

PSG COLLEGE OF ARTS & SCIENCE
(AUTONOMOUS)

MSc DEGREE EXAMINATION MAY 2023
(Second Semester)

Branch – CHEMISTRY

QUANTUM MECHANICS AND GROUP THEORY

Time: Three Hours

Maximum: 50 Marks

SECTION-A (5 Marks)

Answer ALL questions

ALL questions carry EQUAL marks

(5 x 1 = 5)

- 1 Find out the linear operator among the following.
(i) $()^2$ (ii) $k()$
(iii) $\sqrt{()}$ (iv) $\ln()$
- 2 Which of the following is correct about Hamiltonian operator, It is
(i) Total energy operator
(ii) it is equal to sum of kinetic energy and potential energy
(iii) denoted by H
(iv) All the above
- 3 If the total wave function changes its sign due to interchange of coordinates of electrons it is called as ----- wave function.
(i) anti-symmetric (ii) Symmetric
(iii) neither symmetric nor asymmetric (iv) abnormal
- 4 Reflection in the plane causes plane of symmetry and denoted as
(i) σ (ii) i
(iii) E (iv) C_n
- 5 BCl_3 belongs to ----- point group.
(i) C_{2v} (ii) C_{3v}
(iii) D_{3h} (iv) D_{4h}

SECTION - B (15 Marks)

Answer ALL Questions

ALL Questions Carry EQUAL Marks

(5 x 3 = 15)

- 6 a Illustrate linear and non linear, commutator and non- commutator operators with specific examples.
OR
b Derive the Hamiltonian operator using quantum mechanic postulates.
- 7 a Derive Eigen values for a simple harmonic oscillator.
OR
b Use uncertainty relation and quantum mechanical results and show that the zero point energy of rigid rotor is zero, but that of a harmonic oscillator is non-zero.
- 8 a Apply Huckel's molecular orbital method to Butadiene molecule.
OR
b Write the variation principle and apply variation method to anharmonic oscillator.

Cont...

- 9 a Predict the following point groups as abelian or nonabelian groups.
i) C_{3v} ii) C_{2v}
OR
b Prove that if P and Q are matrices related by similarity transformations $Q=B^{-1}PB$ then $XQ=XP$.
- 10 a Explain the symmetry selection rules for Infrared and Raman spectra.
OR
b Explain the classification of vibrational modes present in SO_2 and $POCl_3$.

SECTION -C (30 Marks)

Answer ALL questions

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

- 11 a Derive Schrodinger wave equation for time independent model and determine their solutions.
OR
b Prove the following
(i) Eigen value are linear momentum operator are not quantized
(ii) Hamiltonian operators are Hermitian in nature.
- 12 a Derive an equation for particle in 1D box.
OR
b Prove the following
(i) Eigen functions of harmonic oscillator belong to orthonormal set
(ii) Distortion reduces the degeneracy in 3D cubical box.
- 13 a Derive first order perturbation energy.
OR
b Apply first order perturbation method to Helium atom.
- 14 a Construct the character table for C_{3v} point group using great orthogonality theorem.
OR
b Construct the group multiplication table for C_{2v} point group.
- 15 a Write the steps for the determination of vibrational modes in non-linear molecules using ammonia molecule as an example.
OR
b Construct the hybrid orbitals of water molecule.

Z-Z-Z

END