

STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86  
(For candidates admitted from the academic year 2019-20 & thereafter)

SUBJECT CODE: 19CH/PC/QG24

M. Sc. DEGREE EXAMINATION, APRIL 2023  
BRANCH IV- CHEMISTRY  
SECOND SEMESTER

COURSE : CORE

PAPER : QUANTUM CHEMISTRY AND GROUP THEORY

TIME : 3 HOURS

MAX. MARKS: 100

SECTION – A

ANSWER ALL THE QUESTIONS.

(20 x 1= 20)

Choose the correct answer:

1. Kinetic energy for a rotating system in terms of momentum is given by (i)  $l^2/2I$  (ii)  $L/2I$  (iii)  $P/2m$  (iv)  $P^2/2m$ .
2. Momentum operator is (i)  $-i\hbar d/dx$  (ii)  $i\hbar d/dx$  (iii)  $(i/\hbar)d/dx$  (iv)  $i\hbar d/dx$ .
3. Experimental proof for de Broglie equation was given by (i) Schrodinger (ii) Davisson-Germer (iii) Einstein (iv) None.
4. Point group of ammonia is (i)  $C_{2v}$  (ii)  $C_{3v}$  (iii)  $D_{3h}$  (iv)  $C_{4v}$
5. The degeneracy of the energy level  $6h^2/8ma^2$  corresponding to a three dimensional box is (i) 2 (ii) 3 (iii) 4 (iv) 5.

Fill in the blanks:

6. Number of planes of symmetry in  $CO_2$  is (i) 1 (ii) 2 (iii) 4 (iv) infinite.
7. Molecule having 3-fold axis of symmetry is (i)  $H_2O$  (ii)  $NH_3$  (iii)  $CO_2$  (iv) none of these.
8. An example of a linear operator is -----.
9. Hermite polynomial is-----.
10. Bond order of  $O_2^{2-}$  ion is -----.

State whether true or false:

11. Hamiltonian operator is momentum operator.
12. An acceptable wave function must be finite.
13. Point group of  $BCl_3$  is  $C_{3v}$ .
14. Wave function of an atom must be symmetric according to Pauli.
15. All the four quantum numbers are obtained by solving Schrodinger wave equations.

Answer in a line or two:

16. Evaluate the commutator  $[A,B]$  if  $A = d^2/dx^2$  and  $B = x$
17. Give the radial equation.
18. Define order of a group.
19. Mention the symmetry elements in benzene and methane.
20. Write the secular determinant of naphthalene.

**SECTION – B****ANSWER ANY FIVE QUESTIONS:****(5x8=40)**

21. What are Hermitian operators? Discuss their properties.
22. Solve the Schrodinger wave equation of a particle in a one dimensional box of width 'a'
23. Set up and solve the Schrodinger equation of a simple harmonic oscillator.
24. Discuss the application of HMOT to ethylene.
25. Arrive at the antisymmetric wave functions of excited state of helium atom.
26. (a) Construct the group multiplication table for  $C_{3v}$  point group.  
(b) Explain – axis of symmetry and plane of symmetry.
27. (a) Reduce the given representation to its component irreducible representations of the  $C_{2v}$  point group.  $\Gamma = 3 \ 1 \ -1 \ 1$   
(b) What is direct product? Give its application.

**SECTION – C****ANSWER ANY TWO QUESTIONS:****(2x20=40)**

28. (a) Write the SWE for hydrogen atom in polar coordinates. Separate the resultant equation into three equations using the method of separation of variables.  
(b) The microwave spectrum of HCl consists of a series of equally spaced lines separated by  $6.26 \times 10^{11}$  Hz. Calculate the bond length of HCl.  
(c) Write the first five associated Legendre functions. (10+5+5)
29. (a) Discuss Hartree- Fock self-consistent field theory.  
(b) Apply the variation method to helium atom.
30. (a) Explain the electronic spectra of formaldehyde.  
(b) Obtain the symmetries of vibrational modes in  $BF_3$  molecule.

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