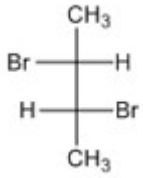
STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI – 86
(For candidates admitted from the academic year 2023 – 2024)

M. Sc. DEGREE EXAMINATION, APRIL 2024
BRANCH IV- CHEMISTRY
SECOND SEMESTER

COURSE : MAJOR CORE
PAPER : QUANTUM CHEMISTRY AND GROUP THEORY
SUBJECT CODE : 23CH/PC/QG24
TIME : 3 HOURS MAX. MARKS: 100

Q. No.	SECTION A (10 x 1 = 10 marks) Answer ALL Questions	CO	KL
1	If $[x,p_x] = i(h/2\pi)$, then $[x^2,p_x]$= ? a) $-i(h/2\pi)$ b) $i(h/2\pi)$ c) $i(h/2\pi)x$ d) $2\,i(h/2\pi)x$	1	1
2	The eigen value correspond to the operator d^2/dx^2 when acting on the function 3sin4x is a) – 48 b) 12 c) 48 d) -16	1	1
3	If the vibrational frequency of a diatomic molecule AB is 2 cm^{-1}, then its zero point energy under the assumption that the molecule behaves as 1D-simple harmonic oscillator is a) 2 hc b) hc c) (1/2) hc d) 4 hc	1	1
4	The quantum number which does not arise out of the solution of Schrodinger equation is a) n b) l c) m d) s	1	1
5	An sp^2 hybrid orbital function of BF_3 molecule is given as $\psi = (1/\sqrt{3})\,\phi_{2s} - (1/\sqrt{6})\,\phi_{2px} + C_2\,\phi_{2py}$, then the coefficient of C_2 is a) $(1/\sqrt{2})$ b) $\sqrt{2}$ c) 1/ 2 d) -1/2	1	1
6	Delocalization energy of 1,3-cyclobutadiene as per Huckel MO theory is a) $2\alpha + 2\beta$ b) $4\alpha + 4\beta$ c) 0 d) 0.472 β	1	1
7	Symmetry number of a molecule that belongs to C_{3v} point group is a) 1 b) 2 c) 3 d) 6	1	1
8	The number of reducible representations possible for C_{3v} point group is a) 3 b) 6 c) 12 d) infinite	1	1
9	The ground vibrational state of a molecule belongs to C_{2v} point group has the symmetry species of a) A_1 b) A_2 c) B_1 d) B_2	1	1
10	Number of irreducible representations of a point group is equal to a) Order of the group b) Number of classes in the group c) Number of rotation operations in the group d) Number of reflection operations in the group	1	1

Q. No.	SECTION – B (10 x 1 = 10 marks) Answer ALL Questions	CO	KL
11	What are orthonormal functions?	2	2
12	The energy of a particle confined in a cubical box with infinite potential barrier outside is 14 ($h^2/8mL^2$). Find the degree of degeneracy associated with this level.	2	2
13	Write the Schrodinger equation for one dimensional simple Harmonic oscillator.	2	2
14	Write the expression for first order correction to the energy of ground state of a system under time independent perturbation theory.	2	2
15	Write the Slater determinantal wave function for the ground state of Helium atom.	2	2
16	Give the point group of C_6H_6.	2	2
17	Find the point group of Methyl chloride.	2	2
18	 Is the above molecule possesses center of symmetry?	2	2
19	What is the symmetry selection rule for a vibrational transition to be active in IR?	2	2
20	Can we predict exact Hybridization of a molecule using symmetry properties?	2	2

Q. No.	SECTION C (4 x 6 = 24 marks) ANSWER ANY FOUR QUESTIONS	CO	KL
21	Normalize the wave function $\psi = e^{im\phi}$ in the range $0 \leq \phi \leq 2\pi$.	3	3
22	Explain Radial probability distribution function.	3	3
23	Derive the expression for the wave functions of Hybrid orbitals of BF_3 molecule.	3	3
24	Reduce the following reducible representation of C2v point group using reduction formula C2v | E C_{2z} $\sigma_v(xz)$ $\sigma_v(yz)$ Γ | 4 0 2 2	3	3
25	n $\rightarrow \pi^*$ transition is electric dipole forbidden transition but it appears in the spectrum with less intensity – Explain.	3	3

Q. No.	SECTION – D (4 x 8 = 32 marks) ANSWER ANY FOUR QUESTIONS	CO	KL
26	a) Write the postulates of quantum mechanics. (5 marks) b) Two operators A and B commute with each other. What do you infer from the statement? (3 marks)	4	4
27	Derive the expression for energy Eigen value of a diatomic molecular rigid rotor in three dimensions.	4	4
28	Derive the expression for wave function and energy of Hydrogen molecular ion using LCAO-MO theory.	4	4
29	Construct the character table for C_{3v} point group.	4	4
30	Find the symmetry species correspond to the Hybrid orbitals of ammonia molecule.	4	4

Q. No.	SECTION – E (2 x 12 = 24 marks) ANSWER ALL QUESTIONS	CO	KL
31 a	(i) An electron is confined in a nanowire of length of 15 Å, calculate the energy of the electron in its first excited state (in eV). (Given: The nanowire can be treated as 1D box) (5 marks) (ii) Find the symmetry species correspond to the normal modes of trans-N_2F_2 molecule and also predict the IR active and Raman active modes among them. (7 marks) (or) (i) An electron in confined to move on a ring of constant radius. If the radius of the ring is 50Å, calculate the energy of the electron in the 2^{nd} excited level (in eV). (5 marks) (ii) Derive the expression for the wavefunction and energy of a particle confined in a cubical box. (7 mark)	5	5
31			
32 a	(i) What is the need for HF-SCF method? (ii) Explain Hartree's Self consisten field method. (iii) Explain Fock's modification of Hartree's SCF procedure. (iv) What is the limitation of HF-SCF method. (v) How will you calculate correlation energy from HF-SCF treatment? (or) (i) Derive the expression for delocalization energy of 1,3-butadiene using HMO Theory. (6 marks) (ii) State "The Great Orthogonality Theorem". Explain the features extracted from this theorem. (6 marks)	5	5
32			