

PSG COLLEGE OF ARTS & SCIENCE  
(AUTONOMOUS)  
MSc DEGREE EXAMINATION MAY 2022  
(Second Semester)

Branch – CHEMISTRY

PHYSICAL CHEMISTRY – II

Maximum: 50 Marks

Time: Three Hours

SECTION-A (5 Marks)

Answer ALL questions

ALL questions carry EQUAL marks (5 x 1 = 5)

- Which one of the following is not a Hermitian operator?  
(i)  $P_x$  (ii)  $L_z$   
(iii)  $H$  (iv)  $iP_x$
- The normalization constant for the wave function of a harmonic oscillator is  
(i) 2 (ii)  $\frac{1}{2} \pi$   
(iii)  $(2\pi)^{-1/2}$  (iv)  $2 \pi$
- Which of the following statement is true regarding Born – Oppenheimer approximation?  
(i) It is valid as long as the energy levels in a molecule are widely separated  
(ii) It is valid as long as the energy levels in a molecule are close to each other  
(iii) It is valid when the energy levels in a molecule are same separation  $b/n$   
(iv) It is valid as long as the energy levels are minimum
- Which of the following is not a symmetry element of the  $C_{3v}$  point group?  
(i)  $E$  (ii)  $C_3$   
(iii)  $S_3$  (iv)  $\sigma$
- The number of vibrational degrees of freedom of ammonia molecule  
(i)  $2A_2+2E$  (ii)  $2A_2+E$   
(iii)  $2A_1+4B_1$  (iv)  $2A_1+2E$

SECTION - B (15 Marks)

Answer ALL questions

ALL questions carry EQUAL Marks (5 x 3 = 15)

- a) Explain the Heisenberg's uncertainty principle.  
(or)  
b) Describe the Hermitian operators.
- a. Explain the eigen functions and eigen values.  
Or  
b. Discuss the quantum numbers.
- a. Explain the antisymmetric nature of wave functions.  
Or  
b. Discuss the perturbation theory.
- a. Explain the symmetry elements and symmetry operations.  
Or  
b. Discuss the rules relating to the determination of point groups of molecules.

Cont...

10. a. Describe the hybrid orbitals in non linear molecules.  
Or  
b. Applying the group theoretical principles, predict the selection rules for IR spectra taking  $\text{H}_2\text{O}$  molecule as an example.

**SECTION -C (30 Marks)**

Answer ALL questions

ALL questions carry EQUAL Marks (5 x 6 = 30)

11. a. Explain the postulates of quantum mechanics.  
OR  
b. Describe the orthogonality and normalization of wave functions.
12. a. Explain how wave mechanics is applicable to simple system such as particle in a one-dimensional box.  
OR  
b. Describe the orthogonality of harmonic oscillator wave functions.
13. a. Describe the Born-Oppenheimer approximation.  
OR  
b. Describe the Huckel's molecular orbital theory of butadiene.
14. a. Derive the character table for  $\text{C}_{3v}$  point group using great orthogonality theorem.  
OR  
b. Discuss the matrix representation of symmetry operations.
15. a. Explain the determination of symmetries of vibrational modes of  $\text{NH}_3$  molecule.  
OR  
b. Discuss the determination of symmetries of vibrational modes of  $\text{POCl}_3$  molecule.

Z-Z-Z END