CHE 501 N

M.Sc. (I[st] 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 <u>one</u> example.

(d) What are the selection rules for IR Spectroscopy.

(e) Prove that :

$\sigma^n = \sigma$ when n is odd.

$\sigma^n = E$ when n is even.

Section-B

Note: Answer all the questions of the following : 4×5=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}	$E2C_3 3\sigma v$		
A_1	1 1 1	Z	$x^2 + y^2, z^2$
A_2	1 1 -1	R_z	
E	2 – 1 0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

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 <u>two</u> questions of the following : 2×20=40

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

(i) CO_3^{2-}

(ii) $HC \equiv CH$

(iii) $H_2 O_2$ (trans planar)

(iv) $C_6 H_6$ (staggered)

(v) $NH_2 Cl$

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

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
Γred	6	0	2	0	2

Find out the values of the following. The character table for Td 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

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