

BACHELORS WITH NANOTECHNOLOGY AS MINOR (CT – I)**2nd SEMESTER****NTY223N: NANOTECHNOLOGY _ ESSENTIALS OF CHEMISTRY IN NANOTECHNOLOGY****CREDITS: THEORY: 04 (60L), PRACTICALS: 02 (60 HRS)****COURSE OBJECTIVES**

This course places emphasis on imparting the essential concepts and principles of Chemistry necessary for comprehending various important and essential aspects of Nanoscience and Nanotechnology.

COURSE OUTCOME

- Successful completion of this course will enable the students to understand the underlying principles of Nanoscience and Nanotechnology.
- This course will also act as the stepping stone for grasping the more advanced concepts encountered towards the end of this programme.

UNIT I**(15 LECTURES)**

Atomic Structure: Wave Mechanical concept of Atomic Structure: de-Broglie's wave equation; derivation and experimental verification. Heisenberg's Uncertainty Principle: Illustration and significance. Confirmation of quantization of angular momentum and its significance. Wavefunction and its significance, radial and angular wave functions for hydrogen atom. Radial and angular distribution curves; Shapes of s, p & d orbitals; Effective nuclear charge and its calculation by Slater rules.

Periodic Properties: Trends in Atomic, Ionic, Metallic and Van der 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 behaviour of elements.

UNIT II**(15 LECTURES)**

Chemical Bonding: 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. Types of intermolecular forces: Hydrogen bonding, Dipole-dipole forces, London forces and ion-dipole forces. Significance of such forces.

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 (BF₃, NH₃, H₂O, SF₄, ClF₃ and XeF₂)

Molecular Orbital Theory: Energy level diagrams, Bond order with its significance and application to simple molecules (N₂, O₂, HCl and CO).

UNIT III**(15 LECTURES)**

Basic Concepts in Organic Chemistry: Inductive and Electromeric effects. Conjugation, Resonance and Hyperconjugation. *Reactive intermediates:* Structure, generation and stability of Carbocations, Carbanions, Free radicals, Carbenes, Benzynes and Nitrenes.

Concept and types of stereoisomerism. Geometrical Isomerism: Configuration of geometrical isomers. E and Z system of nomenclature. 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 racemization. Relative and absolute configurations. D, L and R, S systems of nomenclature.

UNIT IV**(15 LECTURES)**

Essential Concepts in Physical Chemistry: Order of reaction; derivation of rate equations for second and third order reactions (one reactant only). Determination of order of reaction by differential rate, integration, half-life period and isolation methods. Temperature dependence of reaction rates: Arrhenius equation, concept of activation energy.

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.

Equilibrium: Concept of Free energy, Equilibrium constant and free energy change. 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 of Gibbs phase rule, phase diagrams of one component system – water.

Electrochemistry: Arrhenius theory of electrolyte dissociation and its limitations. Migration of ions and Kohlrausch's law, Debye-Huckel-Onsager's equation for strong electrolytes (elementary treatment).

PRACTICALS (2 CREDITS: 60 HOURS)

- Preparation of solutions of different concentrations; Standardization of solutions (acids and bases).
- Volumetric estimation of oxalic acid by titrating it with KMnO₄.
- Determination of ferrous ions by dichromate method using titrimetric method.
- Purification of organic compounds by crystallization (from water and alcohol) and sublimation.
- Detection of N, S and halogens in organic compounds.
- Measurement of density and relative density of various liquids using pycnometer / density bottle.
- Determination of heat capacity of calorimeter for different volumes.
- Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide

BOOKS (PRESCRIBED / RECOMMENDED):

- *Basic Inorganic Chemistry*; F.A. Cotton, G Wilkinson & P.L. Gaus; 3rd ed.; Wiley; 2002.
- *Concise Inorganic Chemistry*; J.D. Lee; 5th ed.; ELBS; 2003
- *Inorganic Chemistry*; D.E. Shriver; P.W. Atkins & C.H. Langford; 4th ed.; Oxford; 2006
- *Principles of Physical Chemistry*; Puri, Sharma and Pathania; S. Nagin Chand & Co; 2011
- *Physical Chemistry; A Molecular Approach*, McQuarrie, Viva Pvt. Ltd., 2021
- *The Elements of Physical Chemistry*; P. W. Atkins; 7th ed., Oxford University Press; 2016
- *Organic chemistry (8th Ed)*; Bruice, Paula Yurkanis, Pearson Prentice Hall, 2007
- *Organic Chemistry by John E McMurry (8th Edition)* Pearson Education, 2011
- *Svehla, G. Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- *Mendham, J. Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- *Comprehensive Practical Organic Chemistry: Qualitative analysis Ahluwalia, V.K. & Sunita Dhingra; Universities Press, India, 2004.*
- *Advanced Practical Organic Chemistry*; N. K. Vishnoi; 3rd Edn; Vikas Publishing, 2009.
- *Advanced Practical Physical Chemistry*; J.B. Yadav; Krishna Prakashan Media (P) Limited, 2015.