Syllabus for
Ph.D. Entrance Exam in
Applied Chemistry
Under the
Faculty of Engineering
Devi Ahilya Vishwavidyalaya,
Indore
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Stereochemistry and Reaction Mechanism

1. Stereochemistry: Configuration and chirality, optical isomerism, R,S-convention, Geometrical isomerism E.Z-convention, Conformational analysis
2. Reactive Intermediates: Generation, structure and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals.
5. Addition to Carbon-Carbon Multiple Bonds: Mechanism, direction and stereochemistry, addition to alkenes and alkynes, Transition metal organometallics.
6. Addition to Carbon-hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles, Addition of Grignard reagents.
7. Elimination Reactions: Reaction mechanism, Direction, stereochemistry, formation of alkenes, alkynes and other multiple bonds.
10. Ring closure and opening reactions: Formation and opening of rings, Dieckmann reaction, Baldwin Rules, Robinson-Annellation, Michael-Robinson addition Thorpe Ziegler reaction, Acylation Cycloaddition, Simmons-Smith reaction
Thermodynamics and Chemical Kinetics


Main Group Chemistry


4. Chemistry of Silicon: Organosilicon Compounds, Silicates and Aluminosilicates. Low-valent silicon compounds, silylens and RsSi-.
5. Inorganic rings, Cages, Clusters and Polymers: Phosphaazenes, Cyclophosphazenes, Polyphosphazenes and the polymers derived from them. Polysilanes.

6. Chemistry of halogens and noble gases: Inter Halogens, Poly Halide Anions, CFC’s, Ozone layer and Clathrates.

7. Chemistry of group 12 elements: Halides & Oxygen compounds, chalcogenides & Related compounds, low-valent compounds & Formation of coordination complexes.

Basic Biological Chemistry

1. Introduction to Biomolecules: Carbohydrates, Proteins, Amino acids, Lipids and phospholipids, Biological membranes, transport across membranes.
2. Nucleic Acids: Base pairing, double helices, DNA replication, transcription and translation.
3. Enzymes: enzyme kinetics and mechanism, nature and application of enzymes.

Quantum Chemistry

2. Linear Motion and harmonic Oscillators: Translation, harmonic, particle in a box a penetration through barriers.
4. Angular momentum: Angular momentum operators, definition of states, Composite systems.
5. Techniques of Approximation: Perturbation theory, variation theory, HF theoretic, time dependent perturbation.
Pharmaceutical Chemistry

1. **Drug Discovery and Drug Development**: Introduction, Present and Past, Drugs and the medicinal chemist, Classification of drugs, Drug targets specification, Choice of Bioassay, In Vivo and in Vitro tests, Pit fails.

2. **Drug Action at Receptors**: Receptor role, Neuro-transmitters and Hormones, Change of shape by the receptors, Design of Agonists and Antagonists, Drug action on DNA and RNA.


4. **Protein-Ligand Interactions**: Concepts and applications.

Surface Chemistry Adsorption and Catalysis

1. **Introduction**: Basics of surface chemistry, surface tension and adsorption.

2. **Surface & Colloids**: Coagulation and kinetics of coagulation, spontaneous aging of colloids.

3. **Aggregation Processes**: Coalescence and particle growth, Stability of colloids, Electric properties, theories of structure of electrical double layer, determination of charge on colloids particle, size and shape of colloids particles.

4. **Association of colloids**: Self-assembly system, Reversal of phase, emulsion, Macro and Micro emulsion and Aerosols, emulsifying agents, theories of emulsification, gels, sol gel transformation thixotropy.

5. **Electrokinetic Effect**: Electrosorption, electrophoresis, streaming potential, Dorn effect, stabilization of surfactant solutions.


7. **Catalysis**: Homogeneous and Heterogeneous Catalysts, Acid base catalysis, Biocatalysts, Micellar catalysis, Mechanism of few catalytic reactions.


Symmetry and Group Theory

1. **Symmetry elements and operations**: Symmetry planes and Reflections, Inversion centre, Proper axes and Proper rotations, Improper axes and Improper rotations.

2. **Relations among Symmetry elements**: Products of symmetry operations, Equivalent symmetry elements and Equivalent atoms, General relations among symmetry elements and operations, symmetry point groups, symmetry classification of molecules.

3. **Representations of groups**: Important rules about irreducible representations and their characters, Relationship between reducible and irreducible representations with examples, construction of character tables.


5. **Molecular orbital theory for Inorganic compounds**: Transformation properties of atomic orbitals, Molecular orbitals for sigma bonding in tetrahedral and octahedral molecules.
6. **Ligand Field theory**: Introduction, Electronic structure of free atoms and ions, splitting of levels and terms in a chemical environment, construction of energy level diagram.

**Chemistry of Transition and Inner - Transition Elements**

1. **Survey of Transition Metal Chemistry** – Electronic configuration, general characteristics, oxidation states, pπ-acid ligands, metal complexes, metal-metal bond, Quadruple bonds.
2. **Chemistry of First Transition Series** – The elements, compounds, complexes, organometallics and bioinorganic chemistry of first transition series in different oxidation states.
3. **Chemistry of Second & Third Transition Series** – The elements, compounds, complexes, organometallics and bioinorganic chemistry of second and third transition series in different oxidation states.
4. **Lanthanides**: Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of lanthanides.
5. **Actinides**: Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of Actinides.
6. **Transition Metal Catalyzed Reactions**: Oxidative addition, Elimination reactions, Migration reactions.
7. **Mechanism of Inorganic Reactions**: Inner sphere, Outer sphere, Trans effect.

**Physical Methods of Structure Elucidation**

1. **Ultraviolet (UV) Spectroscopy**: Principles, origin, effect of structure, solvents, conjugation and Chromophores and Auxochromes, the Woodward-Fieser rules, PES and related spectroscopy.
2. **Microwave Spectroscopy**: Rotation of molecules and rotational spectra- Diatomic molecules, polyatomic molecules-Linear, symmetric top and asymmetric top molecules.
5. **Mossbauer Spectroscopy**: Principles and applications of Mossbauer spectroscopy.
6. **Magnetic Resonance Spectroscopy**: Magnetic resonance- spin angular momentum, Larmor frequency, Relaxation time, NMR spectroscopy of proton and C1 Introduction to ESR. Hyperfine structure and double resonance in ESR. Applications of ESR spectroscopy.
7. **Mass Spectroscopy**: Principles instrumentation and applications.
Analytical Principles and Instrumental Methods of Analysis

1. Atomic Absorption Spectroscopy: General principles, instrumental set up and analytical procedures and applications,
2. Thermo-Analytical Method: Theory, instrumental requirements and methodology for thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), applications
3. Chromatographic Methods: Classification of chromatographic methods according to separation and development procedure, Instrumentation and applications (GC and HPLC)
4. Electrochemical Techniques: Conductometry, pH metry, Karl Fischer titration, cyclic voltametry, Polarography
5. Modern Methods of Surfaces and Crystal Analysis: SEM, TEM, AFM, XRD

Computational Chemistry

1. Operating Systems: Basic understanding of operating systems: DOS, Windows, UNIX, Linux
2. Programming Concepts of Programming languages, use of programming languages (FORTRAN/ C/C++) in making of chemistry programs
3. Mathematical Modeling methods including QSAR/PR/TR (2D & 3D)
4. Drug Design methods Concept of Docking and Virtual Screening
5. Data Analysis: Uncertainties, Errors, calibrations, Mean, Standard Deviation, Least square fit,
6. Concepts of various methods of correlation analysis: Linear and Non-linear regression methods including Multiple Linear Regression (MLR), Artificial Neural Networks(ANN), Support Vector Machine(SVM), Partial Least Squares (PLS)