

CHE 501 N

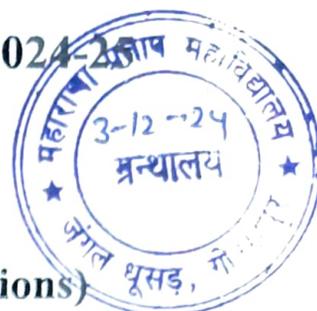
M.Sc. (Ist SEMESTER) EXAMINATION, 2024-25

(CBCS MODE)

CHEMISTRY

(Molecular Symmetry and Molecular Vibrations)

1354



Time : Three Hours]

[Maximum Marks : 75

Note: There are **three** sections (A, B and C) and Candidate has to attempt questions from all section. Marks are indicated against each section.

Section-A

1. Answer all questions : 5×3=15
- (a) Determine the point group in planar zxy_2 , where x is central atom.
 - (b) Explain normal modes of vibration by taking example of your choice.
 - (c) Define group multiplication table with the help of one example.
 - (d) What are the selection rules for IR Spectroscopy.
 - (e) Prove that :

$$\sigma^n = \sigma \text{ when } n \text{ is odd.}$$

$$\sigma^n = E \text{ when } n \text{ is even.}$$

Section-B

Note: Answer all the questions of the following : $4 \times 5 = 20$

2. (a) Explain matrix representations of all the symmetry elements present in water molecule.

Or

- (b) Define irreducible representation and mention its properties.
3. (a) Considering the tetrahedral geometry, prove that C_4 axis and a mirror plane perpendicular to it do not exist independently where as S_4 exists.

Or

- (b) Give the mathematical expression of "the great orthogonality theorem". Explain the meaning of each term.
4. (a) Derive the matrix representation for rotation operation by angle $\Pi/2$ (anti-clockwise) and assuming z-axis as axis of rotation.

Or

- (b) State 'rearrangement theorem' with the help of a multiplication table of your choice.

5. (a) Considering the character table of C_{3v} point group : given below, prove the following :

(i) $A_1 \times A_2 = A_2$

(ii) $A_1 \times E = E$

(iii) $A_2 \times E = E$

C_{3v}	$E2C_33\sigma_v$		
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)	$(x^2 - y^2, xy)(xz, yz)$

Or

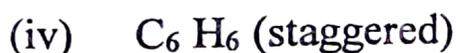
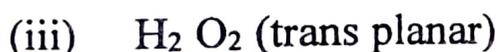
(b) Derive the symmetry types of the normal modes of water molecule by Cartesian coordinate method and discuss their IR and Raman activities. The relevant character table is given below;

C_{2v}	E	$C_{2(z)}$	σ_{xz}	σ_{yz}		
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

Section-C

Note: Answer any two questions of the following : $2 \times 20 = 40$

6. Define the term 'Point group'. Identify the point groups of the following and deduce the symmetry operations :



7. A reducible representation of T_d point group is given below, decompose it into irreducible ones :

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
[red]	6	0	2	0	2

Find out the values of the following. The character table for T_d is given below;

- (i) $A_1 \times E \times E$
 (ii) $A_2 \times T_1 \times T_2$
 (iii) $E \times T_1 \times T_2$

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

8. Explain the following giving a suitable example in each case :

- (a) Dihedral plane of symmetry.
 (b) Rotation reflection axis.
 (c) Order of the group.
 (d) Threefold axis of rotation.

9. Write short notes on any two :

- (a) Cyclic group
 (b) Cubic group
 (c) Similarity transformations

