Dr. A.P.J. Abdul Kalam University, Indore

Semester – I

COURSE	Subject Title	Subject Code
B.Sc. (Major)	**CHEMISTRY**	BSCY-101T

Course Learning Outcomes (CLO)

By the end of this course students will learn the following aspects of chemistry:

1. Ancient Indian chemical techniques.
2. Various theories and principles applied to reveal atomic structure.
3. Significance of quantum numbers.
4. Concept of periodic properties of elements.
5. Theories related to chemical bonding.
6. Acid-base concept, ph, buffer.
7. Factors responsible for reactivity of organic molecules.
8. Basics and mechanism of chemical kinetics.
9. Properties of electrolytes.

CONTENT

Unit - 1

(a) Chemical techniques in ancient India: General Introduction

(b) Contribution of ancient Indian scientists in chemistry eg, metallurgy, dyes, pigments, cosmetics, Ayurveda, Charak Sanhita.

Atomic structure

(i) Review of Bohr's theory and its limitations. Atomic spectrum of Hydrogen. Dual nature of particles and waves, de Broglie's equation, Heisenberg's Uncertainty principle and its significance.

(ii) Quantum numbers and their significance. Rules for filling electrons in various orbitals. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity. Aufbau principle and its limitations, Variation of orbital energy with atomic number.

Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

Unit - 2

Elementary idea of the following properties of the elements with reference to s & p-block elements in periodic table.

- Effective nuclear number (EAN), 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)

Detailed discussion of the following properties of the elements, with reference to s & p-blocks.

- Ionization energy Successive ionization energy and factors affecting ionization energy. Applications of ionization energy.

- Electronegativity-Pauling's/ Mulliken's electronegativity scales.

Variation of electronegativity with bond order, partial charge, hybridization.

Unit - 3

Chemical Bonding

i. Ionic Bonding: General characteristics of ionic bonding.

Ionic bonding &Energy: lattice & solvation energies and their importance in the context of stability and solubility of ionic compounds.

Statement of Born-Landé equation for calculation of lattice energy. Madelung constant. Born-Haber cycle and its applications. Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules.

ii. Covalent bonding: Lewis structure, Valence Bond theory (Heitler- London approach).

Hybridization-Concept, types (SP, SP, SP, dSP d'Sp' with suitable examples of inorganic and organic molecules

Ionic character in covalent compounds- dipole moment and percentage, ionic character,

Valence shell electron pair repulsion theory (VSEPR) theory: Assumptions, need of theory, application of theory to explain geometries or shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear. trigonal planar, square planar. tetrahedral, trigonal bipyramidal and octahedral arrangements such as: NH, HO, SF, CIF). PCs. SF. CIFs, XeF4

*** Molecular orbital (MO) concept of bonding**

The approximations of the theory, Linear combination (LCAO) (elementary pictorial approach)

Rules for the LCAO method, bonding and antibonding MOS. Characteristics for s-s. s-p and p-combinations of atomic orbitals, nonbonding combination of orbitals.

MO diagrams of homonuclear diatomic molecules: H, Li, Beg, B, C, N, O_2, F, and their ions.

Molecular orbitals of heteronuclear diatomic molecules: CO, NO, CN, HF.

*** Bond parameters:**

Definition and factors affecting bond orders, bond lengths, bond angles.

Unit - 4

Acid-Base concept

Arrhenius concept. Bronsted-Lowry's concept, conjugate acids and bases. relative strength of acids, Lewis concept.pH, buffer solutions. Acid-base neutralisation curves, Handerson equation.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values.

Indicator, choice of indicators.

Unit - 5

(a) Fundamentals of Organic Chemistry Structure, shape and reactivity of organic molecules: Physical Effects, Electronic Displacements: Inductive Effect,Electromeric Effect, , Resonance and Hyperconjugation,

Cleavage of Bonds: Homolysis and Heterolysis.

Reactive Intermediates: Carbocations, Carbanions and free radicals, Nucleophiles and electrophiles.

(b) Stereochemistry of Organic compounds:

Concept of isomerism.

Geometrical isomerism:

Determination of configuration of geometric isomers. E & Z system of nomenclature, geometrie isomerism in oximes and alicyclic compounds.

Optical isomerism:

Elements of symmetry, molecular chirality, enantiomers & their properties, stereogeniccentre, optical activity of enantiomers. Concept of chirality (up to two carbon atoms): chiral and achiral molecules with two stereogeniccentres, diastereomers, threo and erythroisomers, meso isomer, resolution of enantiomers, inversion, retention and racemization.

Relative and absolute configuration. sequence rules. D & L and R & S systems of nomenclature.

Conformations and Conformational analysis

Conformations of ethane, butane and cyclohexane. Interconversion of Wedge formula, Newman, Sawhorse and Fischer representations.

Unit - 6

Chemical Kinetics:

Rate of reaction, Definition and difference of order and molecularity. Derivation of rate constants for first, second, third and zero order reactions and examples. Derivation for half-life period. Methods to determine the order of reactions. Effect of temperature on rate of reaction. Arrhenius equation, concept of activation energy.

Ionic Equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Solubility and solubility product of sparingly soluble salts-applications of solubility product.

Practical

Qualitative inorganic analysis

Identification of simple inorganic mixture (5 radicals) with two/three acidic and two/three basic radicals (including typical combinations), special emphasis on learning theoretical concepts of strong, moderate and weak electrolytes, ionic product, common ion effect. Solubility and solubility product.

Qualitative organic analysis

1. Detection of hetero-elements (N, S, Cl, Br. 1) in organic compounds

2. Functional group tests for alcohol, aldehyde, carboxylic acid, carbohydrate, phenols, nitro, amine and amide.

Quantitative analysis of acid, alkali and buffer solutions

Ionic Equilibria

1. Measurement of pH of different solutions of acids and alkalies using pH- meter (may use aerated drinks, fruit juices, shampoos and soaps).

Note - use dilute solutions of soaps and shampoos to prevent damage to the glass electrode.

2. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

3. Preparation of buffer solutions and determination of their pH and buffer capacity:

(i) Sodium acetate-acetic acid

(ii) Ammonium chloride- ammonium hydroxide.

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Semester-I

COURSE	Subject Title	Subject Code
B.Sc. (Minor)	**Chemistry (Analytical Chemistry)-II**	BSCY102T

Course Learning Outcomes (CLO)

By the end of this course students will learn the following aspects of laboratory exercises in chemistry:
1. Basic concepts of Mathematics for Chemists.
2. Fundamentals of analytical chemistry and steps involved in analysis.
3. Basic knowledge of Computer for chemists.
4. Basic Concepts of Chemical equilibrium.
5. Principles of Chromatography and chromatographic techniques.
6. Various techniques of Spectroscopic Analysis.

CONTENT

Unit - 1

Mathematics for Chemists

Straight line equation, Logarithmic relations, curve sketching, linear graphs & calculation of slopes. Differentiation, differentiation of functions like kex". sinx, logx. maxima & minima.partial differentiation. Integration of some useful relevant functions.

Unit - 2

Basic Analytical Chemistry: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures. statistical terms: mean, mean deviation, median, standard deviation, Numerical Problems.

Calculations used in Analytical Chemistry

Some Important units of measurements- SI Units, distinction between mass and weight, mole, milli mole and Numerical Problems.

Solution and their concentrations-Concept of Molarity, molality and normality. Expressing the concentration in parts per million (ppm), parts per billion (ppb). Numerical Problems.

Chemical Stoichiometry- Empirical and Molecular Formulas, Stoichiometric Calculations, Numerical Problems.

Unit - 3

Computer for Chemists

Introduction to computer. Introduction to operating systems like -DOS. Windows, Linux and Ubuntu

Use of computer programs

Running of standard programs & packages such as MS-word, MS-excel. PowerPoint, Execution of linear regression x-y Plot. Use of softwares for drawing structures and molecular formulae.

Unit - 4

Chemical Equilibrium: Equilibrium constant and free energy, concept of chemical potential. Thermodynamic derivation of law of chemical equilibrium. Temperature dependence of equilibrium constant; Van't Hoff reaction isochore, Van't Hoff reaction isotherm. Le-Chatelier's principle and its applications.

Unit - 5

Chromatography

Introduction. Principle and Classification. Mechanism of separation: adsorption, partition & ion-exchange.

Development of chromatograms: frontal. elution and displacement methods.

Paper Chromatography, (ascending, descending and circular). Thin Layer Chromatography (TLC) and Column Chromatography (CC). Gas Chromatography (GC) and High Pressure Liquid Chromatography (HPLC), types of column and column selection, applications, limitations.

Principle and Applications of:

Flash chromatography, lon-exchange chromatography and Chiral chromatography.

Unit - 6

Spectral techniques of analysis

Basics of absorption spectroscopy: Electromagnetic radiation Spectral range. Absorbance. Absorptivity. Molar Absorptivity. Fundamental Laws of Absorption. Lambert-Beer Law and its limitations.

Constitution & working of photometer, spectrometer, colorimeter.

Ultraviolet (UV) absorption spectroscopy-

Presentation and analysis of UV spectra. Types of electronic transitions. Effect of conjugation. Concept of chromophore and auxochrome. Bathochromic, hypsochromic, Hyperchromic and hypochromic shifts. UV spectra of conjugated polyenes and enones.

Infra-red (IR) absorption spectroscopy-

Molecular vibrations, Hooke's law, selection rules, intensity and position of IR bands, Measurement of IR spectrum, finger print region, characteristic absorption of various functional groups and interpretation of IR spectra of simple organic compounds.

Practical

1 **Basic analytical exercises**

Calibration of different weights and glassapparatus (measuring cylinder. burette, pipette, volumetric flasks).

• Preparation of solutions of different molarity/normality by weighing and dilution.

2. Quantitative Analysis

Titrimetric Analysis

- Standardization of NaOH with Oxalic acid.

- Determination of carbonate and hydroxide present in mixture.

- Determinationof carbonate and bicarbonate present in a mixture.

- Determinationof free alkali present in different soaps/detergents.

3. Quantitative Analysis by Colorimetry

- Verification of Lambert-Beer Law

- Determination of concentration of coloured compounds (e.g.. CuSO KMnO4

4. Qualitative Analysis

-Systematic identification of organic compound by qualitative analysis.

- Chromatography:

Identification by determination of the Rvalues of the given organic/ inorganic compounds by paper/ thin layer chromatography.