M.Sc. (Previous)

Paper I

Symmetry & Spectroscopy

1. **Symmetry:** Symmetry elements, Symmetry operations, Symmetry point group, Identification of molecular point group, Molecules of low symmetry, high symmetry and special symmetry (C_n, S_n, D_n, C_{nv}, D_{nh} only)
2. **Group, Classes:** Definition, multiplication table, group generating elements, subgroup, classes, derivation of matrices (C_n, σ, i, S_n), Direct product, Group multiplication basis, matrix representation, Character of an operation, orthogonality projection and shift operators, character table, orthogonality theorem, irreducible representation, Transformation matrices, structure of character table, determination of symmetry species for translations and rotations, construction of character table (C_{2v}, C_{3v})
3. **Valence Bond Theory:** Formation of hybrid orbitals of XY_3 (planar) XY_4 (T_d, square planar). Symmetry of orbital, orbital symmetry properties, Projection to get symmetry orbital, projection operations, basis functions and hybrid orbitals with example
4. **Molecular vibrations:** Internal and symmetry coordinates, SALC's, Symmetric normal vibrations, mixing of linear coordinates in normal modes, determination of symmetry types of normal modes, determination of symmetry types of normal modes, analysis of vibration of 1, 2 dichloro ethylene.
5. **Unifying Principles:** Electromagnetic radiation and its characteristics, Absorption, Emission spectroscopy, Born – Oppenheimer approximation, Rotational, Vibrational and electronic energy levels, Classification of spectra, Region of spectrum.
6. **Infrared Spectroscopy:** Linear harmonic oscillator, Vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, Morse potential, Vibration – rotation spectroscopy, P, Q, R branches, Breakdown of oppenheimer approximation, vibration of polyatomic molecules, selection rules, Group frequencies, Overtones, Hot bands, factors affecting the bond positions and intensities for IR region
7. **Normal Coordinate Analysis:** Cartesian coordinate and internal coordinate methods applied to C_{2v}(Sym XY_2, ZXY_2), $C_{3v}(XY_3)$, T_d (XY_4) and $O_n(XY_6)$ system, IR and Raman activity of some typical molecules (C_{2v}, C_{3v} ,C_{4v}, D_{2h}, D_{3h}, D_{4h} point group)
8. **Raman Spectroscopy:** Classical and quantum theories of Raman effect, Pure rotational, Vibrational and Vibrational – rotational Raman spectra, Selection rule, Mutual exclusion principle, Resonance Raman spectroscopy, CARS
9. **Diffraction Techniques: -**

(A) **X- ray Diffraction:** General Features of diffraction, Powder X-ray diffraction, Single crystal X-ray diffraction: The technique, structure factor, phase problem, brief description of time resolved X- rays diffraction techniques.

(B) **Electron Diffraction:** Scattering intensity vs scattering angle, Wierl equation, Measurement technique, Elucidation of structure of simple gas phase molecules, Low energy electron diffraction structure of surfaces

(C) **Neutron Diffraction:** Brief introduction, difference with X-rays diffractions.

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M.Sc. (Previous)

Paper II

Inorganic Chemistry I

1. **Stereochemistry and bonding:** VSEPR theory- stereochemical rules and explanation of the shapes of molecules and ions of nontransition element with 2-7 valence shell electron pairs, Walsh diagram (Tri and penta atomic molecules) $d\pi-p\pi$ bonds, Bent rule, Energetics of hybridization
2. **Synthesis, Properties and Structures:** Halides and oxides of nontransition elements, silicates and carbides, silicones, phosphazenes, sulphur- nitrogen compounds, Peroxo compounds of B,C and S, Oxyacids of N, P, S and Halogens, interhalogens, Pseudohalides, Noble gas compounds
3. **Structures of 2 to 8 Coordinate Metal Complexes:** Cation –anion ration in various polyhedral, hybrid orbitals and preferred conditions of formation of the complexes of following geometries: CN 2 – Linear, CN 3 – Trigonal planar, Trigonal pyramidal, CN 4 –Tetrahedral, Square planar, CN 5 – Trigonal bipyramidal, Square pyramidal, pentagonal, CN 6 – Octahedral, Trigonal prism, CN 7 – Pentagonal bipyramidal, Capped octahedral, Capped trigonal prism, CN 8- Cubic Tetragonal antiprismatic, Dodecahedral, Hexagonal bipyramidal and bicapped trigonal prism, Stereochemical non- rigidity in four to eight coordinate complexes
4. **Stereoisomerism:** Stereoisomerism in six coordinate octahedral complexes (Ma_3bcd, Ma_2bcde, Mabcdef and complexes containing bi and ter – dentate ligands) intermolecular and intramolecular rearrangements (Bailar and Ray Dutta twist only), mechanism of racemisation in tris(chelate) octahedral complexes, Methods of resolution of optical isomers.

5A. Crystal Fields: Derivation of d orbital splitting patterns of ML_2, ML_3, ML_5 and ML_7 system (energy calculations are not required), the effect of weak field on.

5B. Metal – ligand bonding: Limitation of CFT, Nephelauxetic series, Molecular orbital energy level diagram of octahedral, tetrahedral and square planar complex.

6. **Metal Ligand Equilibria in solution:** Stepwise and overall formation constants and their relations, factors affecting stability of metal complexes with reference to the nature of metal ions and ligands, Determination of stability constants by pH metric and spectroscopic methods.
7. **Kinetics and Mechanism**

   (A). Substitution Reactions: In octahedral Co(III) and Square planar Pt(II) complexes

   (B). Electron Transfer Reactions: Mechanism of one electron reactions (inner and outer sphere mechanisms), factors affecting the rates of direct electron transfer reactions and the Marcus equation, two electron transfer reactions

8. **Electronic spectra of complexes**

   A. Eneregy levels in an atom: Relation between electronic configuration and energy terms, Hund's rules and ground state energy terms, inter electron repulsion parameter, variation of reaction B and C parameters in different transition series, spin orbit coupling parameters

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B. Free ions in crystal fields: Effect of weak crystal field on free ion S, P, D, F and G terms in octahedral, square planar and tetrahedral symmetries, orgel diagrams, mixing of terms, medium and strong field approximation in on point group, transition from weak to strong field and correlation diagram for only d^2case, Non crossing rule, Tanbe sugano diagrams.

C. Interpretation of the spectra: of aqueous solution of $[M(H_2O)_6]^{n+}$, calculation of Dq, and B parameters, John Teller distortions and its effect on electronic spectra.

9. Magnetic Properties of Complexes: Dia, para, ferro and antiferromagnetism, quenching of orbital angular momentum by ligand, The magnetic properties of A, E and T terms.

10. Supramolecular Chemistry: Concept, molecular recognition, nomenclature, metallo –macrocyles as receptors, design of supramolecular through non covalent interaction and their application in transport process.

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