

(6 pages)

Reg. No. : .....

Code No. : 6397

Sub. Code : ZCHM 13

M.Sc. (CBCS) DEGREE EXAMINATION,  
NOVEMBER 2022.

First Semester

Chemistry – Core

QUANTUM MECHANICS AND SPECTROSCOPY – I

(For those who joined in July 2021 onwards)

Time : Three hours

Maximum : 75 marks

PART A — (10 × 1 = 10 marks)

Answer ALL questions.

Choose the correct answer :

1. Schrodinger equation is a \_\_\_\_\_.

- (a) 1<sup>st</sup> order differential equation
- (b) Second order differential equation
- (c) Both (a) and (b)
- (d) None of these

2. Hamiltonian is given by

- (a) sum of K.E. and P.E.
- (b) Difference of K.E. and P.E.
- (c) Product of K.E. and P.E.
- (d) Square root of K.E. and P.E.

3. In one dimensional problem the energy levels of a bound state system are

- (a) Discrete
- (b) Degenerate
- (c) Non degenerate
- (d) Discrete and non degenerate

4. Who discovered the one-dimensional wave function?

- (a) Isaac Newton
- (b) Robert Boyle
- (c) Joseph Fourier
- (d) Jean d'Alembert

5. For what number of zeros, the approximation is poor?

- (a) 1
- (b) 2
- (c) 3
- (d) 4



6. Variational parameters are adjusted until the energy of the \_\_\_\_\_ wave function is minimized.

- (a) Atomic                      (b) Molecular  
(c) Ionic                        (d) Trial

7. Which of the following molecule shows rotational spectra?

- (a) N<sub>2</sub>                            (b) H<sub>2</sub>  
(c) CO<sub>2</sub>                        (d) Co

8. Which of the following is called heat radiation?

- (a) Infrared radiation  
(b) Microwave  
(c) Gamma rays  
(d) X-rays

9. Overtones are mainly observed in \_\_\_\_\_.

- (a) Far IR                        (b) Mid IR  
(c) Near IR                      (d) Not in the IR region

10. In Raman spectroscopy, the radiation lies in the \_\_\_\_\_.

- (a) UV Region                      (b) X-ray region  
(c) Visible region                      (d) microwave region

Page 3                      Code No. : 6397

PART B — (5 × 5 = 25 marks)

Answer ALL the questions, choosing either (a) or (b).

Each answer should not exceed 250 words.

11. (a) Write a note on Hermitian operator.

Or

(b) Comment on quantum mechanical treatment of angular momentum.

12. (a) The ground state wave function of a harmonic oscillator is  $\psi = \exp(-\alpha x^2)$  where

$\alpha = \frac{4\pi^2 m E}{h^2}$  and  $-\infty \leq x \leq \infty$ . Find the most probable value of  $x$ .

Or

(b) Explain the anharmonicity force constant and its significance.

13. (a) Write a note on the approximations used in the HMO method.

Or

(b) Give an account of Heitler - London treatment.

Page 4                      Code No. : 6397

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14. (a) Write briefly on Boltzmann distribution.

Or

- (b) Give an account of rotational spectra of symmetric top polyatomic molecules.

15. (a) Discuss the vibrations in linear molecules and symmetric top molecules.

Or

- (b) (i) Comment on absorption frequencies of any three functional groups for organic compounds.

- (ii) What is meant by Rayleigh scattering?

PART C — ( $5 \times 8 = 40$  marks)

Answer ALL the questions, choosing either (a) or (b).

Each answer should not exceed 600 words.

16. (a) Write a note on postulates of quantum mechanics.

Or

- (b) Discuss in detail the time-dependent and time-independent Schrodinger wave equations.

17. (a) Explain briefly the quantum mechanical treatment of simple harmonic oscillator.

Or

Page 5

Code No. : 6397

- (b) (i) Narrate the radial distribution functions.

- (ii) For a particle in a one-dimensional box of length 'L', find the probability in the region  $0 \leq X \leq L/4$  for  $n = 1$ .

18. (a) Discuss briefly the linear variation method.

Or

- (b) Write an account on Pauli exclusion principle and Slater determinant for He atom.

19. (a) Write notes on the following

- (i) Collision broadening

- (ii) Doppler broadening.

Or

- (b) (i) Comment on transition moment integral.

- (ii) What are the characteristics of an electromagnetic radiation?

20. (a) (i) Stokes lines are more intense than anti-stokes lines. Explain why?

- (ii) State and explain Born – Oppenheimer approximation.

Or

- (b) Describe the theory and principle of vibrational – rotational Raman spectroscopy.

Page 6

Code No. : 6397

