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 $\int\limits_{-a}^{+a} x^3 dx.$ 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.

$(8 \times 1 = 8$ 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 $C_3 v$.

13. Taking the positional coordinates of all atoms of cis butadiens ($C_2 v$) 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 $C_3 v$ character table.

$C_3 v$	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 $C_2 v$ character table.

$C_2 v$	E	C_{2z}	σ_{vxz}	σ_{vyz}^1		
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.

$(6 \times 2 = 12$ 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.

$(2 \times 5 = 10$ weightage$)$