CH2CO5 - APPLICATIONS OF QUANTUM MECHANICS AND GROUP THEORY (3 Credits, 54hrs)

Unit 1: Approximation Methods in Quantum Mechanics (9hrs)

Many body problem and the need of approximation methods; Independentparticle model; Variation method – variation theorem with proof, illustration of variation theorem using a trial function [e.g., x (a-x)] for particle in a 1D-box and using the trial function e $^{-\alpha r^2}$ for the hydrogen atom, variation treatment for the ground state of heliumatom; Perturbation method – time-independent perturbation method (non-degenerate case only), illustration by application to particle in a ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom.

Unit 2: Quantum mechanics of many -electron atoms (9hrs)

Hartree Self-Consistent Field method for atoms; Spin orbitals for many electron atoms, symmetric and antisymmetric wave functions, Pauli's antisymmetry principle; Slater determinants; Hartree -Fock Self- Consistent Field (HF-SCF) method for atoms, Hartree -Fock equations (derivation not required) & the Fock operator; Roothan's concept of basis functions – Slater type orbitals (STO) and Gaussian type orbitals (GTO).

Unit 3: Chemical bonding in diatomic molecule (9hrs)

Schrödingere quation for a molecule, Born – Oppenheimer approximation; Valence Bond (VB) theory – VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2; Molecular Orbital (MO) theory – MO theory of H_2+ ion, MO theory of H2 molecule, MO treatment of homonuclear diatomic molecules – Li_2, Be_2, C_2, N2, O_2 & F_2 and hetero nuclear diatomic molecules – LiH, CO, NO & HF, bond order, correlation diagrams, non-crossing rule; Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories.

Unit 4: Chemical Bonding in polyatomic molecules (hrs)

Hybridization – quantum mechanical treatment of sp, sp2 & sp3 hybridisation; Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion, charge distributions and bond orders from the coefficients of HMO, calculation of free valence, HMO theory of

aromatic hydrocarbons (benzene); formula for the roots of the Hückel determinantal equation, Frost -Hückel circle mnemonic device for cyclic polyenes.

Unit 5: Applications of Group Theory to Molecular Spectroscopy (9hrs)

Molecular vibrations - symmetry species of normal modes of vibration, construction of Γcart, normal coordinates and drawings of normal modes (e.g., H2O and NH3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH4 , SF6), complementary character of IR and Raman spectra.

Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non –vanishing integrals, transition moment integral and spectral transition probabilities, overlap integrals and conditions for overlap.

Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

Unit 6: Applications of Group Theory to Chemical Bonding (9hrs)

Hybridisation - Treatment of hybridization in BF_3 and CH_4, Inverse transformation and construction of hybrid orbitals.   Molecular orbital theory – HCHO and H_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using proj ection operator, use of projection operator in constructing SALCs for the π MOs in cyclopropenyl (C $_3H_3^+$) cation.

References (for Units 1 to 4)

1. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill, 1968.

2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,

3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition,* Pearson Education Inc., 2009.

4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.

5. M.W. Hanna, *Quantum Mechanics in Chemistry* , 2nd Edition, W.A. Benjamin Inc., 1969.

6. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition, Viva books, 2003).

7. Thomas Engel, Quantum Chemistry & Spectro scopy, Pearson Education, 2006.

8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.

9. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.

10. A.K. Chandra, *Introduction to Quantum Chemistry* , 4th Edition, Tata McGraw-Hill, 1994.

11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics* , McGraw-Hill, 1935 (A good source book for many derivations).

12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.

13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.

14. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.

15. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry* , Prism Books Pvt. Ltd.,1998.

16. Jack Simons, *An Introduction to Theoretical Che mistry*, Cambridge University Press, 2003.

For Units 5&6

1.F.A.Cotton, *Chemical applications of Group Theory*, 3rd Edition, John Wiley &Sons Inc. 2003.

2.H. H. Jaffe and M. Orchin, *Symmetry in Chemistry,* John Wiley &Sons Inc., 1965.

3.L.H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill, 1969.

4.R. McWeeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London, 1963.

5.P.H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., NewYork, 1998.

6.Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood 1998.

7.A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry,* PHI Learning Pvt. Ltd. 2010.

8.Arthur M Lesk, *Introduction to Symmetry & Group theory for Chemists*, Kluwer Academic Publishers, 2004.

9.K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009.

10.A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers,1997.