Unit-I: Stereochemistry and Bonding in the Compounds of Main Group Elements. (16 Contact hours)

Valence bond theory- Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, Resonance energy and examples of some inorganic molecules/ions.

Odd electron bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions; Shapes of Trigonal bipyramidal, Octahedral and Pentagonal bipyramidal molecules / ions. (PCl₅, VO₃⁻¹, SF₆, [SiF₆]²⁻, [PbCl₆]²⁻ and IF₇).

Limitations of VSEPR theory.

Molecular orbital theory- Salient features, Variation of electron density with internuclear distance.

Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions.

Molecular orbital diagram of Polyatomic molecules / ions. Walsh diagrams (Concept only).

Delocalized molecular orbitals:- Butadiene, cyclopentadiene and benzene.

Detections of Hydrogen bond: UV – Vis ; IR and X-ray ; Importance of hydrogen bonding.

Unit-II: Bonding in Coordination Compounds and Metal Clusters: (16 Contact hours)

Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn -Teller distortion, spectrochemical series and the nephleuxetic effect.

Evidence of covalent bonding in transition metal complexes; Adjusted crystal field theory.

Molecular orbital theory of bonding in octahedral complexes:- composition of ligand group orbitals;molecular orbitals and energy level diagram for sigma bonded ML₆; Effect of pi-bonding.

Molecular orbital and energy level diagram for Square-planar and Tetrahedral complexes.

Metal Clusters: Introduction to metal clusters; Dinuclear species ; Metal –metal multiple bonds.
Unit-III: Metal- Ligand Equilibria in Solution  


Determination of formation constants by pH- metry and spectrophotometry.

Metal Chelates: Characteristics; Chelate effect and the factors affecting stability of metal chelates.

Applications of metal chelates in chemical analysis and medicine.

Complexes of macrocyclic ligands:- Crown ethers and cryptands.

Unit-IV: $\pi-$ Complexes and Iso- Heteropolymetallates of Transition Metals:  

Transition Metal Carbonyls: Carbon monoxide as ligand; Synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Preparation, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes of transition metals.

Tertiary phosphine as ligand.


Books Recommended:

3. Inorganic Chemistry- G. Wulfsberg ; Viva ; 2002
Course No: CH14102CR
Title: Physical Chemistry (04 Credits)

Max. Marks: 100
External Exam: 80 Marks.
Duration: 64 Contact hours
Internal Assessment: 20 Marks

Unit-I: Quantum Chemistry
(16 Contact hours)

Exact quantum mechanical results:


Unit-II: Surface Chemistry
(16 Contact hours)

Liquid Surface: Surface tension, pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation), Capillary condensation.
Solid liquid interface: Contact angle, young’s equation, wetting, Wetting as contact angle phenomena.

Thermodynamics of Interfaces: surface excess, surface tension and thermodynamic parameters, Gibbs adsorption isotherm.


Unit-III: Statistical Thermodynamics
(16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

Partition function & its significance, translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions with application to isomerization and atomization reactions.
Unit-IV: Chemical kinetics

(16 Contact hours)

Fast reactions: General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis.

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory

Theories of unimolecular reactions (Lindman, Hinshelwood, RRK and RRKM theories), Introduction to potential energy surfaces.


Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions, Hammett equation, Taft equation.

Books Recommended:

Course No. CH14103CR
Title: Laboratory Course in Inorganic Chemistry-I  (04 Credits)

Max. Marks: 100 Duration: 64 Contact hours
External Exam: 80 Marks. Internal Assessment: 20 Marks

I. Preparation of Coordination compounds of Transition metals:
1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:
   i) Mercurytetrathiocyanatocobaltate(II)  : To visualize the complexation process.
   ii) Tristhioureacopper(I)sulphate monohydrate : Insitu generation and Stabilization of unusual oxidation state and re-crystallization/crystal growing.
   iii) Hexaamminecobalt(III) chloride : Multistep synthetic procedure.
   iv) Trisethylenediaminecobalt(III) chloride : Two stage synthesis and aerial oxidation/Resolution of a racemic mixture.
   v) Ammonium dodeca molbedophosphate : Synthesis of a heteroploy metallate/Bonding and structure.

II. Inorganic Quantitative Analyses:
A. Gravimetry:
   i) Skill and importance of weighing in Chemistry, Gravimetric Calculations.
   ii) Precipitation process in homogenous mixtures, Precipitating agents, conditions of precipitation.
   iii) Precipitate processing( Digestion, Ignition); reducing precipitation errors( Co- and post precipitation).

B. Tritimetry:
   i) Types and skill of titration, concept of Complexometric titrations, tritimetric calculations.
   ii) Metallochromic Indicators: selection, structure, and mechanism of action.

III) Role and selection of buffers in Complexometric titrations, EDTA Back titrations.

Separation and estimation of following Binary metal ion systems using Gravimetry&Tritimetry simultaneously:
   i) Silver (Ag⁺) as AgCl and Nickel (Ni²⁺) as [NiEDTA]²⁻ complex.
   ii) Barium (Ba²⁺) as BaSO4 and Zinc as [ZnEDTA]²⁻ complex.
   iii) Barium (Ba²⁺) as BaSO₄ and Nickel (Ni²⁺) as [NiEDTA]²⁻ complex.
   iv) Nickel (Ni²⁺) as Ni (dmg)₂ complex and Magnesium (Mg²⁺) as [Mg EDTA]²⁻ complex.
   v) Copper (Cu⁺) as CuSCN and Magnesium (Mg²⁺) as [MgEDTA]²⁻ complex.

Books Recommended:
Unit-I: Delocalized Chemical bonding (16 Contact hours)


Aromaticity: Huckel rule and concept of aromaticity, Molecular orbital diagram of annulenes, Frost diagram. Relation between NMR and aromaticity.

Annulenes: Systems with electron numbers other than six (2,4,8,10 and more than ten π-electron systems), Aromaticity of hetero annulenes. Carcinogenesis due to aromatic hydrocarbons. Aromaticity in fused ring systems. Aromaticity of ferrocene and azulene. Anti and Homoaromaticity

Tautomerism: Different types including valence tautomerism.

Unit -II : Reactive Intermediates and Reaction Mechanism (16 Contact hours)

Reactive Intermediates: Generation, Structure, fate and stability of carbocations, (Classical and non-classical) carbanions, free radicals, carbenes, nitrenes and radical ions


Unit-III : Aliphatic Nucleophilic Substitutions : (16 Contact hours)

Mechanism and stereocchemical implications of \( S_{N2} \), \( S_{N1} \), \( S_{N\delta} \) and Neighbouring Group Participation (by \( \pi \) and \( \sigma \)-bonds) reactions. Comparison of \( S_{N1} \) and \( S_{N2} \) reactions. Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of \( S_{N1} \) and \( S_{N2} \) reactions. Mixed \( S_{N1} \) and \( S_{N2} \) reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions. Substitutions on other elements. Functional group transformation using \( S_{N2} \) reactions in organic synthesis. Nucleophilic substitutions in biological systems.
**Elimination reactions:** Factors affecting elimination reactions, Mechanism of E1, E2, E1cB and E2C reactions. Competition between substitution and elimination reactions. Stereochemistry and regioselectivity of E2 eliminations, Elimination in cyclic systems and vinyl halides. Mechanism and orientation in pyrolytic eliminations, Shapiro reaction.

**Aliphatic Electrophilic Substitutions**

General mechanism of $S_{E1}$, $S_{E2}$ and $S_{Ei}$ reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-enamine reaction.

**Unit – IV Stereochemistry:**  
(16 Contact hours)

Molecular symmetry and Chirality, Chirality due to chiral carbon in other quadrivalent chiral atoms. Chirality in compounds with tervalent chiral atoms. Chirality in suitably substituted adamantanes. Chirality due to restricted rotation (leading to perpendicular dissymmetric planes), biphenyls and allenes. Chirality due to helical shape. Chirality / optical activity caused by restricted rotation of other types.

Creating a chiral Centre, molecules with more than one chiral centre, Asymmetric synthesis in nature. Enantiotopic diastereoic topic groups and faces. Significance of chirality in biomolecules. Conformational analysis of cycloalkanes, with more than one substituents and decalines. Effect of conformation and reactivity: $SN_1$ reaction and epoxidation reactions.

Conformation and reactivity of cyclohexene and cyclohexanone. Conformation of sugars, steric strain due to unavoidable crowding.

**Books Recommended:**

Course No: CH14105EA
Title: Symmetry and Spectroscopy (04 Credits)

Max. Marks: 100  Duration: 64 Contact hours
External Exam: 80 Marks.  Internal Assessment: 20 Marks

Unit I: Symmetry -I  (16 Contact hours)
Symmetry elements and operations; combination of symmetry operations. Groups, subgroups, classes and group multiplication tables. Symmetry point groups Schoenflies notations of point groups; identification of point groups. Systematic procedure for assignment of point groups to molecules; Symmetry classes and their geometrical significance.

Unit II: Symmetry -II  (16 Contact hours)
Matrices and their combinations, block factored matrices; matrix representation of symmetry operation and point groups. Reducible and irreducible representation, character of a representation, properties of irreducible representations, Mulliken Symbols for IRS. Character table, construction of character tables for C2v, C3v and C4v point groups.

Applications of symmetry: Molecular chirality, Polarity, Fluxionality, and IR and Raman spectroscopy.

Unit III: Electronic Spectroscopy  (16 Contact hours)
Interaction of light with matter, transition probability, transition moment integral, derivation of selection rules.

Intensity of spectral lines; Einstein’s treatment of absorption and emission processes. Oscillator strength.

Natural spectral line width, broadening of spectral lines -Doppler and Collision effects,

Electronic Spectroscopy
Vibronic transitions. Intensity of spectra—the Franck-Condon principle.

Electronic spectra of organic molecules; chromophores , auxochrome, spectral shifts Different types of electronic transitions; nomenclature, symmetry labels of electronic states--spectra of formaldehyde. Effects of solvent, electron withdrawing and electron donating groups, conjugation and extended conjugation on the position of spectral bands.

Photoelectron Spectroscopy
Basic principles- photoionization process; ionization energies; Koopman’s theorem. Photoelectron spectra of simple molecules (N₂, O₂), ESCA - Application.
Unit IV: Infrared and Raman Spectroscopy (16 Contact hours)

**Infrared Spectroscopy**

Linear harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, Morse potential energy levels. Fundamental bands, overtones and hot bands. Vibration-rotation spectra of diatomic molecules; P, Q and R branches; Vibrations of polyatomic molecules: Normal vibrational modes, selection rules; combination and difference bands. Factors influencing the band positions and intensities. Group frequencies and fingerprint region.

**Raman Spectroscopy**

Classical and Quantum theories of Raman scattering, Molecular polarizability, rotational, vibrational, and vibrational-rotational Raman spectra. Selection rules; rule of mutual exclusion. Applications.

**Books Recommended:**

I. Qualitative Analyses by Semi Micro Technique:

1. Discussion about the analysis scheme. Analytical groups and Group reagents.
2. Scales of Analysis, Skill of semi micro technique.
3. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.
4. Identification of four metal ions from different analytical groups with simple and complex combinations:
   (i) Group I and II A
   (ii) Group I, II A and II B
   (iii) Group II A and II B
   (iv) Group I and Group III
   (v) Group II B and Group III
   (vi) Group III only.

II. Chromatography:

A. Paper Chromatography:
   (i) Principle, Separation process, Technique of Paper Chromatography. Design of mobile phase.
   (ii) Methods of paper chromatography (Ascending, Descending and Radial)
   (iii) Comparative mobile phase study of separating mixtures. Chromatogram analysis and Interpretation.

B. Thin layer Chromatography:
   (i) Principle. Skill of TLC, Choice of mobile phase, Comparative mobile phase study of systems.
   (ii) TLC as reaction monitoring tool in synthesis.
   (iii) Selection of locating / visualizing reagents, location by Ultra violet radiation.
   Separation and Identification of Binary and Ternary metal ion mixtures of simple and complex combinations Using Ascending and Radial methods of Paper Chromatography.
   Comparative mobile Phase Study of different Separating Mixtures.
   Monitoring the progress/ completion of a reaction using thin layer Chromatography.

Books Recommended:
1. Vogel's Qualitative Inorganic Analysis; 6th edn; Svehla (Longman, 1994)
Course No: CH14107EO  
Title: Chemistry in Everyday Life-I  (04 Credits)

Max. Marks: 100  
Duration: 64 Contact hours
External Exam: 80 Marks.  
Internal Assessment: 20 Marks

Unit-I:  (16 contact hours)

(a) Household Chemicals
Soaps, detergents, Optical brightens and bleaching agents.
Haircare products: Shampoos, Conditioners, Dyes, Hair curlings and Permanents.
Deodorants and Antiperspirants
Perfumes, Tooth Pastes and Sunscreen lotions.

(b) Agro Chemicals:
Composition and properties of soil, Inorganic and Organic components of soil.
Plant nutrients: Secondary and micro nutrients and their functions.
Fertilizers: Inorganic and Organic fertilizers.
Insecticides, Pesticides and herbicides, Environment and health problems with synthetic
pesticides.
Alternate method of insect control: Pheromones, Hormones and Biological control.
Neem: The Worlds Pharmacy.

Unit II:  (16 contact hours)

Polymers and Plastics: Characteristics and Types of Polymers.
The big six of Polymer: Low Density Polyethylene (LDPE), High Density Polyethylene
(HDPE), Polypropylene PP, Polystyrene (PS), Polyvinyl Chloride (PVC) and Polyethylene-
Tetra phthalate (PET or PETE): their chemical characteristics and uses.
Chemical Features and Applications/Uses of other Polymers: Natural rubber, Synthetic
rubber, Polyesters, Polyamides, Polyurethanes, Polymethylnitrites, Polystyrene and Teflon.
Personal Polymers: Teflon ear bone, Fallopian tube, Heart valve, Contact lenses.
Problems with Polymers: Disposal, Recycling and Environmental concerns.
Ceramics: Composition, structure and properties of ceramics. How to make ceramics.
Silicate Ceramics: Potteries and Clay products. Glass (composition of various glasses),
Cements: Composition of Portland cement.
Unit-III: *(16 contact hours)*

(a) **Carbohydrates**: Definition, classifications. Significance of right and left handedness.
Production through photosynthesis
Composition and functions of Monosaccharides: Glucose, Fructose and Galactose.
Disaccharides: Sucrose, lactose and Maltose. Invert Sugar.
Polysaccharides: Starch, glycogen and Cellulose.
Aerobic and Anaerobic metabolism

(b) **Lipids**: Oils and Fats: Fatty acids and Triglycerides. Saturated and Unsaturated fatty acids (MUFA and PUFA). Rancidity of Oils & Fats. Absorption of toxic substances by fat.
**Steroids**: Cholesterol, transport of Cholesterol in blood stream. Cholesterol and heart diseases, Recommended values of HDL and LDL, Steroidal hormones and anabolic steroids

Unit-IV: *(16 contact hours)*


**Enzymes**: Classification. Theories of mechanism of action of Enzymes; Fisher Lock and Key Theory, Koshland’s Induced Fit Theory. Mechanism of action of Chymotrypsin and Carboxypeptidase.

**Nucleic acids**: Features and functions of DNA and RNA.

**Vitamins**: Classes of Vitamins and their functions. Vitamin deficiency diseases.

**Minerals**: Macro and Micro minerals. Their functions and diseases caused by their deficiencies.

**Books Recommended**:

4. www.chemistryincontext (American Chemical Society)