UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS ANDBIBLIOGRAPHY

Subject	
Code	**Name**
QF536	Quantum Chemistry

Vector
OF:S-5 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement	MA311 QI245 *F 328

Summary

The postulates of Quantum Mechanics. The Schrodinger Equation. Exact solutions and approximation methods. The Hydrogen atom and multi-electronic atoms. Methods to obtain the electronic structure of molecular systems.

Program

Historical aspects, properties of waves: Wavelength, wave number, period, frequency, velocity of propagation. Fundamental equations of the old quantum theory: Planck and de Broglie.
I. The first postulate of Quantum Mechanics: The stationary wave function and is propagation in time. Probability densities and probabilities. Normalized and non-normalized wave functions. Well behaved wave functions: continuous, single-valued and finite.
II. The second postulate of quantum mechanics: Operators. The linear momentum operator. Definition of operators from classical concepts: the potential energy operator, the kinetic energy operator, and the Hamiltonian. Sum and multiplication of operators. Linear operators. The eigenvalue equation. Hermitian operators and orthogonal functions.
III. Some fundamental theorems: Orthogonality. Set of orthogonal functions (Kronecker's Delta). Expansion in a base. Commutation. Heisenberg's uncertainty principle. Commutation of two operators in a set of eigenfunctions. Commutators and the uncertainty principle.
IV. Third postulate: Mean value theorem. Average values and probability for discrete and continuous variables. Eigenvalues and average values.
V. Fourth postulate: The Schrodinger Equation. The time-dependent Schrodinger Equation. Separation of variables. The time-independent Schrodinger Equation. Solution of the differential equation for time. The global wave time-dependent wave function.
VI. Analytical solution for the uni-dimensional particle in a box problem. Definition of the potential. Building the Hamiltonian and the Schrodinger equation. Analytical solution of the differential equation: Using boundary conditions. Energy levels, wave function: normalization and nodes. Average value of the momentum operator. Average value of the position: mean value and most probable value.
VII. Analytical solution of the particle in box in two dimensions. Building the Hamiltonian and the Schrodinger equation. Variable separation. Degeneracy. Computing average values for more than one coordinate.
VIII. Analytical solution of the particle in a ring. Circular movement in the xy plane, constructing the kinetic energy operator: momentum of inertia and angular momentum. Plane-polar coordinate system and the transformation of Cartesian (xy) and plane-polar (r,theta) coordinates. Solution of the Schrodinger equation and boundary conditions: quantization of the energy, degeneracy, quantum numbers and angular momentum in the z coordinate.
IX The rigid rotor. Rigid rotor with two masses, center of mass for two bodies, change of origin of the coordinate system, representing the rotational kinetic energy in three

dimensions: reduced mass, momentum of inertia, and angular momentum. Angular momentum and the construction of the angular momentum operator in Cartesian coordinates. Spherical coordinates and the transformation of the angular momentum operator. Solution of the Schrodinger equation for the rigid rotor, separation of variables and energy quantization. Wave equations for the rigid rotor: Legendre functions and spherical harmonics. Quantum numbers and angular momentum.
X. Harmonic Oscillator. Solution of the classical harmonic oscillator equation: fundamental frequency and force constant. Solution of the Schrodinger equation for the harmonic oscillator involving two masses: The Hermite differential equation and the quantization of energy.
XI. Variational Principle and Perturbation Theory
XII. The Hydrogen and Multi-electronic atoms.
XIII. The Hartree Model. Definition of spin-orbitals and the the wave function as the product of Hartree using spin-orbitals. Determination of the mean value of the electronic energy of a multi-electronic atom using the Hartree product. Integration of the spin coordinates and the mean value of the energy in terms of orbital functions. A simplified deduction of the Hartree method: the model for independent particles, orthonormal spin-orbital functions, Coulomb integrals and the Hartree equations. Interpretation of the Hartree equations: the mean field ans self-consistent model. Distribution of Fermions and Bosons: symmetry and anti-symmetry of the wave function. Wave function for He atoms in fundamental and excited states.
XIV. The Hartree-Fock methods. Anti-symmetric wave functions for many electrons. Slater determinants. The Pauli exclusion principle.
XV. Molecular Orbital Theory.

Bibliography

1. McQuarrie, D. A.; Simon, J. D. Physical chemistry: a molecular approach; University Science Books: McGuire, Ann Editor, 1997.
2. Chandra, A. K. Introductory quantum chemistry; Tata McGraw-Hill, 1994.
3. Levine, I. N. Quantum Chemistry; volume I Academic Press: New York, 1993.
4. McWeeny, R.; Sutcliffe, B. T. Methods of Molecular Quantum Chemistry; Academic Press: London, 1969.
5. Szabo, A.; Ostlund, N. S. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory; MacMillan Publishing Co., Inc.: 866 Third Av., New York, N. Y., 10022, 1982.
6. D.A.McQuarrie and J.D.Simon, Physical Chemistry: A Molecular Approach, University Science Books; 1a. edição (1997).
7. Oswaldo Sala, Fundamentos da Espectroscopia Raman e no Infravermelho; Ed.Unesp, 1ª. Edição (1996).
8. G. N. Barrow, Introduction to Molecular Spectroscopy; McGraw-Hill Education, (1962).

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures. For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.