009**
5. **Inorganic Chemistry ; D.E. Shriver ; P.W. Atkins & C.H. Langford ; 4th ed.; Oxford; 2006**
6. **Concepts and models of Inorganic Chemistry ; B. Douglas ; D.Mc. Daniel & J. Alexander; 3rd ed.; Wiley; 2001.**
7. **Advanced Inorganic Chemistry ; Volume 1; S. Prakash; G.D. Tuli ; S.K. Basu & R.D . Madan; S.Chand & Company Ltd.**
8. **Vogel's Qualitative Inorganic Analysis; Svehla; 7th ed.; Orient Longman; 2004.**
9. **Advanced Practical Inorganic Chemistry; Gurdeep Raj; 24th ed.; Goel Publishing House; 2012.**

Syllabus for B.Sc 1st year (Semester-II)

Subject: Chemistry

Effective from Academic Session-2015

Organic Chemistry

Unit-I Localised and Delocalised chemical bonds and Methods of determination of reaction mechanism: (16 Contact Hours)

Localised and delocalised chemical bonds: **Recapitulation and applications of Inductive and Electromeric effects. Conjugation, Resonance and Hyperconjugation.**

Dipole-dipole interactions: **Hydrogen bond, Van der Waal's and London forces and their significance with respect to organic compounds.**

Aromaticity: **Requirements of aromaticity. Huckel's rule and its significance. Explanation using molecular orbital diagram of benzene. Aromaticity of non-benzenoid compounds like pyrrole, thiophene, furan and aromatic ions (3, 5 and 7-membered rings).**

Reactive intermediates: **Structure, generation and stability of Carbocations, Carbanions, Free radicals, Carbenes, Benzynes and Nitrenes.**

Methods of determination of reaction mechanism: **Identification of Products, Isotope labeling, Sterochemical and Kinetic evidences.**

Unit-II Stereochemistry: (16 Contact Hours)

Stereochemistry: **Concept and types of stereoisomerism.**

***Geometrical Isomerism*: Configuration of geometrical isomers. *E* and *Z* system of nomenclature.Geometrical isomerism in oximes and disubstituted cycloalkanes.**

Optical Isomerism: **Elements of symmetry, molecular chirality, chiral and achiral molecules with two stereogenic centers.Enantiomers, diastereoisomers and Meso compounds. Resolution of enantiomers. Inversion, retention and recemisation. Relative and absolute configurations. *D, L* and *R, S* systems of nomenclature.**

Structure and Stereochemistry of Alkanes: **Conformational analysis of *n*-butane and 1,2-dibromoethane using Newman, Sawhorse and Fischer Projection formulae. Conformations of cyclohexane and methylcyclohexane. Relative stabilities of 3 to 6- membered cycloalkanes. Baeyer's strain theory and its limitations. Strains in smaller rings including cyclopropane. The banana bonds.**

Unit-III Structure, Synthesis and Reactions of Alkenes, Dienes, Alkynes and Alkyl halides: (16 Contact Hours)

Alkenes: **Preparation of alkenes from alcohols and alkyl halides through elimination reaction.Hoffman and Saytzev's rules. Mechanism and Stereochemical implications. Mechanistic details including regioselectivity and stereochemical implications of halogenation, hydrohalogenation, hydroboration, epoxidation, hydroxylation and ozonolysis. Substitution at allylic and vinylic positions of alkenes.**

Dienes: **Structure of isolated, conjugated and cumulative dienes. 1,2 and 1,4-additions of 1,3-butadiene. Mechanism and Stereochemistry of Diels's-Alder reaction. Mechanism of Birch reduction.**

Alkynes: **Structure and acidic character of alkynes. Mechanisms of addition of halogens, hydrogen, halides, hydration, hydroboration and catalytic and metal-ammonia reductions of alkynes.**

***Alkyl halides*: Classification,methods of preparation and reactions of alkyl halides. Mechanistic details of S_N1 and S_N2 E1 and E2 reactions. Effects of structure of alkyl halides, nature of nucleophiles, leaving groups, solvent and stereochemical implications of S_N reactions. Substitution versus Elimination.**

Unit-IV Aromatic Compounds and Oxygen Bearing Compounds-I:

(16 Contact Hours)

***Aromatic Electrophilic Substitution Reactions*: General mechanism of aromatic electrophilic substitution reactions. Formation of Sigma and pi-complexes with energy profile diagram. The second substitution-concept and role of activating and deactivating groups. *Ortho* and *para* ratio. Mechanisms of Fries and Claisen rearrangements and Gatterman, Huben-Hoesch,**

Veils-Meir-Haack and Riemer-Tieman reactions.

Aromatic Nucleophilic Substitution Reactions:

***Aryl halides:* Methods of preparation of aryl halides with mechanistic details of the reactions involved. Addition-Elimination and Elimination-Addition mechanisms of nucleophilic aromatic substitution reactions involving aryl halides. Mechanism of nucleophilic aromatic substitution reaction in nitroarenes.**

Oxygen bearing compounds-I:

***Alcohols:* Classification. Methods of formation of monohydric alcohols through reduction of aldehydes, ketones, carboxylic acids and esters using different reducing agents including mechanistic details of the reactions involved. Reactions of alcohols including Pinacole-Pinacolone rearrangement with mechanism. Methods of formation and the oxidative cleavage reactions of diols.**

***Epoxides:* Methods of formation and mechanism of acid/base catalysed ring openings of epoxides. Reactions of Grignard and organolithium reagents with epoxides.**

***Ethers:* Mechanisms involved in the synthetic procedures of ethers, their cleavage and auto-oxidation.**

Books Recommended

1. **A textbook of Organic Chemistry; R.K. Bansal; 4th ed.; Wiley-Eastern; 2003.**
2. **Organic Chemistry; Vol I & II; I. L. Finar; 6th ed.; ELBS; 2004.**
3. **Organic Chemistry; Morrison and Boyd; 6th ed.; PHI; 2003.**
4. **Organic Chemistry Reaction Mechanism; R. K. Bansal; 3rd ed., 2003.**
5. **Advanced Organic Reaction Mechanism; Peter Sykes; 6th ed.; Orient Longmann; 2007.**
6. **Reaction Mechanismin in Organic Chemistry;Mukherji and Singh; 3rd ed.; Macmillan; 2007.**
7. **Advanced Organic Chemistry; Jerry March, 6th ed.; Wiley; 2001.**
8. **Chemistry of Organic Compounds; Eliel; TMH; 2003.**
9. **Organic Chemistry; Vol I & II; Roger Macomber; Viva Books private Ltd; 2004.**
10. **Organic chemistry; I.G.Wade; 5th ed.; Prentice Hall; 2004.**
11. **Organic Chemistry; Solomons and Fryhle; 10th ed.; John-wiley; 2012.**

Chemistry
Effective from academic session-2016
B.Sc. III Semester
Physical Chemistry

Course No: CHB-301 ***Max. Marks: 100***
Course Weightage: 04 Credit ***End Term Exam: 80***
No. of Contact Hours: 64 ***Continuous Assessment: 20***

Unit- I Mathematical Concept& Chemical Kinetics: (16 Contact Hours)

Mathematical Concepts: Mathematical functions; Important families of functions - linear and quadratic algebraic functions; logarithmic, exponential and trigonometric functions – and their graphical representation. Calculation of slopes of linear functions. Differentiation of functions like kx, x^n, e^x, sinx, cosx, logx, u.v u/v; rules for differentiations. Geometrical interpretation of the derivative, maxima and minima, partial differentiation.

Integration of some useful functions- x^n, 1/x, $1/x^n$, lnx, sinx, cosx, e^x ,1/[x(x-a)] – rules of integration, integration by substitution; indefinite and definite integral. Permutations and combinations.

Chemical Kinetics: Order of reaction; derivation of rate equations for second (two reactants) and third order reactions. Determination of order of reaction by differential rate, integration, half life period and isolation methods.

Techniques for kinetic investigation: Conductometry, Potentiometry, Polarimetry and Spectrophotometry.

Temperature dependence of reaction rates:-Arrhenius equation, concept of activation energy.

Unit-II Gaseous and Liquid State: (16 Contact Hours)

Gaseous State: Deviation of gases from ideal behavior, van der Waal's equation of state.

Critical Phenomenon**:** PV isotherms of real gases, continuity of states, the isotherms of van der Waal's equation. Relationship between critical constants and van der Waal's constants, the law of corresponding states, reduced equation of state.

Molecular velocities**:** Root mean square, average and most probable velocities; qualitative discussion of the Maxwell's distribution of molecular velocities. Collision number, mean free path and collision diameter.

Liquid State: Liquification of gases and adiabatic expansion. Intermolecular forces.Structure of liquids (a qualitative description), structural differences between solids, liquids and gases.

(16 Contact

Unit-III Liquid Crystals and solid state:

Hours)

Liquid crystals: Differences between liquid crystal, solid and liquid. Classification of liquid crystals based on structure - nematic, smectic and cholesteric phases Thermography and seven segment cell.

Solid State: Laws of crystallography: (i) Law of constancy of interfacial angles (ii) Law of rational indices and (iii) Law of symmetry

Symmetry elements in crystals, Lattice planes and Miller indices. X-ray diffraction by crystals, derivation of Bragg's equation and its application. Interplanar distances in terms of miller indices. Determination of crystal structure by Laue's method and powder method. Systematic absence of diffraction lines in the X-ray pattern of cubic crystals with reference to NaCl, KCl & CsCl. Point defects in solids: Schottky and Frenkel ; Semiconductors: intrinsic and extrinsic

Unit- IV Thermodynamics: (16 hrs)

Thermodynamic functions: State and path functions and their differentials. Thermodynamic processes. Concept of heat and work.Heat capacity, heat capacities at constant volume and constant pressure and their relationship.Joule's law, Joule-Thomson coefficient and inversion temperature.Calculation of ΔU &ΔH for the expansion of ideal and non-ideal (van der Waals) gases under isothermal and adiabatic conditions.Temperature dependence of enthalpy, Kirchhoff's equation.

Bond dissociation energy and its calculation from thermo-chemical data with applications.

Second law of thermodynamics: Need for the law, different statements of the law. Carnot cycle and its efficiency, Carnot theorem.Thermodynamic scale of temperature.

Concept of entropy, entropy as a function of V&T, and as a function of P&T. Clausius inequality; entropy as criteria for spontaneity and equilibrium. Entropy change in physical processes, ideal gas expansion and entropy of mixing of ideal gases.

Third law of thermodynamics: Gibbs function (G) and Helmholtz function (A) as thermodynamic quantities, Nernst heat theorem, third law of thermodynamics, concept of residual entropy, evaluation of absolute entropy from heat capacity data. ΔG &ΔA as criteria for thermodynamic equilibrium and spontaneity.their advantage over entropy change. Variation of G and A with P, V and T, Gibbs-Helmholtz equation.

Books Recommended:

1. Principals of Physical Chemistry; Puri, Sharma and Pathania; S. Nagin Chand & Co; 2011.
2. The Elements of Physical Chemistry; P. W. Atkins; Oxford University Press;
3. Physical Chemistry; G. M. Barrow; McGraw-Hill; 5th ed.;International Student edition; 1992.
4. Physical Chemistry; R. A. Alberty; Wiley; Eastern Ltd.
5. Essentials of Physical Chemistry; Vols III & IV; K. L. Kapoor; 2nd ed.; Macmillan India Ltd; 2005.
6. Physical Chemistry through Problems; S. K. Dogra; Wiley Eastern Ltd; 1991.
7. University general Chemistry; C. N. R. Rao; MacMillan.

B.Sc. IVth Semester

Inorganic Chemistry

Course No: CHB-401 ***Max. Marks: 100***
Course Weightage: 04 Credit ***End Term Exam: 80***
No. of Contact Hours: 64 ***Continuous Assessment: 20***

Unit-I p-Block Elements (16-18) and Nuclear Chemistry: (16 Contact Hours)

p-Block Elements (16-18):

Oxygen**:** Chemistry of different forms (atomic , molecular and ozone).
Oxides, Fluorides and Oxyacids of Sulphur: Properties, Structure & Bonding.
Hydrogen Peroxide: Preparation, Properties and Uses.

Halogens: Comparative chemical reactivity, Types, Properties, Structure & Bonding of hydrogen halides, Interhalogens and Polyhalides. Oxyacids of Chlorine: Structure and Bonding.

Noble gases*:* Isolation and importance of noble gases in theoretical chemistry.
Fluoride, oxides and oxyfluorides of Xenon: Structure and bonding (VB and MO treatment) ***Nuclear Chemistry*****:** Nuclear Reactions: Types, Compound nucleus, Threshold energy and Nuclear cross section.

Isotope Separation Methods**:** Gaseous and thermal diffusion; electromagnetic and chemical exchange methods.

Applications of Radioisotopes**:** Chemistry, Industry, Agriculture and Medicine. Neutron activation and Isotope dilution analyses.

Detection and measurement of radiation**:** Gas ionization detectors and Scintillation counters. ***Radiation Chemistry***: Units of radiation; LET and G-Value. Radiation Chemistry of oxygen and water.

Unit-II Transition and Inner-Transition Elements: (16 Contact Hours)

Transition Elements**:** Variation in atomic and ionic sizes, Ionization enthalpies, Variable oxidation states. Standard electrode Potentials of M^{2+} / M and M^{3+} / M^{2+} systems.
Ionic / Covalent and Acidic / Basic character of transition metal oxides in various oxidation states. Stabilization of unusual oxidation states.
Spectral and Magnetic Properties; Calculation and Uses of magnetic moment value.
Interstitial Hydrides, Carbides and Oxides of first transition series:- Preparation, Properties & Uses.

Inner-Transition Elements: Electronic Configuration, Oxidation States, Magnetic Properties and Complexing behavour of inner transition elements.
Cause and Consequences of Lanthanoid / Actinoid Contraction.

Separation of Lathanoids: Fractional Crystallization, Ion–exchange and Solvent extraction methods.

Unit-III Coordination and Bioinorganic Chemistry: (16 Contact Hours)

Coordination Chemistry:

Experimental verification of Werner's theory. Effective Atomic number: Concept and its significance.

Stereochemistry of Coordination compounds: With coordination numbers 2-6; Optical and Geometrical isomers of MA_4B_2, MA_3B_3 and MABCD type Complexes.

***Bonding in Complexes*:** Comparison of valence bond and Crystal field theories; CFT of tetrahedral, square planner and octahedral systems. Factors affecting magnitude of Δ ; pairing energy and CFSE of weak and strong field ligands.

Limitations of Crystal field theory. Applications of Coordination compounds.

Bioinorganic Chemistry:

Biomolecules and their Metal coordination behaviour: Proteins, Nucleic acids and Lipids.

Abundance of elements in living systems; Concept and Criteria for essentiality of elements in living systems.

Distribution and biological role of essential elements in life: Na^+, K^+, Ca^{2+}, Mg^{2+}, Fe^{2+} and halogens.

Hemoglobin & Chlorophyl : Structure and Biological role.

Unit-IV Inorganic Quantitative Analyses: (16 Contact Hours)

Gravimetry: Definition, Preparation of standard solution and precipitation methods.

Physical properties of precipitates: Appearance, particle size and purity; Fractional precipitation.

Colloidal State: Supersaturation, Precipitate formation, Co-precipitation and Post– precipitation; Digestion, Washing, Ignition and Gravimetric Calculations.

Titrimetry: Definition, Types, Primary and Secondary standard substances and preparation of standard solutions.

Indicators: Types, Criteria of selection, Mechanisms of action (Acid base and Redox). Theory of visual titration of acids and bases.

Precipitation Titrations: Underlying principles and detection of equivalence points (Mohr, Volhard, Fajan's and Nephelometric methods).

***Redox Reagents*:** Their equivalent weights, Redox potentials and applications in Volumetric Analysis.

***Data Evaluation*:** Accuracy and precision, Types of errors; Mean and standard deviations.

Books Recommended

1. Basic Inorganic Chemistry; F.A . Cotton; G. Wilkinson & P.L. Gauss; 3rd ed.; Wiley; 2002.
2. Chemistry of Elements; Greenwood Earnshaw; 2nd Ed.; Butterworth; 2000.
3. Advanced Inorganic Chemistry; Volume 1; S. Prakash, G.D. Tuli, S.K. Basu & R.D . Madan; S.Chand & Company Ltd;

4. Essentials of Nuclear Chemistry; H.J.Arnikar; 4th ed.; New Age; 2002.
5. Principles of Radiation Chemistry; O. Donnell, Sangster & Edward Arnold; 1970.
6. Introduction to Nuclear Chemistry; D.J.Carswell; Elsevier; 1967.
7. Coordination Chemistry; D.Banerjee; Tata Mc Graw Hill; 1997.
8. Concise Coordination Chemistry; R. Gopalan & V. Ramalingam; Vikas; 2003.
9. The Biological Chemistry of Elements; J.J. R. Frausto de Silva & R.J.P. Williams; Oxford; 1994.
10. Bio-inorganic Chemistry of Elements; K. Hussain Reddy; New Age; 2005.
11. Vogel's Text of Quantitative Inorganic Analysis; J. Bassett; R.C. Denny; 6th ed.; ELBS; 2007.
12. Analytical Chemistry; G.D. Christian; 6th ed.; Wiley; 2008.

B.Sc. Vth Semester

Organic Chemistry

Course No: CHB-501 ***Max. Marks: 100***
Course Weightage: 04 Credit ***End Term Exam: 80***
No. of Contact Hours: 64 ***Continuous Assessment: 20***

Unit-I Oxygen bearing Compounds-II :

(16 Contact Hours)

Aldehydes and Ketones: Structure and reactivity of carbonyl groups. Synthesis of aldehydes starting from acid chlorides and those of ketones from nitriles, carboxylic acids and 1,3-dithianes. Stereochemistry and mechanism of nucleophilic additions to carbonyl groups. Cram's rule.

Mechanisms involved in Benzoin, Aldol/Cross Aldol, Perkin,Knoevenegal,Cannizzaro and Mannich condensations/reactions. Meerwein-Pondroff-Verly, Clemmenson and Wolf-Kishner reductions and Baeyer-Villegar & Oppenaur Oxidations. Mechanisms of acid and base catalysed halogenation in aldehydes and ketones.

Carboxylic acids and their derivatives**:** Structure of carboxylic group. Factors affecting strength of carboxylic acids. Mechanistic details of preparation of carboxylic acids using Grignard reagent and from hydrolysis of nitriles. Mechanisms involved in the HVZ reaction, conversion of acids to corresponding chlorides, esters, anhydrides and amides. Relative stabilities and interconversion of acid derivatives into one another. Reduction of carboxylic acids and their derivatives. Transesterification and hydrolysis of esters.

Applications of Ethylacetoacetate and Malonic ester in organic synthesis.

Unit-II Amines and Nitrogen bearing Heterocyclic compounds:

(16 Contact Hours)

Amines: Classification and factors affecting basicity of amines.Mechanistic detailes(wherever applicable) of methods of formation of alkyl and arylamines through reduction of nitro compounds and nitriles.Gabriel-Phthalamide reaction and Hofmann rearrangement. Mechanisms involved in the formation and reactions of arenediazonium salts including Azo coupling.

Heterocyclic compounds bearing one nitrogen atom: Stuctural features of pyrrole,pyrrolidine, pyridine and piperidine and comparative account of their basic strength.Aromaticity and electrophilic substitution reactions of pyrrole and their comparison with those of furan and thiophene.Mechanisms involved in the preparations of Indole and quinoline using Fischer-Indole and Bishlier-Napierlaski syntheses.

Unit-III Biomolecules: (16 Contact Hours)

Carbohydrates: Introduction, classification, D&L-system of Nomenclature, and Cyclisation of Monosaccharides. Determination of ring size of D-glucose. Mechanisms of formation of

osazones, glycosides, acetates and methyl ethers of monosacchrides. Chain lengthening and shortening processes of aldoses. Mechanism of Mutarotation. Chemistry of sucrose, maltose and lactose.

Nucleic Acids: Introductions, structural features of Nucleosides, Nucleotides, RNA and DNA.

Amino acids, Peptides & Proteins: Introduction, classification, structure and stereochemistry of amino acids. Acid-base behaviour and isoelectric points. Methods of formation and reactions of alpha-amino acids. Structure determination of dipeptides through end group analysis and selective hydrolysis and their classical and solid phase syntheses. Primary, Secondary, Tertiary and Quaternary structures of proteins.

Lipids: Definition and classification. Structural features of triglycerides. Common fatty acids in Naturally Occurring Fats and Oils. Hydrogenation of Oils. Saponification, Iodine and Acid values and their significance.

Unit-IV Organic Spectroscopy: (16 Contact Hours)

Ultraviolet Spectroscopy: The electromagnetic spectrum. Beer-Lambert law, molar absorptivity, presentation and analysis of electronic spectra. Types of electronic excitations. Effects of conjugation and solvents on absorption. Chromophores and auxochromes. Bathochromic and hypsochromic shifts. Ultraviolet spectra of enes and enones. Prediction of maxima of enes and enones using Woodward's rules.

Infrared spectroscopy: The infrared region, Molecular vibrations, significance of Hook's law and selection rules. The infrared spectrum. Fingerprint region and its significance. Effect of resonance, inductive effect and H-bonding on infrared absorptions. Characteristic absorptions of Alkanes, alkenes, alkynes, alcohols, ethers, carbonyl compounds, amines and carboxylic acids and their derivatives.

Nuclear Magnetic Resonance Spectroscopy: Basic principles of NMR spectroscopy. Shielding and deshielding of protons. The chemical shift. Equivalent and non-equivalent protons. Spin-spin splitting, coupling constants for vicinal, geminal and long range couplings. Characteristic functional group NMR absorptions. The NMR spectra of ethyl bromide, ethanol, acetaldehyde, ethyl acetate, methyl propionate, toluene and acetophenone.

Books Recommended

1. A textbook of Organic Chemistry; R.K. Bansal; 4th ed.; Wiley-Eastern; 2003
2. Organic Chemistry; Vol I & II; I. L. Finar; 6th ed.; ELBS; 2004.
3. Organic Chemistry; Morrison and Boyd; 6th ed.; PHI; 2003.
4. Organic Chemistry Reaction Mechanism; R. K. Bansal; 3rd ed.; 2003.
5. Advanced Organic Reaction Mechanism; Peter Sykes, 6th ed.; Orient Longmann; 2007.
6. Reaction Mechanism in Organic Chemistry; Mukherji and Singh., 3rd ed.; Macmillan; 2007.
7. Chemistry of Organic Compounds; Eliel; TMH; 2003.
8. Organic Chemistry; Vol I & II; Roger Macomber; Viva Books private Ltd; 2004.
9. Organic Chemistry; I.G.Wade; 5th ed.; Prentice Hall; 2004.
10. Fundamentals of Organic Chemistry; Solomons and Fryhle; 10th ed.; John-Wiley; 2012.

B.Sc. VIth Semester

Physical Chemistry

Course No: CHB-601 ***Max. Marks: 100***
Course Weightage: 04 Credit ***End Term Exam: 80***
No. of Contact Hours: 64 ***Continuous Assessment: 20***

Unit- I Equilibrium & Solution thermodynamics: (16 Contact Hours)

Equilibrium: Equilibrium constant and free energy change. Thermodynamic derivation of law of mass action.Reaction isotherm and reaction isochore, Clapeyron equation and Clausius-Clapeyron equation, applications.

Phase rule*:* Meaning of the terms: phase, component and degree of freedom, statement and derivation of Gibbs phase rule, phase diagrams of one component system – water andsulphur systems.

Phase equilibria of two component system: solid-liquid equilibria, simple eutectic system (Pb-Ag), desilverisation of lead.

Solid solutions - compound formation with congruent melting point (Mg-Zn) and incongruent melting point ($FeCl_3$-H_2O systems). Freezing mixtures, acetone- dry ice.

Liquid-liquid mixtures: Ideal liquid mixtures, Raoult's and Henry's law. Non-ideal systems, azeotropes (HC1-H_2O and C_2H_5OH-H_2O systems.)

Partially miscible liquids: Lower and upper consolute temperatures, (examples of phenol-water, trimethylamine-water, nicotine-water systems).

Nernst distribution law: Statement and thermodynamic derivation, applications.

Thermodynamics of Solutions**:** Thermodynamics of elevation in .boiling point and depression in freezing point. Activity and activity coefficient, determination of activity and activity coefficient with freezing point and EMF methods. Excess thermodynamic functions of non-ideal solutions.

Unit-II Electrochemistry: (16 Contact Hours)

Migration of ions and Kohlrausch's law, Arrhenius theory of electrolyte dissociation and its limitations. Debye-Huckel-Onsager's equation for strong electrolytes (elementary treatment without derivation). Transport number, definition and determination by Hittorf's and moving boundary methods. Application of conductivity measurements: determination of degree of dissociation and dissociation constants of acids, solubility product of a sparingly soluble salt, conductometric titrations.

Types of reversible electrodes (half-cells): metal-metal ion, gas-metal-ion, metal-insoluble salt-anion and redox electrodes. Standard hydrogen electrode, glass electrode, reference electrodes (calomel, Ag/AgCl). Electrode reactions, Nernst equation and cell E.M.F. Electrochemical series and its significance.

Electrolytic and Galvanic cells.Measurement of EMF of a cell.Concentration cells, electrolyte concentration cell (with and without transport), electrode concentration cell.

Application of standard potentials: determination of thermodynamic functions of cell reactions (ΔG, ΔH and K.), pH and pKa, solubility product and activity coefficient; potentiometric titrations.

Unit-III Chemical kinetics &Photochemistry: (16 Contact Hours)

Theories of chemical kinetics*:* Simple collision theory based on hard sphere model, evaluation of rate constants of atomic reactions, extension to molecular reactions, limitations. Brief idea of transition state theory (equilibrium hypothesis).

Catalysis: Characteristics of catalyzed reactions, Acid-Base catalysis with examples

Photochemistry: Interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry.Grothus-Drapper law, Stark-Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing) quantum yield, photosensitized reactions, energy transfer processes (simple examples).

Kinetics of photochemical reactions: Photochemical decomposition of hydrogen iodide. Hydrogen-chlorine and hydrogen-bromine reactions, Comparison with thermal decomposition reactions

Unit- IV Quantum Chemistry& Spectroscopy: (16 Contact Hours)

Limitation of Classical mechanics**:** Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids and atomic spectra.

Introduction to operators. Linear and Hermitian operators, Hamiltonian operator, commutation of operators. Schrodinger wave equation and its importance, physical interpretation of the wave function, postulates of quantum mechanics, detailed treatment of particle in a one dimensional box.

Molecular orbital theory; basic ideas, criteria for forming M.O's from AO's. Construction of M.O's by LCAO, H_2^+ ion(expressions for bonding and antibonding MOs and their energies), physical picture of bonding and antibonding wave functions, concept of σ, σ^*, π and π^*orbitals and their characteristics.

Spectroscopy**:** Electromagnetic radiation, regions of the spectrum, basic features of different spectrometers. Statement of Born-Oppenheimer approximation.

Rotational spectrum**:** Moment of inertia, classification of molecules on the basis of moment of inertia. Energy of a rigid diatomic rotor, selection rules for rotational transition and associated spectrum, relative population of rotational levels and spectral intensity, determination of bond length.

Vibrational Spectrum*:* Classical and quantum mechanical (qualitative) treatment of simple harmonic oscillator, selection rules for vibrational transition, pure vibrational spectrum of a diatomic molecule, determination of force constant, relation of force constant with bond length and bond energy, vibrational degrees of freedom, idea of vibrational frequencies of different functional groups.

Books Recommended:

1. Principals of Physical Chemistry; Puri, Sharma and Pathania; S. Nagin Chand & Co; 2011.
2. The Elements of Physical Chemistry; P. W. Atkins; Oxford University Press;
3. Physical Chemistry; G. M. Barrow; McGraw-Hill; 5th ed.;International Student edition; 1992.
4. Physical Chemistry; Alberty , Selby etc ; Wiley Eastern Ltd.
5. Physical Chemistry through Problems; S. K. Dogra; Wiley Eastern Ltd; 1991.
6. Physical Chemistry; Monk, John Wiley & Sons
7. Physical Chemistry; A Molecular Approach, McQuarie, Viva Pvt. Ltd.
8. Physical Chemistry; Ball, Cengage Learning.
9. University general Chemistry; C. N. R. Rao; MacMillan.