

D2ACH2301

(2 Pages)

Name.....

Reg.No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2024
(Regular/Improvement/Supplementary)

CHEMISTRY
FCHE2C05: GROUP THEORY AND CHEMICAL BONDING

Time: 3 Hours

Maximum Weightage: 30

Section A: Short answer questions. Answer any *eight* questions. Each carries 1 weightage.

1. Explain the term abelian group. Write one example.
2. What are subgroups and classes of a group?
3. Show that 120° and 240° rotations are conjugate elements of C_{3v} point group.
4. Define S_5 axis of symmetry. Find the distinct operations generated by S_5 axis.
5. Explain the term "block diagonalization".
6. Determine the point group of $B(OH)_3$ assuming that it is a planar molecule.
7. What are group orbitals? Give example.
8. Give group theoretical explanation for Laporte selection rule.
9. What is the term symbol for the first excited state of H_2 molecule.
10. State and explain non-crossing rule.
11. Write the normalized functions of sp hybridization.
12. What is Frost-Huckel circle mnemonic device for cyclic polyenes.

(8 × 1 = 8 weightage)

Section B: Short essay questions. Answer any *four* questions. Each carries 3 weightage.

13. Explain the rules associated with direct product and direct sum of square matrices.
14. Set up group multiplication table of C_{2h} point group.
15. H_2O belongs to C_{2v} point group. Find the group orbitals involved bonding with O atom orbitals.
16. Rationalize rule of mutual exclusion principle using group theory.
17. Discuss the MO treatment of CO and NO.

(P.T.O.)

18. Write the Hückel determinant of 1,3-butadiene. Obtain HMO coefficients.
19. Apply HMO method to find π -molecular orbitals and their energy values for allyl cation.

(4 × 3 = 12 weightage)

Section C: Essay questions. Answer any two questions. Each carries 5 weightage.

20. State Great Orthogonality Theorem. Using this derive C_{2v} character table. Also include the IR corresponding to the vectors x, y, z and their products.
21. Predict the hybridization in BF_3 and obtain the hybrid orbitals by SALC and projection operator method.
22. (a) Explain the selection rules for Raman and electronic spectroscopy.
(b) Determine the vibrational modes of ammonia molecule.
23. Compare VB and MO methods of bonding as applied to H_2 . Which is found better? Justify your answer.

(2 × 5 = 10 weightage)

Character tables of C_{3v} and D_{3h} point groups

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	$2C_3$	$3C_2'$	σ_h	$2S_3$	$3\sigma_v$		
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)	(xz, yz)