SEMESTER I

Paper: CHM701C (Core)
Inorganic Chemistry I

Credits: 3+1+0=4

Theory: 60 Lectures

Unit 1: Chemical Bonding

Molecular Orbital Theory: Introduction, qualitative molecular orbital treatment for homonuclear and heteronuclear diatomic molecules (N_2, O_2, CO, NO, HF), Bonding in polyatomic molecules (H_2O, BeH_2, H_2O, CO_2, NO_2, NH_3) based on the concept of hybridization and LCAO-MO. Molecular shape in terms of molecular orbitals – Walsh diagrams.

Correlations in Bond properties- Bond length, Bond Order and Bond Strength. Hydrogen bonding interactions. Effect of hydrogen bonding and other chemical forces on melting and boiling points and solubility.

(14 lectures)

Unit 2: Structure of Simple Solids

Packing of spheres – hexagonal and cubic close packing, tetrahedral and octahedral holes in close-packed structures- metals and alloys, solid solutions. The ionic model for the description of bonding in ionic solids. Characteristic structures of ionic solids- the NaCl and CsCl types, the sphalerite and wurtzite types of ZnS, the NiAs structure type, The perovskite and spinel structure types of mixed-metal oxides- importance ionic radii and the radius ratios in determining structure type among ionic solids. Lattice energy considerations, Thermal stability and solubility of inorganic solids.

(12 lectures)

Unit 3: Acid Base and Redox Chemistry

Hard and soft acid-base (HSAB) concept and its applications. Strength of oxo acids and halo acids, strength of inorganic bases- periodic trends in acidity and basicity of hydrides, oxides, oxyacids of non-transition elements. Relevance of acidity and basicity in catalysis. Nonaqueous solvents.

Standard electrode potentials, pH dependence of electrode potentials. Redox stability of metal ions in water, oxidation by atmospheric oxygen. Applications of Latimer and Frost diagrams,Rredox behaviour of non-transition elements based on electrode potential data.

(12 lectures)

Unit 4: Chemistry of Inner Transition Elements

Lanthanides and Actinides: Extraction and separation, periodic properties, redox Chemistry, magnetic and spectral properties, analytical applications (Lanthanide Shift Reagents).

(10 lectures)

Unit 5: Coordination Chemistry: Bonding and Magnetic properties

Crystal field theory of bonding in octahedral, tetrahedral and square planar transition metal complexes. Factors affecting crystal field splitting, Crystal field stabilization energy, Spectrochemical series. Jahn Teller Distortion, Ligand field theory of metal complexes.

Magnetic properties of transition metal complexes.

(12 lectures)

Paper: CHM702C (Core)
Organic Chemistry I

Credits: 3+1+0=4

Theory: 60 Lectures

Unit :1 Kinetics and Energetics of Reaction Mechanism

TST theory of reaction rates: kinetics & thermodynamics of activation. Reaction profiles for multistep reactions, Hammond postulate, Curtin-Hammett Principle; kinetic and thermodynamic control.

Linear free energy relationships (LFER): Hammett equation - substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds; kinetic isotope effects in organic reactions.

Effects of conformation on reactivity: anomeric effect, stereoelectronic effects, neighbouring group participation.

(12 Lectures)

Unit 2: Stereochemistry

Classification of organic molecules into different Point Groups, R/S, E/Z nomenclature in C, N, S, P containing compounds; concept of absolute and relative configuration; chirality in molecules devoid of chiral centers- allenes, spiranes and biphenyls (atropisomerism), binaphthyls.

Concepts of stereogenic center – chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochirality etc.); optical purity and enantiomeric excess; conformation of acyclic organic molecules, chirality of

conformers, cyclohexane (di- and tri- substituted), cyclohexanone and decalins.

(16 Lectures)

Unit 3: Stereodifferentiating reactions

Stereospecific and Stereoselective synthesis; classification of stereoselective synthesis, diastereoselective, enantioselective and double stereo-differentiating reactions, nucleophilic addition to aldehyde and acyclic ketones– Cram, Felkin and Felkin-Anh model, Prelog's rule, Stereoselective nucleophilic addition to cyclic ketones (Cram and Felkin-Anh models).

Acyclic stereoselection: reactions at α-and β-positions of a chiral center.

(11 Lectures)

Unit 4: Aromaticity

Aromaticity of benzenoid and non-benzenoid compounds including monocyclic and fused ring systems, molecular orbital description, Frost's model, non-aromatic and antiaromatic compounds, molecular stability and reactivity, aromaticity driven reactions including acid-base reactions; aromaticity of higher annulenes; Homoaromatic compounds.

(8 Lectures)

Unit 5: Heterocyclic chemistry

Heterocyclic compounds containing two or more hetero atoms: Synthetic methods of preparation, properties and applications in medicinal chemistry e.g., azoles (pyrazole, imidazole, oxazole and thiazole derivatives), diazines (pyrazine, pyrimidine and pyridazine derivatives), benzo-diazines, heterocyclic compounds containing one nitrogen atom and an oxygen or sulphur atom (oxazine, phenoxazine and thiazine derivatives), triazines and tetrazines.

(13 Lectures)

Paper: CHM703C (Core)
Physical Chemistry I
Credits: 3+1+0=4

Theory: 60 Lectures

Unit 1: Equilibrium and Non-Equilibrium Thermodynamics

Non-ideal systems: Fugacity and fugacity coefficients for gases, activity and activity coefficients for non-ideal solutions – the different scales of activity and activity coefficients.

Phase equilibrium: Application of Gibbs phase rule to three component systems, triangular plots, water-acetic acid chloroform and ammonium chloride-ammonium sulphate water system.

Non-equilibrium thermodynamics: Concept of internal entropy production in irreversible processes. Generalised forces and flows, coupled forces and flows, phenomenological relations, statement of Onsager's reciprocal relation. Non-equilibrium stationary states in some open systems – statement of Prigogine's principle of minimum entropy production, the explanation of sustenance of highly ordered biological organisms in spite of continual increase of entropy.

(18 Lectures)

Unit 2: Statistical Thermodynamics

Statistical thermodynamics: Molecular energy levels and concept of distribution of gas molecules in energy levels. Concept of macrostate, microstate and thermodynamic probability. Concept of ensembles – micro-canonical, canonical and grand canonical ensembles, definition of canonical ensemble partition function Q. Ideas of Maxwell-Boltzmann, Fermi-Dirac, Bose-Einstein and the corrected-Boltzmann statistics, question of indistinguishability of particles.

Boltzmann distribution in a pure gaseous system, the molecular partition function q and its significance, relation between Q and q for a pure gas. Molecular significance of heat and work. Translational, electronic, nuclear, rotational and vibrational partition functions of gas molecules. Thermodynamic functions of monatomic, diatomic and polyatomic gases – calculation of equilibrium constants of gaseous reactions, residual entropy calculations.

(20 Lectures)

Unit 3: Polymer Chemistry

Some basic concepts: Monomers, repeat units, degree of polymerization, concepts of linear, branched and network polymers with examples. Classifications of polymers with examples: natural and synthetic polymers, thermoplastic and thermosetting polymers, classification on the basis of use as fibres, elastomers and plastics.

Polydispersity and average molecular weight concept. Number, weight and viscosity average molecular weights – numerical calculations, polydispersity index. Determination of molecular weights: viscosity, osmotic pressure and light scattering methods.

Polymers in solutions: Chain configuration of macromolecules – root mean square end to end distance and radius of gyration; random flight model and chain stiffness concept, short range and long range effects, average dimension of polymer chains, concept of theta solvent.

Chain and step polymerisation, introductory concepts of cationic, anionic and coordination chain polymerisation and ring-scission step polymerisation. Review of free-radical chain polymerisation kinetics, kinetics of step polymerisation and of chain copolymerisation.

(22 Lectures)

Paper: CHM704C (Core)
Group Theory and Molecular Spectroscopy
Credits: 3+1+0=4

Theory: 60 Lectures

(Note: Separate answer-scripts to be supplied for Part A and Part B during examination.)

Part A: Group Theory

Unit 1: Molecular symmetry and symmetry groups

Concept of group theory, Symmetry elements and symmetry operations, Classes of symmetry operation, Symmetry point groups, Assignment of point groups to simple molecules, Structure and symmetry of Inorganic complexes (coordination number 2-6), Shapes and Symmetry of s, p and d orbitals.

(8 lectures)

Unit 2: Representation of groups

Matrix representation of symmetry operations, The Great Orthogonality Theorem Reducible and Irreducible representation of groups, Features and Construction of Character tables ($C_{2v,}$ C_{3v} and C_{2h}).

(8 lectures)

Unit 3: Applications of Group Theory and Symmetry

Molecular Vibrations- determining symmetry types of normal modes of vibrations with selected examples, Selection rules for Fundamental Vibrational Transition (IR and Raman).

(8 lectures)

Part B: Molecular Spectroscopy

Unit 4: Introduction

Electromagnetic spectrum, Representation of spectra, Signal-to–noise ratio: Resolving power, The Width and Intensity of Spectral transitions, Fourier Transform Spectroscopy, Enhancement of Spectra: computer averaging.

(8 lectures)

Unit 5: Rotational (Microwave) Spectroscopy

Classification of molecules according to their moments of inertia, Rotational spectra of the rigid diatomic molecules (eg. HCl), selection rule, intensity and the effect of isotopic

substitution, Rotational spectra of diatomic molecule as non rigid rotator, spectra of symmetric top molecules, asymmetric top molecules, Stark effect.

(12 lectures)

Unit 6: Infrared and Raman Spectroscopy

Harmonic and Anharmonic oscillators, The diatomic vibrating rotator, The vibration-rotation spectrum of diatomic molecules, fundamental vibration frequencies, overtone and combination frequencies, P, Q, R branches, Modes of vibrations in polyatomic molecules (e.g. CO_2, NH_3) and their symmetry, the influence of rotation on spectra of polyatomic molecules, the influence of Nuclear spin.

Molecular Polarizability, Pure Rotational Raman spectra of Linear, symmetric and asymmetric Top molecules, Raman activity of vibrations, Rule of Mutual Exclusion, Stokes' and Anti-Stokes' lines, Structure determination of selected molecules/ions from IR and Raman Spectroscopy (CO_2, SO_2, N_2O, NO_3^-, ClO_3^-, ClF_3).

(16 lectures)

Paper: CHM705L (Lab Course)
Organic and Physical Chemistry Practical
Credits: 0+0+4=4

Practical: 120 Hours

Unit 1: Organic Chemistry Practical **90 Hours**

A. Qualitative organic analysis

Binary mixtures of organic compounds, covering compounds with major functional groups, should be given with an objective to train students in

i. Qualitative separation by physico-chemical methods and
ii. Identifying the compounds by chemical analysis.

B. Organic estimation

i. Glycine by sodium hydroxide in the presence of formaldehyde
ii. Amino acid by colorimetric method using ninhydrin
iii. Glucose and sucrose in a mixture

C. Chromatographic application

Separation and identification of amino acids present in a ternary mixture by paper chromatography

D. Organic preparation: Two-step preparation

i. Benzanilide from benzophenone
ii. Benzilic acid from benzoin
iii. Anthranilic acid from phthalic anhydride

Unit 2: Physical Chemistry Practical **30 Hours**

(1) Study of the ternary phase equilibrium of acetic acid-chloroform-water at room temperature and construction the triangular plot phase diagram.

(2) Study of the complex formation between Cu^{2+} ion and ammonia by distribution method using water-chloroform mixtures and hence to find the composition of the complex.

(3) Study of the equilibrium between iodine, iodide ion and tri-iodide ion by distribution method and determination of the equilibrium constant of the reaction.

(4) Determination of the viscosity-average molar mass of a polymer by viscometric method.

(5) Determination of the dissociation constant of a weak acid using Hendersen's equation.

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