UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I

CH1CO1 - QUANTUM CHEMISTRY AND GROUP THEORY (3Credits, 54 hrs)

Unit 1: Introduction to Quantum mechanics (9hrs)

Black body radiation and Planck's quantum postulate. Einstein's photoelectric equation, de Broglie's matter waves, Uncertainty principle, Schrodinger's wave mechanics, Deduction of Schrodinger wave equation from classical wave equation- Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, eigen functions of commuting operators; Expectation value postulate; Postulate of time-dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((L_x, L_y, L_z), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.

Unit 2: Quantum mechanics of Translational & Vibrational motions (9hrs)

Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a one-dimensional box with one finite potential wall, Particle in a rectangular well, (no derivation), Significance of the problem, Introduction to tunneling; Particle in a three dimensional box, Separation of variables, degeneracy. Symmetry breaking.

One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, wave functions and energies, important features of the problem, harmonic oscillator model and molecular vibrations.

Unit: 3 Quantum mechanics of Rotational motion (9hrs)

Co-ordinate systems:- Cartesian, cylindrical polar and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution of the Phi-equation, One particle Rigid rotator (non planar rigid rotator or particle on a sphere) (complete treatment): Angular momentum in spherical polar co-ordinate, The wave equation in spherical polar coordinates, wave functions in the real form;

separation of variables, the Phi-equation and the Theta-equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms),Converting imaginary functions to real form, polar diagrams of spherical harmonics. Spherical harmonics as eigen functions of angular momentum operators Lz and L^2.

Unit 4: Quantum Mechanics of Hydrogen-like Atoms (9hrs)

Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots. angular functions (spherical harmonics) and their plots. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), spin orbitals, construction of spin orbitals from orbitals and spin functions.

Unit 5: Foundations of group theory & molecular symmetry (9hrs)

Basic principles of group theory - the defining properties of mathematical groups, finite and infinite groups, Abelian and cyclic groups, group multiplication tables (GMT), similarity transformation, sub groups & classes in a group;

Molecular Symmetry & point groups - symmetry elements and symmetry operations in molecules, relations between symmetry operations, complete set of symmetry operations of a molecule, point groups and their systematic identification, GMT and classes of point groups;

Mathematical preliminaries - matrix algebra, addition and multiplication of matrices, inverse of a matrix, square matrix, character of a square matrix, diagonal matrix, direct product and direct sum of square matrices, block factored matrices, solving linear equations by the method of matrices;

Matrix representation of symmetry operations.

UNIT 6: Representations of point groups & corresponding theorems (9hrs)

Representations of point groups - basis for a representation, representations using vectors, atomic orbitals and cartesian coordinates positioned on the atoms of molecule (H_2O as example) as bases, reducible representations and irreducible representations (IR) of point groups, construction of IR by reduction (qualitative demonstration only), Great orthogonality theorem (GOT) (no derivation) and its consequences, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2V}, C_{3V},

C_{2h} and C_{4V} and C_3 as examples), nomenclature of IR - Mulliken symbols, symmetry species;

Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g., Γ_{cart}) using the reduction formula;

Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

Reference 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 6 th 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 & Spectroscopy, 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., New York, 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.