MASTER OF SCIENCE (CHEMISTRY)

CHM–6111

INORGANIC CHEMISTRY- I

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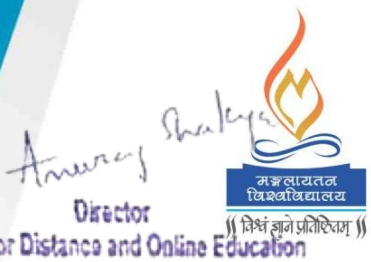

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3. Dr. Deepmala
4. Ms. Rainu Verma
5. Mr. Ripudaman Singh
6. Mr. Rohit Kumar

Block I: Structure and Bonding in Main Group Compounds

Unit 1: Bonding in Inorganic Molecules

Various Theories of Bonding in Inorganic Molecules, Limitations and Applications - (VBT, CFT, and LFT), Hybridization.

Unit 2: VSEPR Theory

VSEPR, Walsh Diagram (Triatomic and Penta-Atomic Molecules), dπ-pπ Bond, Bent Rule and Energetic Of Hybridization, Some Simple Reactions of Covalently Bonded Molecules.

Unit 3: Phosphorus-Nitrogen Compounds

Synthesis, Structure, Bonding and Uses of Phosphorus-Nitrogen Compounds: Cyclo and Linear Phosphonitrilic Compounds.

Unit 4: Phosphorus-Sulphur and Sulphur-Nitrogen Compounds

Synthesis, Structure, Bonding and Uses of Phosphorus-Sulphur Compounds, Sulphur- Nitrogen Compounds, Ring and Chain Compounds S_2N_2, S_4N_4. $(SN)_X$ etc.

Block II: Alkali and Alkaline Earth Metal Complexes

Unit 5: Coordination Chemistry of Alkali and Alkaline Earth Metals

General Properties and Coordination Behavior, Factors Affecting Coordination Number and Geometry, Common Ligands: Crown Ethers, Cryptands, Calixarenes, and their Selectivity for Alkali and Alkaline Earth Metals, Chelate Effect in Complexes of Alkali and Alkaline Earth Metals.

Unit 6: Structure and Stability

Mononuclear, Polynuclear, and Cluster Complexes, Thermodynamic Stability Constants: Stepwise and Overall Stability of Complexes, Role of Hard and Soft Acids and Bases (HSAB) Theory in Predicting Stability, Influence of the Size, Charge Density, and Polarization of Cations on Complex Stability, Solvation Effects And Ion-Pair Formation.

Unit 7: Reactivity and Catalysis

Reactivity Patterns of Alkali and Alkaline Earth Metal Complexes in Aqueous and Nonaqueous Media, Organometallic Compounds of Alkali and Alkaline Earth Metals: Preparation and Stability. Catalytic Roles in Hydrogenation, Hydroboration, Deprotonation and Enolate Formation, Cross-coupling Reactions (e.g., Kumada and Negishi reactions), Activation of Small Molecules (e.g., H_2, CO_2, and N_2) Using Alkali and Alkaline Earth Metal Complexes.

Unit 8: Biological, Industrial and Environmental Applications

Complexes of Alkali and Alkaline Earth Metals in Enzymatic Processes and Biomimetic Systems, Industrial applications: Complexes in Ion-exchange Processes, Phase-transfer catalysis, and as Desiccants, Environmental Applications: Metal Ion Complexes in Water Softening, and Pollutant Sequestration.

Block III: Metal pi-Complexes

Unit 9: Metal Carbonyls

Metal Carbonyl: Preparation, Properties, Structure and Bonding, Vibrational Spectra of Metal Carbonyls for Bonding and Structural Elucidation, Important Reactions of Metal Carbonyls.

Unit 10: Other Transition Metal

Preparation, Bonding Structure and Important Reactions of Transition Metal Nitrosyl, Dinitrogen and Dioxygen Complexes; Tertiary Phosphine as Ligand.

Unit 11: Metal-Alkene and Metal-Alkyne Complexes

Preparation, Properties, Structure and Bonding of Metal-Alkene Complexes, Preparation, Properties, Structure and Bonding of Metal-Alkyne Complexes, Important Reactions and Applications of Metal-Alkene and Metal-Alkyne Complexes in Catalysis and Organic Synthesis, The Dewar-Chatt-

Duncanson Model for Metal-Alkene Bonding, Analysis of Vibrational Spectra for Structural Elucidation of Metal-Alkene and Metal-Alkyne Complexes.

Unit 12: Metallocenes and Sandwich Complexes

Preparation, Properties, Structure, And Bonding of Ferrocene and other Metallocenes, Structure and Bonding of Sandwich Complexes, Including Examples like Dibenzene Chromium and Dibenzene Titanium, Reactivity and Applications of Metallocenes in organic Synthesis and Industrial Catalysis, Concepts of Aromaticity in Metallocenes and their Electronic Structures, Spectroscopic Methods (NMR, IR, UV-Vis) for the Characterization of Metallocenes and Sandwich Complexes.

Block IV: Metal Clusters

Unit 13: Introduction to Metal Clusters

Definition and Classification of Metal Clusters, Structure of Clusters, Electron Counting In Clusters, Distinction between Low-Valency Metal Clusters (e.g., Metal Carbonyl Clusters) and High-Valency Metal Clusters (E.G., Metal Halide Clusters).

Unit 14: Preparation and Reactions of Metal Clusters

General Methods for Preparation of Metal Cluster Complexes: Pyrolysis, Electrolytic Reduction, Nucleophilic Attack On Clusters, Reductive Elimination Processes, Reactions Of Metal Clusters: With Electrophiles and Nucleophiles, Oxidative Addition and Reactions on M-M Multiple Bond.

Unit 15: Structure and Bonding

Structural Aspects of Various Metal Clusters, Metal-Metal Bonding; Including Single, Double, Triple, and Quadruple Bonds, Application of Wade's Rules for Predicting Structures in Higher Boranes and Carboranes.

Unit 16: Boranes and their Derivatives

Synthesis, Properties, Structure, Bonding, Uses of Higher Boranes, Carboranes, Metalloboranes and Metallocarboranes, Compounds with Metal-Metal Multiple Bonds.

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Block I: Metal-Ligand Bonding

Unit 1: Theories of Metal-Ligand Bonding

Crystal Field Theory and its Limitations, Molecular Orbital Theory, Octahedral, Tetrahedral and Square Planar Complexes, Jahn-Teller Effect, pi-Bonding and Molecular Orbital Theory, Spectrochemical Series, Low Spin and High Spin Complexes.

Unit 2: Crystal Field Stabilization and Related Aspects

Crystal Field Stabilization Energy, Spectrochemical Series, Weak and Strong Field Complexes, Thermodynamic and Related Aspects of Crystal Fields, Ionic Radii, Heats of Ligation, Lattice Energies, Site Preference Energies.

Unit 3: Stability of Metal Complexes

Factors Affecting the Stability of Metal-Ligand Complexes Including Charge Density, Ligand Size, and Electronegativity, Chelate Effect and Thermodynamic Origins.

Block II: Electronic Spectroscopy and Magnetism

Unit 4: Electronic Spectroscopy of Transition Metal Complexes

Fundamentals of Electronic Spectra, Absorption of Light and Electronic Transitions, Types of Electronic Transitions: d-d, Charge Transfer (MLCT and LMCT) and Others, Crystal Field Theory and Spectra, Term Symbols and Multiplicity, Selection Rules.

Unit 5: Interpretation of Electronic Spectra

Spectroscopic Ground States, Correlation, Orgel and Tanabe-Sugano Diagrams for Transition Metal Complexes (d^1-d^9 States), Calculations of Racah Parameters.

Unit 6: Applications of Electronic Spectroscopy

Spectroscopic Method of Assignment of Absolute Configuration in Optically Active Metal Chelates and their Stereochemical Information, Electronic Spectra of Metalloproteins and Enzymes, Time-Resolved Spectroscopy, Analysis of Complex Spectra, Comparative Study of High Spin vs. Low Spin Systems.

Unit 7: Fundamentals of Magnetism in Transition Metals

Definition and Types of Magnetism: Diamagnetism, Paramagnetism, Ferromagnetism, Antiferromagnetism and Ferrimagnetism, Origin of Magnetic Moments, Determination of Magnetic Moments Using the Gouy Balance Method and the Faraday Method, Concept of Magnetic Susceptibility, Application of the Curie and Curie-Weiss Laws.

Unit 8: Magnetic Behavior of Transition Metal Complexes

Magnetic Properties of Complexes of Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn, Spin Crossover and Jahn-Teller Effect, Introduction to Molecular Magnets, Single-Molecule Magnets (SMMs) and Single-Chain Magnets (SCMs).

Block III: Reaction Mechanisms of Metal Complexes

Unit 9: Substitutions in Square Planar Complexes

Mechanisms of Substitution Reactions of Square Planar complexes: Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects, Berry's Pseudo Rotation Mechanism; Factors Affecting the Reactivity of Square Planar Complexes, Swain-Scott Equation.

Unit 10: Substitutions in Square Pyramidal and Trigonal Bipyramidal Complexes

Mechanisms of Substitution Reactions of Square Pyramidal and Trigonal Bipyramidal Complexes: Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects.

Unit 11: Substitutions in Octahedral and Tetrahedral Metal Complexes

Mechanisms of Substitution Reactions of Octahedral Complexes: Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects, Trans Effect and its Application to Synthesis of

Complexes; Stereochemical Changes in Substitution Reactions of Octahedral and Tetrahedral Complexes.

Unit 12: Molecular Rearrangements

Molecular Rearrangement Processes; Electron Transfer Reactions (Outer and Inner Sphere); HOMO and LUMO of Oxidant and Reductant, Chemical Activation, Precursor Complex Formation and Rearrangement; Nature of Bridged Ligands; Fission of Successor Complexes, Two-Electron Transfers.

Block IV: Bioinorganic Chemistry

Unit 13: Fundamentals of Bioinorganic Chemistry

Historical Development and Significance, Role of Metal Ions in Biological Systems, Metal Ion Transport and Storage, Metal Ion Interactions with Nucleic Acids.

Unit 14: Metalloproteins and Their Functions

Hemoglobin and Myoglobin, Iron-Sulfur Proteins, Copper Proteins, Zinc Proteins.

Unit 15: Metalloenzymes and Catalysis

Mechanisms of Metalloenzymes, Role of Metal Ions in Enzyme Catalysis, Structure and Function of Key Metalloenzymes, Biomimetic Models and their Applications.

Unit 16: Medicinal Aspects of Bioinorganic Chemistry

Metal-Based Drugs and their Mechanisms of Action, Diagnostic Applications of Metal Complexes (e.g. MRI Contrast Agents), Advanced Spectroscopic Techniques in Bioinorganic Chemistry: X-Ray Crystallography, NMR, EPR and Mössbauer Spectroscopy for Studying Metalloprotein Structures and Functions.

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