

**PSG COLLEGE OF ARTS & SCIENCE**  
(AUTONOMOUS)  
**MSc DEGREE EXAMINATION MAY 2019**  
(Second Semester)

Branch – CHEMISTRY

**PHYSICAL CHEMISTRY – II**

Time: Three Hours

Maximum: 75 Marks

**SECTION-A (10 Marks)**

Answer ALL questions

ALL questions carry EQUAL marks

(10 x 1 = 10)

- 1 What is the eigen value of function,  $y = \sin ax$ , for operator  $\frac{d^2}{dx^2}$ ?
 

(i) $a$	(ii) $-a^2$
(iii) $a^2$	(iv) None
- 2 The condition for well-behaved wave function is
 

(i) single valued	(ii) not continuous
(iii) multivalued	(iv) none
- 3 The zero point energy of simple harmonic oscillator is
 

(i) $h\nu$	(ii) $\frac{3}{2}h\nu$
(iii) $\frac{1}{2}h\nu$	(iv) zero
- 4 The orbital shapes are obtained from
 

(i) radial function	(ii) angular function
(iii) distribution function	(iv) none
- 5 The total wave function is
 

(i) symmetric	(ii) spatical
(iii) antisymmetric	(iv) none
- 6 What is the variation parameter in the wave function of helium atom?
 

(i) $z$	(ii) perturbation
(iii) electron correlation	(iv) none
- 7 The point group symmetry of  $\text{PH}_3$  is
 

(i) $C_2$	(ii) $C_3$
(iii) $C_{3v}$	(iv) done
- 8 If all the symmetry elements do not commute with each other, then the group is
 

(i) Abelian	(ii) Cyclic
(iii) non-Abelian	(iv) none
- 9 In general, all 'u' type of modes should be found to be IR.
 

(i) active	(ii) inactive
(iii) exclusive	(iv) none
- 10 For non-polarisable molecule, the Raman modes are
 

(i) inactive	(ii) active
(iii) allowed	(iv) none

Cont...

**SECTION - B (25 Marks)**

Answer ALL questions

ALL questions carry EQUAL Marks (5 x 5 = 25)

- 11 a What are Hermitian operators? Give their significance.  
OR  
b Derive time independent Schrodinger equation using separation of variables procedure.
- 12 a Obtain and solve the Schrodinger equation for simple harmonic oscillator.  
OR  
b Explain the degeneracy in particle in a 3D box.
- 13 a Using HMO theory, calculate the delocalization energy in  $\frac{1}{3}\lambda$  butadiene.  
OR  
b State and explain variation method.
- 14 a Sketch the flow chart for deducing the point group symmetry of the molecule.  
OR  
b Define and explain Great Orthogonality theorem.
- 15 a How do you determine the vibrational modes in  $\text{NH}_3$  molecule using group theory?  
OR  
b Apply group theory to deduce the hybrid orbitals in  $\text{BF}_3$  molecule.

**SECTION - C (40 Marks)**

Answer ALL questions

ALL questions carry EQUAL Marks (5 x 8 = 40)

- 16 a Describe the essential postulates of quantum mechanics.  
OR  
b Explain the following:  
(i) Commutator operators. (4)  
(ii) Heisenberg's uncertainty principle. (2)  
(iii) Well-behaved wave function. (2)
- 17 a Set up and solve the Schrodinger equation of a particle in 3D box.  
OR  
b Derive an expression for energy of a rigid rotator from the Schrodinger wave equation.
- 18 a Describe the following:  
(i) Approximation methods (4) (ii) Slater determinants (4)  
OR  
b Explain the perturbation method and illustrate its application to He atom.
- 19 a Apply group theory to construct the character table for  $\text{C}_{3v}$  point group symmetry.  
OR  
b Define and explain:  
(i) Symmetry elements and operations. (4)  
(ii) Reducible and irreducible representations. (4)
- 20 a (i) How are vibrational modes for  $\text{SO}_2$  classified? (4)  
(ii) Explain the symmetry selection rules for Raman Spectra. (4)  
OR  
b By applying group theory, how do you obtain the hybrid orbitals in  $\text{NH}_3$  molecule?