QP Code: P25B003

Reg. No : .....
Name : .....

ST MARY'S COLLEGE (AUTONOMOUS), THRISSUR-20
II SEMESTER (CBCSS-PG) DEGREE EXAMINATION, MARCH 2025
M Sc Chemistry
CHE2C05 : GROUP THEORY AND CHEMICAL BONDING
2024 Admission Onwards
(Credits: 3)

Time: 3 Hours **Maximum Weightage: 30**

Section A

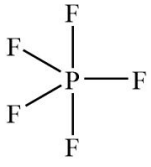
Answer **any eight** questions. Weightage **1** for each question. **(8x1 = 8 Weightage)**

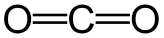
1. Find schoenflies symbol of point group for [BTL1]
   i) CH_2Cl_2 ii) Allene
2. Classify the following molecules into Abelian and Non-abelian groups [BTL4]
   i) H_2O ii) NH_3
3. Show that $\sigma_{xy} \times \sigma_{xz} = C_2(x)$. [BTL2]
4. Define representation of point groups using translational vector as basis taking H_2O as an example. [BTL1]
5. Can wave functions be used as bases for irreducible representations? Explain. [BTL1]
6. Construct the character table for C_{2h} point group. [BTL3]
7. What is Laporte selection rule for centrosymmetric molecules. [BTL1]
8. You are given $\int_{-a}^{+a} x^3 dx$ .Predict whether it is a vanishing integral or not. Justify. [BTL5]
9. Draw the MO energy level diagram of **HCHO** molecule. Also mention the symmetry of atomic orbitals. [BTL3]
10. Illustrate the MO treatment for homonuclear diatomic molecule- Be_2 . [BTL2]

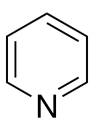
Section B

Answer **any six** questions. Weightage **2** for each question. **(6x2 = 12 Weightage)**

11. Show that the four symmetry operations E, $C_2(z)$, σh (xy) and i forms a mathematical group under multiplication. [BTL1]
12. Identify the schoenflies symbol for the point group to which the molecules belong in each of the following cases [BTL2]

i) 

ii) 

iii) 

Turn Over

13. Ethylene belongs to D_{2h} (E, C_2 (x), C_2 (y), C_2 (z), σ_{xy}, σ_{xz}, σ_{yz} and i).Taking the positional coordinates of all atoms generate a reducible representation. [BTL4]

14. Derive reduction formula using GOT. [BTL5]

15. Find IR and Raman active vibrations of NH_3. Use C_{3v} character table [BTL1]

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

16. Explain the terms SALC and projection operator. [BTL1]

17. Determine the spectroscopic term symbol for [BTL3]
    i) H_2 ii) O_2^+ iii) O_2^- iv) C_2 v) O_2

18. Use 2s and $2p_z$ orbitals to construct [BTL3]
    i) Two equivalent sp hybrid orbitals
    ii) Three equivalent sp^2 orbitals

Section C

Answer **any two** questions. Weightage **5** for each question. **(2x5 = 10 Weightage)**

19. Explain Great Orthogonality Theorem. What are the consequences of the theorem? Use the theorem to derive C_{4v} character table. [BTL2]

20. Make use of the Td character table and find the hybridized orbitals of CH_4 [BTL3]

Table 1: Character table for T_d point group

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xz, yz, xy)

21. Discuss the MO theory of bonding as applied to H_2 molecule. [BTL5]

22. Analyse the HMO for butadiene and find out free valence of carbon atoms [BTL4]

$\Phi_1 = 0.372\,p_1 + 0.602\,p_2 + 0.602p_3 + 0.372p_4$

$\Phi_2 = 0.602p_1 + 0.372\,p2 - 0.372\,p3 - 0.602p4$

$\Phi_3 = 0.602p_1 - 0.372p2 - 0.372p3 + 0.602p4$

$\Phi_4 = 0.372p_1 - 0.602p2 + 0.602p3 - 0.302p4$

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