



## CHEMISTRY

(Major)

(1<sup>st</sup> Semester)

Course No.: CHM-DSC-101

(Inorganic Chemistry -I)

*Atomic Structure, Chemical Bonding and Metallurgy*

**Contact Hours: 45; Credits: 03**

**Full Marks = 100**[End Semester Exam (70) Internal Assessment (30)]

**Pass Marks = 40** [End Semester Exam (28) Internal Assessment (12)]

### UNIT-1: 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  $\psi$  and  $\psi^2$ . Quantum numbers and their significance. Normalized and orthogonal wave functions. 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-2: Periodicity of Elements

s-, p-, d-, f- block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to s- & p- block.

- 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 electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity.

### UNIT-3: Chemical Bonding-I

(i) *Ionic bond*: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(ii) *Covalent bond*: Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Resonance and



resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules  $N_2$ ,  $O_2$ ,  $C_2$ ,  $B_2$ ,  $F_2$ ,  $CO$ ,  $NO$ , and their ions;  $HCl$ ,  $BeF_2$ ,  $CO_2$ , (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding ( $\sigma$ - and  $\pi$ - bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

#### **UNIT-4: Chemical Bonding-II**

(i) *Metallic Bond*: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

(ii) *Weak Chemical Forces*: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Hydrogen bonding (theories of hydrogen bonding, valence bond treatment).

#### **UNIT-5: Oxidation-Reduction and Principles of Metallurgy**

Redox equations, Standard Electrode Potential and its application to inorganic reactions.

Principles involved in volumetric analysis: Fe (II) and oxalic acid using standardized  $KMnO_4$  solution, Fe (II) with  $K_2Cr_2O_7$  solution.

General Principles of Metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic processes and Mond's process, Zone refining.

#### **Reference Books:**

- Puri, Sharma, Kalia; Principles of Inorganic Chemistry, Vishal Publishing Co.
- Lee, J. D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B. E. and Mc Daniel, D. H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
- Day, M. C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.