BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: IMSc/MSc **SEMESTER : X/IV**
BRANCH: CHEMISTRY **SESSION : SP/2025**

SUBJECT: CH514 CHEMICAL APPLICATION OF GROUP THEORY

TIME: 3 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			CO	BL
Q.1(a)	With the help of character table of H_2O molecule, determine which of the vibrational modes are IR-active and Raman-active?	[5]	1	2
Q.1(b)	Find the symmetries of all vibrational motions of water.	[5]	1	3
Q.2(a)	Show the symmetry factoring of secular equations in cis-butadiene.	[5]	2	2
Q.2(b)	Show that, the symmetry of π orbitals of naphthalene belongs to B_{2g}, B_{3g}, A_u, and B_{1u} representation.	[5]	2	2
Q.3(a)	Show the SALC on the basis of *p*-orbitals of three terminal fluorine atoms which are bonded with sp^2 hybridized B-atom in BF_3 with A'_1 and E′ symmetry.	[5]	2	2
Q.3(b)	Draw the correlation diagram of water molecule which follows A_1 and B_2 symmetry.	[5]	2	3
Q.4(a)	Determine the term and draw correlation (Orgel) diagram for d^1 configuration.	[5]	2	2
Q.4(b)	Show that in BrF_5 the central atom adopts dsp^3 hybridization.	[5]	2	3
Q.5(a)	What are the seven crystal lattices possible in 3D unit cell? Explain. What are Bravais lattices?	[5]	2	2
Q.5(b)	Proves that 5-fold rotational axis is not possible in crystal symmetry.	[5]	2	2

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CHARACTER TABLES

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma'_v(yz)$		
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

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

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)

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	−1	−1	R_z	
B_1	1	−1	1	1	−1		x^2-y^2
B_2	1	−1	1	−1	1		xy
E	2	0	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)