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

M. Sc. DEGREE EXAMINATION, APRIL 2026
BRANCH IV- CHEMISTRY
SECOND SEMESTER

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

Q. No.	SECTION A **Choose the correct answer. (10 x 1 = 10 marks)**	CO	KL
1.	Which of the following principles relates the position and momentum of a particle? a) Pauli's Principle b) Uncertainty Principle c) Variation Principle d) Aufbau Principle	1	1
2.	What is the condition for two wavefunctions Ψ_i and Ψ_j to be considered orthogonal? a) Their product integral is zero b) Their product integral is one c) They have the same eigenvalue d) They are physically unacceptable	1	1
3.	The wave function of rigid rotator is called as spherical harmonics because a) it doesn't contain normalization constant b) it contains square root term c) they represent harmonic waves on the surface of the sphere d) all of these	1	1
4.	The wave function of a rigid rotator is referred to as: a) Hermite polynomial b) Spherical harmonics c) Laguerre polynomial d) associated Legendre	1	1
5.	Which theory determines the wavefunction of many – electron atoms using a self- consistent field? a) LCAO – MO b) Hartree – Fock c) Perturbation d) Valence Bond	1	1
6.	The sp^2 hybrid orbitals are associated with which type of molecular geometry? a) linear b) Trigonal Planar c) Tetrahedral d) Octahedral	1	1
7.	Which symmetry element involves rotation followed by reflection in a plane perpendicular to the axis? a) Centre of Inversion b) Proper Axis c) Improper Axis d) Identity	1	1

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8.	The C_{2v} point group is associated with which molecule? a) NH_3 b) H_2O c) CH_4 d) BF_3	1	1
9.	Group theory predicts the number of active modes in which type of spectroscopy? a) Mass b) Vibrational c) NMR d) Photoelectron	1	1
10.	Which molecule's electronic spectra is specially mentioned as an application in the syllabus? a) Benzene b) HCHO c) CH_4 d) H_2O	1	1
Q. No.	**SECTION B** **Answer ALL the questions. (10 x 1 = 10 marks)**	**CO**	**KL**
	Fill in the blanks.		
11.	A wavefunction is said to be _____ if the integral of its square over all space is equal to unity.	2	2
12.	In a Rigid Rotator model, the diatomic molecule is assumed to have a fixed _____.	2	2
13.	According to Pauli's Exclusion Principle, a total wavefunction must be _____ with respect to the exchange of any two electrons.	2	2
14.	A _____ table summarizes the symmetry operations and irreducible representations of a point group.	2	2
15.	In the C_{2v} point group of water, the number of _____ during a symmetry operation is used to determine the reducible representation.	2	2
	Answer in a line or two.		
16.	Define an Operator as per quantum mechanical formalism.	2	2
17.	What is a "node" in the context of atomic orbitals?	2	2
18.	Why is the Hartree – Fock method called a self-consistent Field method?	2	2
19.	Define a "Subgroup" in group theory.	2	2
20.	State the point group of the BF_3 molecule.	2	2
Q. No.	**SECTION C** **Answer any FOUR questions. (4 x 6 = 24 marks)**	**CO**	**KL**
21.	Explain the properties of wave functions and the conditions for a complete orthonormal set of functions.	3	3

22.	Describe the Variational Method and its application to the ground state of a Helium atom.	3	3
23.	Explain the concept of hybridization and derive the wave functions for sp^2 hybrid orbitals.	3	3
24.	Explain the Systematic Point Group Classification for molecules with examples.	3	3
25.	Discuss the applications of Group Theory in the electronic spectra of Formaldehyde (HCHO).	3	3
Q. No.	**SECTION D** **Answer any FOUR questions. (4 x 8 = 32 marks)**	**CO**	**KL**
26.	An electron is confined to a 1D box of length L. If the photon emitted during the transition from n=2 to n=1 has a wavelength of 400nm, calculate the length of the box L.	4	4
27.	Solve the Schrödinger Wave Equation for a Harmonic Oscillator and explain the physical significance of energy eigenvalues.	4	4
28.	Describe the LCAO-MO approximation for the Π-system of Ethylene and Butadiene.	4	4
29.	State and explain the Great Orthogonality Theorem (GOT) and its importance.	4	4
30.	Determine the hybridization scheme for the CH_4 molecule using Group Theory principles.	4	4
Q. No.	**SECTION E** **Answer the following questions. (2 x 12 = 24 marks)**	**CO**	**KL**
31. 32.	Discuss the postulates of Quantum Mechanics and explain the Hermitian properties of operators. **(OR)** Discuss the application of Schrödinger Wave Equation to Hydrogen-like atoms and explain the splitting into R, θ, and ϕ equations.	5	5
33. 34.	Elaborate on the Hartree-Fock Self-Consistent Field (SCF) theory and discuss the excited states of the Helium atom. **(OR)** Construct the Character Table for C_3v and use Group Theory to analyse the Vibrational Spectra of H_2O.	5	5

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