

C 83026

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Name.....

Reg. No.....

SECOND SEMESTER M.A./M.Sc./M.Com. DEGREE EXAMINATION, JUNE 2020

(CBCSS)

Chemistry

CHE 2C 05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admissions)

Time : Three Hours

Maximum : 30 Weightage

**Section A**

*Answer eight questions.*

*Each question carries a weightage of 1.*

- Write Schoenflies symbol of point group for :  
(a)  $\text{XeOF}_4$ . (b)  $\text{H}_2\text{O}_2$ .
- Which of the following does not have inversion centre ?  
(a) Td. (b)  $D_{3d}$ .  
(c)  $C_{2h}$ . (d)  $D_{2d}$ .
- Generate matrices using positional co-ordinates  $x, y, z$  :  
(a)  $C_4$ . (b)  $S_3$ .
- Trans dichloro ethylene belongs to  $C_{2h} (E, C_{2z}, \sigma_{hxy}, i)$ . Find the symmetry species to which rotation about  $z$ -axis  $R_z$  belongs.
- Ethylene belongs to  $D_{2h}$ . Find the character under E in the gamma cart.
- Explain with one example 'vanishing integral'.
- Write projection operator  $\hat{P}_{A_1}$  for  $c_{2v}$ .
- Arrange  $\text{O}_2, \text{O}_2^+$  and  $\text{O}_2^-$  in the increasing order of stability. Justify your answer.
- The  $\Pi(pi)$  bond energy of benzene are  $\alpha + 2\beta, \alpha + \beta, \alpha + \beta, \alpha - \beta, \alpha - \beta, \alpha - 2\beta$ . Find delocalization energy.
- Write trial function for bonding in  $\text{H}_2$  by V.B. approach.

(8 × 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  $E, C_{2z}, \sigma_{vzx}$  and  $\sigma'_{vyz}$  form a mathematical group under multiplication.
12. Set-up group multiplication table for  $C_{3v}$ .
13. Cis butadiene belongs to  $C_{2v}$ . Taking the positional co-ordinates of all atoms generate a reducible representation. Reduce it with its IR components.
14. Rationalise mutual exclusion principle using group theory.
15. Find  $\Pi(pi)$  molecular orbitals and the corresponding energies using HMO method for allylation.
16. Find allowed electronic transition of carbonyl group. Use  $C_{2v}$  character table.
17. With the help of correlation diagram, explain non-crossing rule.
18. The Pi molecular orbitals of butadiene are given below. Find the free valence on each C atom :

$$\Phi_1 = 0.372p_1 + 0.602p_2 + 0.602p_3 + 0.372p_4$$

$$\Phi_2 = 0.602p_1 + 0.372p_2 - 0.372p_3 - 0.602p_4$$

$$\Phi_3 = 0.602p_1 - 0.372p_2 - 0.372p_3 + 0.602p_4$$

$$\Phi_4 = 0.372p_1 - 0.602p_2 + 0.602p_3 - 0.372p_4$$

(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 IR and Raman active vibrations of  $NH_3$ . Use  $C_{3v}$  character table.
21. Find hybridized orbitals of B in  $BF_3$ . Use  $D_{3h}$  character table.
22. Discuss M.O. theory of bonding on applied to  $H_2^+$ .

$C_{2v}$	E	$C_{2z}$	$\sigma_{vzx}$	$\sigma'_{vyz}$		
$A_1$	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	$y, R_x$	$yz$

$C_{3v}$	E	$2C_3$	$3\sigma_v$		
$A_1$	1	1	1	$z$	$x^2 + y^2, z^2$
$A_2$	1	1	-1	$R_z$	
E	2	-1	0	$(x, y)$ $(R_x, R_y)$	$(x^2 - y^2, xy)$ $(xz, yz)$

$D_{3h}$	E	$2C_3$	$3C_2$	$\sigma_h$	$2s_3$	$3\sigma_d$		
$A_1'$	1	1	1	1	1	1		$x^2 + y^2, z^2$
$A_2'$	1	1	-1	1	1	-1	$R_z$	
$E'$	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	$(R_x, R_y)$	$(xy, yz)$

(2 × 5 = 10 weightage)