

**2025/TDC (CBCS)/ODD/SEM/
CHMHCC-502T/438**

TDC (CBCS) Odd Semester Exam., 2025

**CHEMISTRY
(5th Semester)**

Course No. : CHMHCC-502T

**[Physical Chemistry—V (Quantum Chemistry
and Spectroscopy)]**

Full Marks : 50

Pass Marks : 20

Time : 3 hours

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

UNIT—I

1. Answer any *two* of the following questions :
2×2=4

(a) Explain the concept of zero-point energy in the context of a quantum mechanical system like the particle in a box.

- (b) Write down the time-independent Schrödinger equation and identify its components.
- (c) Explain why energy levels of vibrating molecules are equally spaced.

2. Answer any *one* of the following questions : 6

- (a) (i) Using Schrödinger wave equation, derive an expression for the energy of a particle of mass m in 1D-box of length a and also calculate the eigenvalue. 3+1=4

- (ii) A particle of mass m is confined in a 1D-box of length a . Calculate the probability of finding the particle in the region

$$0 \leq x \leq \frac{a}{2} \quad 2$$

- (b) (i) Obtain an expression for energy of rigid rotator by considering quantum mechanical approach. 5
- (ii) Write the condition for an operator to be Hermitian operator. 1

(3)

UNIT—II

3. Answer any *two* of the following questions :
2×2=4

- (a) In the context of hydrogen atom, what is the physical meaning of the radial part of the wave function?
- (b) State the variation theorem and explain why it is a useful tool in quantum chemistry.
- (c) Write the total Hamiltonian of He atom considering all interactions.

4. Answer any *one* of the following questions : 6

- (a) (i) Explain with diagram the electron probability distribution of bonding and anti-bonding orbitals of H_2^+ molecule. 3
- (ii) Explain the basic difference between LCAO-MO and VBT by taking a suitable example. 3
- (b) (i) Obtain the expression for energy of H_2 molecule by solving Schrödinger equation with the help of VBT. 4
- (ii) Draw the molecular orbital diagram of HF. 2

UNIT—III

5. Answer any *two* of the following questions :

2×2=4

- (a) How can the bond length of a diatomic molecule be determined from its rotational spectrum?
- (b) Explain the concept of group frequencies in vibrational spectroscopy.
- (c) How is the force constant of a diatomic molecule related to its vibrational frequency?

6. Answer any *one* of the following questions : 6

- (a) (i) Explain the difference between classical and quantum mechanical treatments of diatomic vibrator. 4
- (ii) Show that the lines of rotational spectra are equally spaced. 2
- (b) (i) Explain why homonuclear diatomic molecule does not show vibrational spectra. 2
- (ii) Show that the zero-point energy of a harmonic oscillator is not zero. What does this non-zero value of zero-point energy signify? 1+1=2

- (iii) Explain the significance of Born-Oppenheimer approximation in simplifying the study of molecular spectra.

2

UNIT—IV

7. Answer any *two* of the following questions :

2×2=4

- (a) Differentiate between stokes and anti-stokes lines in a Raman spectrum in terms of energy exchange and frequency shift.
- (b) Define singlet and triplet state of electron.
- (c) What is the basic principle of NMR-spectroscopy?

8. Answer any one of the following questions : 6

- (a) (i) State and explain the Franck-Condon principle of electron transition.

3

- (ii) Explain why TMS is used as internal standard in NMR spectroscopy.

3

- (b) (i) Explain the phenomenon of fluorescence and phosphorescence in terms of molecular energy state and transition. 3
- (ii) Explain the rule of mutual exclusion with an example. 3

UNIT—V

9. Answer any *two* of the following questions :
2×2=4

- (a) State the two laws of photochemistry.
- (b) Explain photosensitized reaction with an example.
- (c) Explain the term quenching in photochemistry.

10. Answer any *one* of the following questions : 6

- (a) (i) Explain the importance and limitations of Beer-Lambert law. 2+2=4
- (ii) Explain the physical significance of absorption coefficient. 2

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- (b) (i) Define quantum yield. Explain abnormal quantum yields by giving at least two examples. 1+3=4
- (ii) Define the term chemiluminescence with an example. 2

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