C 42743 (Pages : 3) Name.....

Reg. No.....

SECOND SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, APRIL 2023

(CBCSS)

Chemistry

CHE2C05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admission onwards)

Time : Three Hours Maximum : 30 Weightage

Section A

Answer any **eight** *questions.*
Each question carries a weightage of 1.

1. Find Schoenflies symbol of point group for :
   (a) CH_2Cl_2. (b) Allene.
2. Generate matrices (3 × 3) for (a) C_4 ; (b) S_4.
3. Distinguish between degenerate and nondegenerate representations.
4. State rules for assigning Mulliken's symbols for irreducible representations.
5. You are given $\int_{-a}^{+a} x^3 dx$. Predict whether it is a vanishing integral or not. Justify.
6. Write projection operator for A_1 symmetry $\left(\hat{P}_{A_1}\right)$ for C_2v molecule.
7. Arrange O_2, O_2^+ and O_2^- in the increasing order of stability. Justify your answer.
8. Write spectroscopic term symbol for (a) O_2 ; (b) C_2.
9. The energy of $\pi(\rho_1)$ molecular orbitals of benzene are $\alpha+2\beta, \alpha+\beta, \alpha+\beta, \alpha-\beta, \alpha-\beta$ and $\alpha-2\beta$. Find the delocalization energy.
10. State and explain Born–Oppenheimer approximation.

(8 × 1 = 8 weightage)

Turn over

Section B

Answer any **six** *questions.*
Each question carries a weightage of 2.

11. Show that the four symmetry operations $E, C_2\,z, \sigma_h\,xy$ and i form a Mathematical group under multiplication.

12. Generate group multiplication table for C_3v.

13. Taking the positional coordinates of all atoms of cis butadiens (C_2v) generate a reducible representation. (characters only).

14. State great orthogonality theorem. Use the theorem to derive C_3 character table.

15. Find IR and Raman active vibrations of NH_3. Use C_3v character table.

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	Rz	
E	2	-1	0	(x,y) (Rx, Ry)	$(x^2 - y^2, xy)$ (xz, yz)

16. Find molecular orbitals of H_2O. Use C_2v character table.

C_2v	E	C_{2z}	σ_{vxz}	σ^1_{vyz}		
A_1	1	1	1	1	z	$x^2,\ y^2, z^2$
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

17. Briefly discuss Sp^2 hybridization.

18. Find $\pi(\rho_i)$ molecular orbitals and the corresponding energies of allyl cation using HMO method.

(6 × 2 = 12 weightage)

Section C

Answer any **two** *questions.*
Each question carries a weightage of 5.

19. Find hybridized orbitals of CH4. Use Td character table :

Td	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	(Rx, Ry, Rz)	
T_2	3	0	−1	−1	1	(x, y, z)	(xy, xz, yz)

20. Briefly discuss MO theory of bonding as applied to H_2^+.

21. Find allowed electronic transitions in formaldehyde. Use C_2v character table.

22. (a) Generate gamma cart for H_2O. Reduce it into its IR components. Use C_2v character table.

(b) Explain the term 'block diagonalization'. Discuss its impoprtance in group theory.

(2 × 5 = 10 weightage)