24P210 (Pages: 3) Name : .....

Reg. No : .....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2025

(CBCSS-PG)

(Regular/Supplementary/Improvement)

CC19P CHE2 C05 - GROUP THEORY AND CHEMICAL BONDING

(Chemistry)

(2019 Admission onwards)

Time: 3 Hours Maximum: 30 Weightage

Section A

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

1. What is meant by the term inverse of a group element? What is the inverse of the element C_3?
2. What is meant by conjugate elements?
3. Derive the transformation matrix for improper axis of rotation.
4. Consider the BCl_3 molecule. What will be the reducible representation, if 3N cartesian coordinates are used as basis set?
5. Describe the nature of functions that are placed in the last two columns of the charatcter tables of the point groups.
6. Using the reduction formula reduce, reducible following represenations, Γ_a and Γ_b of C_{3v} point group into irreducible representation of the point group.

C_{3v}	E	$2C_3$	3σ
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
Γ_a	5	2	-1
Γ_b	7	1	-1

7. Define projection operator. What is its significance?
8. Give the MO diagram of CO.
9. What is non-crossing rule?
10. Give the Huckel matrix for benzene molecule.
11. Phosphorus pentachloride, PCl_5 is a trigonal bipyramidal molecule. To what point group does it belong?
12. What are Coulomb integrals? Explain using H_2^+ as an example.

(8 × 1 = 8 Weightage)

Section B

Answer any ***four*** questions. Each question carries 3 weightage.

13. List and depict all symmetry elements of (i) XeF_4 (ii) BF_3

14. Write matrices corresponding to all symmetry operations in C_{2v} point group and using mtrices prove that (i) $\sigma_{xz}\,\sigma_{yz} = C_2$ (ii) $\sigma_{xz}\,C_2 = \sigma_{yz}$.

15. Find the symmetries of vibrational modes of water molecule. Depict the transformation of these vibrational modes under each symmetry operation and assign symmetries to each vibrational mode (C_{2v} Table is given).

16. Taking of trans N_2F_2 as an example, find the symmetries of normal modes and illustrate the rule of mutual exclusion (C_{2h} Table is given)..

17. State and explain Laporte selection rule using a suitable example.

18. Water belongs to C_{2v} point group. Find the symmetry species of MO's (C_{2v} Table is given).

19. What are the approximations introduced by Huckel to MO theory of conjugated molecules?

(4 × 3 = 12 Weightage)

Section C

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

20. Sate Great Orthogonality Theorem. Using GOT derive the C_3V character table.

21. Using group theory determine the atomic orbitals of carbon atom involved in hybridization in CH_4 molecule. Using inverse transformation procedure determine the contribution of each atomic orbital toward hybrid orbitals.

Table 1: Character table for T_d point group

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

22. Discuss the VB treatment of H_2 molecule.

23. Discuss the LCAO method for H_2^+ system.

(2 × 5 = 10 Weightage)

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Refer Character table for required questions:

Character table for C_{2v} point group

	E	C_2 (z)	σ_v(xz)	σ_v(yz)	linear, rotations	quadratic
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

Character table for C2h point group

C_{2h}	E	C_2 (z)	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x or R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x or y	

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