

(4)

5. Find out the direct product $T_1 \times T_2$ in Td point group and decompose it. 3

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

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Ex/SC/CHEM/PG/TH/I/2025

M. SC. CHEMISTRY EXAMINATION, 2025

(1st Semester)

CHEMISTRY

PAPER : PG/TH/I

(Theoretical Chemistry)

Time : Two Hours

Full Marks : 40

20 marks for each unit

Use a separate Answer Script for each Unit.

UNIT—1011

Answer any **four** questions.

1. (a) The operator $\left(x + \frac{d}{dx}\right)$ has eigenvalue α . Derive the eigenfunction. 3

- (b) Prove that the Hermitian operator gives real eigenvalues. 2

2. (a) Verify that $\hat{L}_z$ is Hermitian using spherical coordinates. 3

- (b) Show that $\psi(\xi) = e^{-\xi^2/2}$ is an asymptotic solution to following equation :

$$\frac{d^2\psi}{d\xi^2} + \left(\frac{\lambda}{\alpha} - \xi^2\right)\psi(\xi) = 0 \quad 2$$

(2)

3. (a) For a simple one-dimensional harmonic oscillator, find the average values of $\langle x \rangle$ and $\langle x^2 \rangle$, in its n^{th} quantum state. 3
- (b) Using definition of the Hermite polynomial, generate $H_0(\xi)$, $H_1(\xi)$ $H_2(\xi)$. 2
4. (a) Calculate the probability that an electron described by a Hydrogen atomic 1s wave function will be found within one Bohr radius of the nucleus. 3
- (b) Write and expand the Slater determinant for the ground-state He atom. 2
5. (a) Write down the time-independent Schrödinger equation of the spherically symmetrical potential (H atom) and separate it into three equations. 3
- (b) Construct Pauli spin matrices for spin angular momentum operators $\hat{S}^2$ and $\hat{S}_z$. 2
6. (a) Using the LCAO for the wave function for He^+ obtain the normalized wave function for the bonding MO and anti-bonding MO. 3
- (b) Show that $\hat{P}_{12}$ and $\hat{P}_{23}$ do not commute with each other.

UNIT—1012

1. (a) Draw the stereographic projection for D_{3h} and C_{4v} . 2

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[Continued]

(3)

- (b) Determine the Mulliken symbol of Γ_{IR} with justification. 2

E	$2C_4(z)$	$C_2(z)$	$2C_2'$	$2C_2''$
1	1	1	1	1
1	1	1	-1	-1
1	-1	1	1	-1
1	-1	1	-1	1
2	0	-2	0	0

- (c) List all symmetry operations present in D_{3d} point group. How many classes are there? 2

2. Show that any group of order 4 is an Abelian group. 3

3. Find out the pi-SALCs for C_4H_4 system. Use C_4 point group for the calculation. 4

	E	C_4^1	C_4^2	C_4^3
A	1	1	1	1
B	1	-1	1	-1
E {	1	i	-1	$-i$
	1	$-i$	-1	i

4. Identify the point groups of the following molecules (any four). 4

(i) $\text{I}_3^{(-)}$ (ii) $\text{fac}[\text{CoF}_3(\text{NH}_3)_3]$ (iii) cis-platin

(iv) $\text{H}_3^{(+)}$ (iv) XeOF_4 (vi) $\text{SO}_4^{(2-)}$

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[Turn Over]