C 4712

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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}, $\sigma_h x_y$ 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.

$(8 \times 1 = 8$ weightage)

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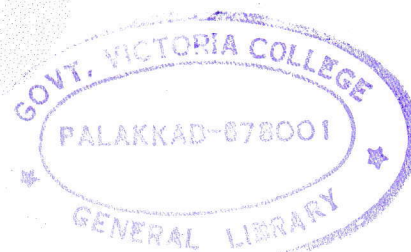
Section B

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 Td 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}	$\sigma_v x_z$	$\sigma' vyz$		
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
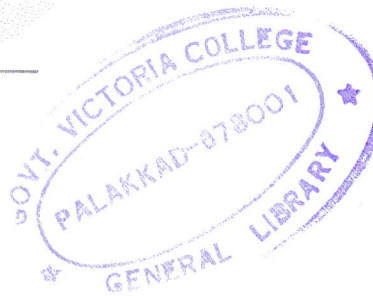
T_d	E	$8c_3$	$3c_2$	$6s_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2 - x^2 - y^2)$
T_1	3	0	-1	1	-1	(Rx, Ry, Rz)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

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