D 122468   (Pages : 4)   Name...

Reg. No....................................

SECOND SEMESTER M.Sc. DEGREE REGULAR/SUPPLEMENTARY EXAMINATION, APRIL 2025

(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. Assign Schoenflies symbol of point group for :

    (a) CH_2Cl_2.   (b) Cyclohexane (chair form),

2. Generate 3 × 3 matrices for :

    (a) C_3.   (b) S_3.

3. Distinguish between degenerate and nondegenerate representations with examples.

4. State rules for assigning Mulliken's symbol for symmetry species.

5. You are given $\int\limits_{-a}^{+a} x^3 dx$. Predict whether it is a vanishing integral or not. Justify.

6. State Laporte selection rules for electronic transitions.

7. Write projection operator $\hat{P}_{A_1}$ for A_1 symmetry under C_2v point group.

8. Arrange O_2, O_2^+ and O_2^- in the increasing order of stability. Justify your answer.

Turn over

9. Write spectroscopic term symbol for :

   (a) C_2.   (b) O_2.
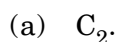
10. The energy of $\pi(\rho i)$ molecular orbitals of benzene are $\alpha+2\beta, \alpha+\beta, \alpha+\beta, \alpha-\beta, \alpha-\beta$ and $\alpha-2\beta$. Find the delocalization energy.

                                                 ($8 \times 1 = 8$ weightage)

Section B

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

11. List the symmetry elements and operators associated with D_3h point group. Classify them into different classes of operations.

12. Taking the positional coordinates of all atoms of cis butadiene (C_2v) generate a reducible representation (Characters only).

13. Derive C_4v characters table.

14. Predict IR and Raman active vibrations of NH_3. Use C_3v character table :

C_3v	E	$2\rho_3$	$3\sigma_v$		
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, E_y)	$\left(x^2-y^2, xy\right)(xz, yz)$

15. Find the molecular orbitals of H_2O. Use C2v character table :

C_2v	E	C_2z	σ_{vxz}	$\sigma'_v yz$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

16. With the help of correlation diagram explain noncrossing rule.

17. Find $\pi(\rho i)$ molecular orbitals of cyclo propenyl cation $(C_3H_3)^+$. Use C_3 or D_3h character table :

C_3	E	C_3	$C_3{}^2$			
A	1	1	1	z, Rz	x^2, y^2, z^2	$\varepsilon = e^{i(2\pi/3)}$
E	1	ε	ε^*	(x, y)		
	1	ε^*	ε	(Rx, Ry)	$\left(x^2 - y^2, xy\right)(xz, yz)$	

18. Find the hybridized orbitals of C in CH_4 from quantum mechanical approach.

$(6 \times 2 = 12$ weightage$)$

Section C

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

19. Find hybridized orbitals of B in BF_3. Use D_3h character table :

D_3h	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(Rx, Ry)	(xz, yz)

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

21. Find the energy of $\pi(\rho i)$ molecular orbitals of butachene using HMO method. Also find any one of the π molecular orbitals.

22. Discuss briefly :

    (a) Block diagonalization.

    (b) Frost Hückel circle mnemonic device.

$(2 \times 5 = 10$ weightage)