U.G. 1st Semester

Paper: CHM101C (Core)
Inorganic Chemistry I

Credits: 5 = 4+0+1 (60 Lectures)

Theory: 60 Lectures

Unit 1: Atomic Structure (10 Lectures)

Review of Bohr's theory and its limitations, atomic spectrum of hydrogen, Wave mechanical model of atom: de Broglie equation, Heisenberg's Uncertainty Principle and concept of probability.

Schrodinger's wave equation, Significance of ψ and ψ^2, Quantum numbers and their significance, Normalized and orthogonal wave functions, Radial and angular wave functions for Hydrogen atom, Radial distribution curves, Shapes of s, p, d and f orbitals.

The concept of spin and the spin quantum numbers s and m_s (outlines only).

Pauli's exclusion Principle, Hund's rule, Aufbau principle and electron configuration of many electron atoms.

Unit 2: Periodicities of Elements (14 Lectures)

Brief discussion of the periodicity in following properties of s and p block elements:

(a) Electronic configuration, Effective nuclear charge – shielding and screening effect, Slater's rules, Variation of effective nuclear charge in periodic table.

(b) Atomic and ionic radii

(c) Ionisation enthalpy and electron gain enthalpy

(d) Electronegativity of elements – Pauling, Mulliken and Allred-Rachow's electronegativity scales, variation of electronegativity with bond order, partial charge, hybridisation, group electronegativity.

(e) Melting point and boiling point of elements and their compounds.

(f) Catenation and inert-pair effect

Unit 3: Chemical Bonding – I (14 Lectures)

Covalent bond**:** Valence Bond theory and its limitations, Types of Hybridization and shapes of simple molecules, Bent's rule, Resonance and resonance energy , Formal charge, electro neutrality principle, covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and its consequences, Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions including H_2O, NH_3, NO_2, NO_2^-, NO_2^+, PCl_3, PCl_5, SF_4, SF_6, ClF_3, I_3^-, BrF_2^+, PCl_6^-, ICl_2^-, ICl_4^-, SO_4^{2-}, CO_3^{2-} and OCF_2.

Ionic bond: types and characteristics of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Structures of common binary ionic crystals – CsCl structure, NaCl structure, ZnS structures and fluorite structure. Common ternary ionic crystals: spinel and perovskite structures. Lattice energy of ionic solids; Born-Landé equation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

Unit 4: Chemical Bonding – II (12 Lectures)

Molecular orbital theory (LCAO method) of bonding, Molecular Orbital energy level diagrams and electronic configuration of ground states of Homonuclear and Heteronuclear diatomic molecules/ions (N2, O2, C2, B2, F2, CO, NO, HCl) and simple polyatomic molecules (BeH_2, H_2O), Multiple bonding (σ and π bond approach) and bond lengths. Multicentre bonding in Diborane

Bonding in metals - Qualitative idea of valence bond theory and band theory. Semiconductors and insulators, defects in solids.

Weak Chemical Forces: Vander Waal's forces, ion-dipole forces, dipole-dipole interactions, induced dipole interaction. Hydrogen bonding (theories of hydrogen bonding, valence bond treatment). Effects of weak chemical forces, melting and boiling points, solubility, energetics of dissolution process.

Unit 5: Acid- Base Concept and Redox Chemistry (10 Lectures)

Bronsted-Lowry concept of acids and bases: relative strengths of acids, amphoterism, levelling solvents, pH and pK_a, buffer solutions. Lewis concept of acids and bases: classification of Lewis acids. Hard and soft acids and bases (HSAB) principle, application of HSAB principle.

Non-aqueous solvents: liquid ammonia, liquid sulphur dioxide, liquid HF and liquid N_2O_4.

Electrode potentials and redox behaviour in aqueous solutions. The Latimer diagram and Frost diagram, their uses.

Practical: 30 Hours

Unit 6: Inorganic Chemistry Lab (1 Credit)

(a) To determine the water of crystallization of hydrated salts (e.g. blue vitriol) by ignition and weighing.

(b) To determine the total hardness of water by titration with EDTA.

(c) To determine the water of crystallization of green vitriol by titration with $KMnO_4$ solution.

List of Suggested Books:

1. Basic Inorganic Chemistry by F.A. Cotton, G. Wilkinson, P.L. Gaus (John Wiley and Sons Ltd., Indian Edition)
2. Concise Inorganic Chemistry by J.D. Lee (John Wiley and Sons Ltd., Indian Edition)
3. Inorganic Chemistry by G.L. Meissler and D.A. Tarr (Pearson)
4. Shriver and Atkins's Inorganic Chemistry by P. Atkins, T. Overtone, J. Rourke, M. Weller and F. Armstrong (Oxford University Press, Indian Edition)
5. Inorganic Chemistry by G.D. Tuli, Manik and R.D. Madan (S. Chand)

Paper: CHM102C (Core)
Physical Chemistry I

Credits: 5=3+0+2 (45 Lectures)

Theory: 45 Lectures

Unit 1: Chemical Thermodynamics – I (15 Lectures)

Definition of thermodynamic terms: isolated, closed and open systems; the surroundings. Concepts of system internal energy U, heat transfer q and work done w; state and path functions; intensive and extensive variables (state functions). The zeroth law and the concept of temperature.

The first law (with old and new notations about the work done w), enthalpy H and its significance. Concept of thermodynamic reversibility, calculations of w, q, ΔU and ΔH during reversible, irreversible and free expansion of an ideal gas under isothermal and adiabatic conditions.

State functions and differentials; variation of internal energy and enthalpy with temperature – the heat capacities C_p and C_v; Joule-Thomson experiment and liquefaction of gases; relation between C_p and C_v in general and for ideal gases. Relation between P, V, T for adiabatic processes in an ideal gas.

Thermochemistry – standard states; standard enthalpy changes for formation, combustion, etc. Reactions. Relation of reaction enthalpy with changes in internal energy. Hess's law and Kirchhoff's law – their derivations and use in numerical problems. Calculation of bond dissociation energies from thermochemical data.

Unit 2: The Gaseous State (16 Lectures)

Distribution of molecular speed – Maxwell's speed distribution law. Concept of mean, root mean square (r.m.s.) and most probable speeds – their expressions from the speed distribution law. Kinetic theory of gases: Postulates, expression of pressure in terms of the r.m.s. speed of gas molecules. Interpretation of the ideal gas law PV = nRT in terms of the kinetic theory expression. Degrees of freedom, principle of equipartition of energy, molecular basis of the heat capacity of gases.

Deviation from ideal behaviour of gases: van der Waals equation of state, virial equation of state, critical phenomena, equation of corresponding states.

Collision among gas molecules: collision cross-section, collision frequency, collision density and mean free path. Variation of the mean free path on pressure and temperature.

Concepts of transport properties of gases, flux and the Fick's law of diffusion. Rate of diffusion, thermal conductivity and coefficient of viscosity of a gas; relations for these three transport properties without derivation. Variation of the coefficient of viscosity on pressure and temperature.

Unit 3: Liquids and Solids (14 Lectures)

Qualitative discussion of the structure of liquids, the structure of liquid water and ice. Physical properties of liquids: vapour pressure, surface tension and viscosity. Determination of surface tension and the coefficient of viscosity of a liquid. Effect of addition of various solutes on surface tension and viscosity. Liquid crystals: elementary ideas of structure, physical properties and uses of liquid crystals.

Solids: Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices. Elementary ideas of symmetry, symmetry elements and symmetry operations; qualitative idea of point groups and space groups; the seven crystal systems and the fourteen Bravais lattices; X-ray diffraction, Bragg's law. Idea of close packing of spheres – CCP model, octahedral and tetrahedral voids.

Practical: 60 Hours

Unit 4: Physical Chemistry Lab (2 Credits)

(1) Determination of heat capacity of a calorimeter using hot water and cold water.
(2) Determination of enthalpy of neutralisation of HCl solution with NaOH solution.
(3) Determination of enthalpy of ionisation of ethanoic acid solution.
(4) Determination of the specific rotation of an optically active substance by polarimetry.
(5) Determination of surface tension of several aqueous solutions of ethanoic acid (of concentrations not beyond 25% w/w) by drop number method using a stalagmometer and hence to determine the concentration of a solution of unknown strength.
(6) Determination of coefficient of viscosity of aqueous solutions of ethanol using an Ostwald viscometer and hence to determine the concentration of a solution of unknown strength.

(Any new experiments may be added from time to time)

List of Suggested Books:

1. Atkins's Physical Chemistry by P. Atkins and J.D. Paula (Oxford University Press)
2. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand (New Age International)
3. A Textbook of Physical Chemistry (Volume 1) by K.L. Kapoor (MacMillan)
4. An Advanced Course in Practical Chemistry by A.K Nad, Ghosal and Mahapatra (New Central Book Agency)

Paper Code - CHM103M (Modular General Elective)
Chemistry – I

Credits: 4=4+0+0 (60 Lectures)

Theory: 60 Lectures

Unit 1: Fundamentals (10 Lectures)

Definition and importance of chemistry. Chemistry in daily life (cleansing action of surfactants, use of ion-exchange resin, etc.).

Pure substances, mixtures, homogeneous mixtures (solutions, alloys) and heterogeneous mixtures. Atoms and molecules, covalent bonds between atoms in a molecule, intermolecular interactions between molecules. Electrons, protons and neutrons in an atom – example of H, C, N and O atom. Atomic and molecular masses, actual masses of atoms and molecules, calculation of number of atoms and molecules in a sample.

Unit 2: Chemicals and Chemical Structures (20 Lectures)

Elements and compounds, symbols and molecular formula. Structures of simple molecules – H_2O, CH_4, CO_2, CO, NO_2. Simple reactions: combustion reactions of H_2, CO and CH_4. Names and structure of organic molecules – C-1 to C-4 alkanes, ethylene and acetylene. Structures of ethanol, acetic acid, benzene and phenol. Idea of catalysis, enzyme-catalysed reactions in the production of ethanol from molasses.

Structures of crystalline solids – ordered arrangements of atoms, ions or molecules. Idea of unit cells – examples of bcc crystal structure of iron and interpenetrating fcc structure of sodium chloride. Crystalline solids and amorphous solids, their examples.

Structures and uses of polymers – polyethene, polyethylene terephthalate (PET), polyvinyl chloride, polystyrene (polystyrene foam), teflon, linear polypeptide proteins, natural rubber, vulcanisation of natural rubber giving network polymers. Advent of biodegradable polymers – names of examples. Classification of polymers into fibres, elastomers and plastics.

Unit 3: Chemistry of Petroleum Fuels and Environmental Pollution (15 Lectures)

Qualitative idea about compositions of natural gas, LPG, petrol and diesel. Introduction to power alcohol. Quality of petrol: concept of flash point, knocking and octane number. Introduction to catalytic cracking and reforming of petroleum fuels.

Production of pollutant gases in combustion: exhaust hydrocarbons, CO, NO_x and SO_x – their physiological effects on humans. Role of catalytic converters to minimize the polluting exhaust gases. Brief ideas about environmental pollution issues regarding toxic heavy metals (Pb, Hg and Cd), chemical fertilizers and detergents (eutrophication) and pesticides. Greenhouse effect – role of CH_4 and of increasing levels of CO_2 in atmosphere, measures for its solution.

Unit 4: Elementary Medicinal Chemistry (15 Lectures)

Definition of drugs and medicines. Idea of classes of medicines: analgesics, antacids, antiparasitics, antibiotics, antiseptics and disinfectants. Examples of each of these classes (chemical structures of the examples not required). Concept of brand name and chemical name.

Carbohydrate, protein, fat, the two essential fatty acids, the vitamins and the common mineral elements necessary for human nutrition.

List of Suggested Books:

1. General Chemistry by D. D. Ebbing and S. D. Gammon (Cengage India, New Delhi)

2. CBSE Chemistry Class XI (Vol. I & II) and Class XII (Vol. I & II) (NCERT, New Delhi)