

C 4712

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Name.....

Reg. No.....

**SECOND SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY)
EXAMINATION, APRIL 2021**

(CBCSS)

Chemistry

CHE 2C 05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admissions)

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. 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. Assign Schoenflies symbol of point group :
(a) Allene. (b) Dichloromethane.
2. Find the similarity transform of any one of the vertical planes in NH_3 .
3. Generate matrices using positional co-ordinates x, y, z :
(a) S_4 . (b) C_3 .
4. Distinguish between degenerate and non-degenerate representations with examples.
5. Explain with one example non-vanishing integral.
6. Cis butadiene belongs c_{2v} point group. Find the character under E in the gamma cart.
7. Write projection operator \hat{P}_{Ag} for c_{2h} . The operations are E, c_{2z} , $\sigma_h \alpha_y$ and i .
8. State and explain Born–Oppenheimer approximation.
9. Write spectroscopic term symbol of :
(a) O_2 . (b) N_2 .
10. State and explain Laporte selection rules.

(8 × 1 = 8 weightage)

Turn over

Section B

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

11. Explain the importance of block diagonalization in solving quantum mechanical problem using group theory.
12. Derive C_3 character table.
13. Find IR and Raman active vibrations of H_2O (c_{2v}).
14. Find molecular orbitals of HCHO. Use c_{2v} character table.
15. Find bond energy of π – molecular orbitals of benzene by HMO method.
16. Discuss Frost Hückel mnemonic device for cyclic polymers.
17. Show that the four symmetry operations E, c_{2z} , $\sigma_h x_y$ and i form a mathematical group under multiplication.
18. List the symmetry operations possible on D_{4h} . Classify them into different classes of operations.
(6 × 2 = 12 weightage)

Section C

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

19. Find hybridized orbitals of C in CH_4 . Use T_d character table.
20. Find $\pi(pi)$ molecular orbitals of *cis butadiene* by HMO method. Use c_{2v} character table.
21. Discuss V.B. method of bonding as applied to H_2 .
22. (a) Setup group multiplication tables for c_{3v} .
(b) State and explain rules for assigning Mulliken's symbol for symmetry species.

c_{2v}	E	c_{2z}	$\sigma_v x_z$	$\sigma' v yz$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	Rz	xy
B_1	1	-1	1	-1	x, Ry	xz
B_2	1	-1	-1	1	y, Rx	xyz

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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	$(2z^2 - x^2 - y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)
T_2	3	0	-1	-1	1	(x, y, z)

 $(2 \times 5 = 10 \text{ weightage})$