



**Avinashilingam Institute for Home Science and Higher Education for Women**  
(Deemed to be University under Category 'A' by MHRD, Estd. u/s 3 of UGC Act 1956)  
Re-accredited with A++ Grade by NAAC. Recognised by UGC Under Section 12B  
Coimbatore - 641 043, Tamil Nadu, India  
**Continuous Internal Assessment –II October 2025**

**II Semester**

**Class : III UG**  
**Branch : Chemistry**

**Time : 2 hours**  
**Max. Marks : 60**

**23BCHC09 Introduction to Quantum Chemistry**

CO1: Understand the basics of quantum mechanics  
CO2: Identify the steps involved in studying a system quantum mechanically  
CO3: Apply Schrödinger wave equation to Simple harmonic oscillator and Rigid rotor models  
CO4: Apply Schrödinger wave equation to hydrogen and hydrogen like ions  
CO5: Generalize the VB and MO treatment of H<sub>2</sub> species

**Part-A**

**Answer the following**

**6×1=6**

- Which of the following is the fundamental equation of quantum mechanics?  
a) Newton's Law                      b) Maxwell                      c) Schrödinger                      d) Euler's Formula                      CO4K1
- In a rigid rotator distance between two particles is \_\_\_\_\_  
a) Variable                      b) Zero                      c) Infinite                      d) constant                      CO3K2
- What is the ground state energy of the quantum mechanical harmonic oscillator?  
a)  $E_0 = hv/2$                       b)  $E_0 = 0$                       c)  $E_0 = hv$                       d)  $E_0 = v^2$                       CO3K4
- What is the type of polynomial function in harmonic oscillator wavefunction?  
a) Binominal                      b) Hermite                      c) Monomial                      d) Trinomial                      CO3K1
- What is the expression for reduced mass,  $\mu$  for two particles in a system of mass  $m_1$  and  $m_2$ ?  
a)  $\mu = m_1m_2$                       b)  $\mu = m_1 \times m_2 / m_1 + m_2$                       c)  $\mu = m_1 + m_2$                       d)  $\mu = 1/m_1 \times m_2$                       CO4K1
- What is the mathematical definition of angular momentum  $L$  for a classical particle in terms of moment of inertia  $I$  and angular frequency  $\omega$ ?  
a)  $L = I^2\omega$                       b)  $L = I\omega^2$                       c)  $L = I/\omega$                       d)  $L = I\omega$                       CO3K4

**Part-B**

**3x6=18**

**Answer all Questions**

**Each answer should not exceed 200 words or one page**

- a. Write an equation for finding total energy of Hydrogen atom                      CO4K2  
(or)  
b. Enumerate on constructive and destructive overlap                      CO5K4
- a. Discuss about Average and most probable distances of electron from nucleus                      CO4K3  
(or)  
b. Deliberate on limitations of VB theory                      CO5K3
- a. Compare LCAO- MO and VB treatments of H<sub>2</sub>                      CO5K3  
(or)  
b. Discuss the transformation from cartesian coordinates to spherical coordinates                      CO3K3

**Part – C**

**3x12=36**

**Answer ALL Questions**

**Each answer should not exceed 600 words or three pages**

- a. Discuss in detail about Quantitative treatment of simple harmonic oscillator model                      CO3K4  
(or)  
b. Enumerate on Rigid rotator model                      CO3K4
- a. Give a detailed account of setting up of Schrödinger equation in spherical polar coordinates for Hydrogen atom                      CO4K4  
(or)  
b. Discuss in detail about separation of variable and solution for Hydrogen atom                      CO4K4
- a. Derive Secular equation                      CO5K4  
(or)  
b. Explain in detail about radial and angular parts of atomic orbitals                      CO4K4

**No of Copies: 20      Staff in-charge: Dr.A.Prithiba**