

5 SEM TDC CHMH (CBCS) C 12

2023

(November)

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) Quantum mechanical operator for momentum is

(i) $\frac{h}{2\pi i} \nabla$

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

(iii) $-\frac{h^2}{8\pi^2 m} \nabla^2$

(iv) $\frac{h}{2i} \nabla$

(2)

(b) The energy required to excite (to first excited state) a particle of mass m confined in a length l is

(i) $\frac{3h^2}{8ml^2}$

(ii) $\frac{h^2}{8ml^2}$

(iii) 0

(iv) h^2

(c) The number of NMR signals formed by 2-chloropropene is

(i) 2

(ii) 3

(iii) 1

(iv) None of the above

(d) Some chemical reactions take place not by the absorption of light by one of the reactants but by a third substance which transfers the absorbed energy to the reactants. This process is known as

(i) quenching

(ii) photosensitization

(iii) chemiluminescence

(iv) None of the above

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(3)

2. Answer any four questions from the following : 2×4=8

(a) Why is $\psi\psi^*$ taken instead of ψ^2 ? What is angular part of wave function?

(b) What is zero-point energy? What is its significance?

(c) Why is TMS used as a reference standard in NMR spectroscopy?

(d) Describe Born-Oppenheimer approximation with its importance.

(e) What is the basic difference between fluorescence and phosphorescence?

UNIT—I

3. Answer any four questions from the following : 4×4=16

(a) Solve Schrödinger's wave equation for a particle moving freely in a three-dimensional cubic box. 4

(b) Write Schrödinger's wave equation for rigid rotator system and separate the variables. 4

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(Turn Over)

(4)

- (c) (i) Write a short note on eigenfunctions and eigenvalues. Normalize the function $\psi = x^2$ over the interval $0 \leq x \leq k$, where k is a constant. 2
- (ii) What will happen if the walls of the one-dimensional box are suddenly removed? 2
- (d) (i) What does angular part of wave function depict? 2
- (ii) How can spherical harmonics wave function for hydrogen atom be written? 2
- (e) (i) Write down Schrödinger's wave equation for H-atom in polar coordinates. 2
- (ii) Write a short note on orthogonal wave function. 2

UNIT—II

4. Answer any four questions from the following : 4×4=16

- (a) (i) Discuss about the interaction of electromagnetic radiation with a rotating molecule. 2
- (ii) Microwave studies are done only in gaseous state. Explain why. 2

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(5)

- (b) (i) Explain fundamental frequencies and overtones with examples. 2
- (ii) Calculate the force constant for H^{35}Cl from the fact that the fundamental vibrational frequency is $8.667 \times 10^{13} \text{ s}^{-1}$. 2
- (c) Discuss the relaxation processes in NMR spectroscopy. What is chemical shift? 3+1=4
- (d) Write short notes on the following : 2×2=4
- (i) Chromophores
- (ii) Bathochromic shift
- (e) (i) What are P, Q and R branches of vibrational rotational spectrum? 3
- (ii) Why is electronic spectrum a band spectrum? 1

UNIT—III

5. Answer any two questions from the following : 4½×2=9

- (a) What is Beer-Lambert law? Explain. What are the limitations of Beer-Lambert law? 2½+2=4½

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(Turn Over)

(6)

(b) What is the role of photochemical reactions in biochemical process? $4\frac{1}{2}$

(c) What is meant by photostationary state? What is chemiluminescence?
 $3+1\frac{1}{2}=4\frac{1}{2}$
