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**5 SEM TDC CHMN (CBCS) C 12**

**2025**

( Nov/Dec )

**CHEMISTRY**

( Core )

Paper : C-12

**( Physical Chemistry, Quantum Chemistry  
and Spectroscopy )**

Full Marks : 53

Pass Marks : 21

Time : 3 hours

*The figures in the margin indicate full marks  
for the questions*

1. Choose the correct answer from the following : 1×4=4

(a) The momentum operator in one-dimension is

(i)  $\frac{h}{2\pi} \frac{\partial}{\partial x}$

(ii)  $\frac{2\pi i}{h} \frac{\partial}{\partial t}$

(iii)  $\frac{h}{2\pi i} \frac{\partial}{\partial x}$

(iv)  $\frac{2\pi i}{h} \frac{\partial}{\partial x}$

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(b) Which of the following statements about the hydrogen atom in groundstate is incorrect?

(i) It is described by the quantum number  $n = 1, l = 0, m = 0$

(ii) The electron's angular momentum equals to  $h/2\pi$

(iii) The radial distribution function has its maximum at the Bohr radius

(iv) The wave function is spherically symmetrical

(c) The movement of nuclei is negligible during the time taken by an electronic transition. It is called

(i) Born-Oppenheimer approximation

(ii) Franck-Condon principle

(iii) Lambert-Beer law

(iv) None of the above

(d) The photochemical decomposition of a substance is called

(i) thermal dissociation

(ii) photolysis

(iii) photosensitization

(iv) thermolysis

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2. Answer any *four* of the following :  $2 \times 4 = 8$

(a) Show that  $e^{-\alpha x^2}$  ( $\alpha$  is a constant) in an eigenfunction of the operator  $\frac{1}{x} \cdot \frac{d}{dx}$

but not of  $\frac{d^2}{dx^2}$ .

(b) Write two postulates of quantum mechanics.

(c) What is the significance of  $\psi$  and  $\psi^2$ ?  
What is an operator?  $1+1=2$

(d) What does angular part of wave function depict?

(e) What is Born-Oppenheimer approximation?

(f) State Einstein law of photochemical equivalence.

3. Answer any *four* of the following :  $4 \times 4 = 16$

(a) Solve Schrödinger wave equation for a particle moving freely in a three-dimensional cubic box.

(b) What are normalized and orthogonal wave functions? Explain with suitable examples.  $2+2=4$

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(c) What is a harmonic oscillator? Set up Schrödinger equation for a linear harmonic oscillator. 1+3=4

(d) Normalize the wave function  $\psi = A \sin \frac{\pi nx}{l}$  for a particle in one-dimensional box of length  $l$ . What is probability distribution function? 2+2=4

Show that zero-point energy of the harmonic oscillator is consistent with uncertainty principle.

(f) Write the Schrödinger equation for hydrogen atom in terms of polar coordinates. Write the expression for the energy of electron in hydrogen and hydrogen-like atoms. 2+2=4

4. Answer any four of the following : 4×4=16

(a) Discuss the effect of isotopic substitution on the rotational spectra of a diatomic molecule.

(b) The fundamental vibrational frequency of CO is  $2140 \text{ cm}^{-1}$ . Calculate the force constant of the molecule. Define hot bands. 3+1=4

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(c) State and explain Franck-Condon principle. Define chromophore with example. 3+1=4

(d) Discuss the principle of NMR spectroscopy. What is chemical shift? 3+1=4

(e) Describe the terms 'chromophores', 'auxochromes', 'bathochromic shift' and 'hypsochromic shift' giving examples.

5. Answer any two of the following :  $4\frac{1}{2} \times 2 = 9$

(a) What is quantum yield? What are the causes of low and high quantum yield? What is photochemical equilibrium?  $1+2\frac{1}{2}+1=4\frac{1}{2}$

(b) Discuss the mechanism of photosensitization and quenching. Write Beer-Lambert law.  $4+\frac{1}{2}=4\frac{1}{2}$

(c) Write short notes on any three of the following :  $1\frac{1}{2} \times 3 = 4\frac{1}{2}$

(i) Photostationary state

(ii) Jablonski diagram

(iii) Intersystem crossing

(iv) Chemiluminescence

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