DISCIPLINE SPECIFIC CORE COURSE-15 (DSC-15): Quantum Chemistry and Organic Chemistry IV Covalent bonding

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Quantum Chemistry and Covalent bonding (DSC-15, Physical Chemistry V)	**04**	**03**	**--**	**01**	**Class 12th with Physics, Chemistry, Mathematics**	

Learning objectives

The objectives of this course are as follows:

- To make students understand the limitations of classical mechanics and the need of quantum chemistry
- To familiarize the students with the postulates of quantum chemistry
- To explain how to apply the postulates to derive equations for various models and extend to hydrogen atom and hydrogen like atoms.
- To explain the valence bond and molecular orbital theories and their applications to simple molecules
- To explain the use of some computational software

Learning outcomes

By studying this course, students will be able to:

- Explain the limitations of classical mechanics and solution in terms of quantum mechanics for atomic/molecular systems.
- Develop an understanding of quantum mechanical operators, quantization, probability distribution, uncertainty principle
- Set up Schrodinger equations for different types of systems
- Explain the concept of covalent bonding based on valence bond theory and molecular orbital theory.
- Perform calculations using different software and plot different wavefunctions and probability distribution curves.
- Perform simple calculations using appropriate quantum mechanical methods in different computational software

SYLLABUS OF DSC-15

Unit-1: Quantum Chemistry **(Hours: 22)**

Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrödinger equation and its application to free particle and particle in a box rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties, Extension to two and three- dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar coordinates (derivation not required). Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).

Unit-2: Hydrogen atom (Hours: 08)

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Zeeman effect, Introduction of spin quantum number and magnetic spin quantum number Setting up of Schrödinger equation for many electron atoms (He, Li), Indistinguishability of electrons and Pauli exclusion principle, Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Unit-3: Covalent bonding (Hours: 15)

Setting up of Schrödinger equation, Born-Openheimer approximation, LCAO-MO treatment of H_2^+ and its qualitative extension to H_2, Valence bond (VB) treatment of H_2, Comparison of LCAO-MO and VB wave functions of H_2 and their refinements, Qualitative description of LCAO-MO of homonuclear and heteronuclear diatomic molecules-HF and LiH.

Practical component

Practical: Credits: 01

(Laboratory periods: 15 classes of 2 hours each)

1. Plot the radial wavefunctions and probability distribution for H atom's 1s, 2s, 2p orbital using software like EXCEL.
2. Using a software such as ArgusLab, plot HOMO, LUMO and ESP maps of various molecules.
3. Draw probability plots for a particle in a 1-dimensional box for different values of quantum number n - commenting on the number of points of zero probability and then correlate them with the correspondence principle.
4. Plot the electron density contour maps of sigma molecular orbitals for diatomic homonuclear molecules.
5. Plotting of the wave function and probability curve for simple harmonic motion and interpret the results for first two levels.

6. Plotting energy as a function of distance for simple harmonic motion - parabolic curve.
7. Using software such as ArgusLab calculate properties such as dipole moment and Mulliken charges using quantum mechanical methods.

Note: Any other suitable software may also be used .

Essential/recommended readings

Theory:

1. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
2. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier.
3. McQuarrie, D.A. (2016), **Quantum Chemistry**, Viva Books.
4. Chandra, A. K. (2001), **Introductory Quantum Chemistry**, Tata McGraw-Hill.
5. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier

Suggested Readings

1. Atkins, P.W.; Friedman, R. (2010), **Molecular Quantum Mechanics**, 5th Edition, Oxford University Press.

Practical:

1. McQuarrie, D. A. **Mathematics for Physical Chemistry** University Science Books (2008).
2. Mortimer, R. **Mathematics for Physical Chemistry**. 3rd Ed. Elsevier (2005).
3. Steiner, E**. The Chemical Maths Book** Oxford University Press (1996).
4. Yates, P. **Chemical Calculations**. 2nd Ed. CRC Press (2007).
5. Levie, R. de, **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press (2001) 487 pages.
6. Noggle, J. H. **Physical Chemistry on a Microcomputer**. Little Brown & Co. (1985).

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.