

Elective Paper I (Group C)

Advanced Quantum Chemistry:

(Pre-requisite: Mathematics at least upto First year B.Sc. level is necessary. At least one PC among 4-students should be available) in future so as to undertake specified course of computer experiments.

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| I. Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory | 12 hrs |
| Review of the principles of quantum mechanics, Born-Oppenheimer approximation, Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Rothan equation. | |
| II. Configuration Interaction and MC-SCF | 12 hrs. |
| Introduction to CI; full and truncated CI theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods. | |
| III. Valence Bond and Molecular Orbital Treatment of Hydrogen Molecule/ion: | 12 hrs. |
| Overlap, coulomb and exchange integrals. Singlet and Triplet state of hydrogen molecule (Heitlers – London theory). Simple MO treatment of hydrogen ion for bonding and antibonding orbitals. Normalization of LCAO and MO Functions. | |
| IV. Semi-Empirical Theories | 12 hrs. |
| A review of the Huckel, EHT and PPP treatments. ZDO approximation, detailed treatment of CNDO and M INDO theories. A discussion of electronic energies and properties. | |
| V. Density Functional Theory | 12 hrs. |
| Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory. | |

Books Suggested

1. Modern Quantum Chemistry, N.S. Ostlund and A.Szabo, McGraw Hill.
2. Methods of Molecular Quantum Mechanics, R.McWeeny and B.T.Sutcliffe, Academic Press.
3. Density Functional Theory of Atoms and Molecules, R.G.Parr and W.Yang, Oxford.
4. Exploring Chemistry with Electron Structure Methods, J.B.Foresman and E.Frish, Goussian Inc.
5. Semi-empirical MO Theory, J.Pople and D.L.Beveridge.