C 23313 (Pages : 3) 24 Name.....

Reg. No.....

SECOND SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, APRIL 2022

(CBCSS)

Chemistry

CHE 2C 05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admission onwards)

Time : Three Hours Maximum : 30 Weightage

General Instructions

1. In cases where choices are provided, students can attend **all** questions in each section.
2. The minimum number of questions to be attended from the Section/Part shall remain the same.
3. The instruction if any, to attend a minimum number of questions from each sub section/sub part/ sub division may be ignored.
4. There will be an overall ceiling for each Section/Part that is equivalent to the maximum weightage of the Section/Part.

Section A

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

1. List the symmetry elements and operations associated with D_3d.
2. Explain with example (a) cyclic group ; (b) abelian group.
3. State and explain rearrangement theorem.
4. Show that $\sigma_{xy} \times \sigma_{xz} = c_2(x)$.
5. Generate matrices for (a) c_6 ; (b) σ_{xy} using positional coordinates x, y, z.
6. Explain 'transition moment integral'.
7. Distinguish between symmetric direct product and ordinary direct product.
8. O_2^+ is more stable than O_2^-. Why ?

Turn over

9. The energy of $\pi(p_1)$ molecular orbitals of benzene are $\alpha+2\beta, \alpha+\beta, \alpha\times\beta, \alpha-\beta$ and $_0$ delocalization energy.

10. Write spectroscopic term symbol of c_2.

(8 × 1

Section B

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

11. Show that the four symmetry operations $E, C_2(x), C_2(y)$ and $C_2(z)$ form a mat under multiplication.

12. Ethylele belongs to $D_2h(E, C_2(x), C_2(y), C_2(z))$ $\sigma_{xy}, \sigma_{xz}, \sigma_{yz}, i$. Taking the positio of all atoms generate a reducible representation.

13. Rationalize mutual exclusion principle using group theory.

14. Find $\pi(p_1)$ molecular orbitals and their energies for allyl anion using HMO meth

15. Find allowed electronic transitions of Carbonyl group. Use C_2v 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	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

16. 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)	(x^2-y^2, xy)
				(R_x, R_y)	(xz, yz)

17. The Pi molecular orbitals of *cis* butadiene are given below. Find the free valence around each *c* atom.

$\Phi_1 = 0.372\ P_1 + 0.602\ P_2 + 0.602\ P_3 + 0.372\ P_4$

$\Phi_2 = 0.602\ P_1 + 0.372\ P_2 - 0.372\ P_3 - 0.602\ P_4$

$\Phi_3 = 0.602\ P_1 - 0.371\ P_2 - 0.372\ P_3 + 0.602\ P_4$

$\Phi_4 = 0.372\ P_1 - 0.602\ P_2 + 0.602\ P_3 - 0.372\ P_4$

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

(6 × 2 = 12 weightage)

Section C

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

19. State Great Orthogonality Theorem. What are the consequences of the theorem ? Use the theorem to derive C_4v character table.

20. Find the molecular orbitals of H_2O. Use C_2v character table. Predict allowed electronic transitions.

21. Find the hybridized orbitals B in BF_3. Use D_3h character table :

D_3h	E	$2C_3$	$3C_2$	σ_h	$3S_3$	$3\sigma_d$		
A_1'	1	1	1	1	1	1		$x^2+y^2-z^2$
A_2'	1	1	−1	1	1	−1	Rz	
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	(R_x, R_y)	(xz, yz)

22. Compare V.B. and M.O. theory of binding as applied to H_2. Which is found better ?

(2 × 5 = 10 weightage)