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

CLASS: MSc. **SEMESTER: IV**
BRANCH: Chemistry **SESSION: SP/22**

SUBJECT: CH514 Chemical Applications of Group Theory

TIME: 2 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.

Q.1(a) Use the 3N Cartesian basis and the appropriate Character table to determine the symmetries of vibrational modes of H_2O. [5]

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

Q.1(b) Express the symmetry coordinates as SALCs of the internal coordinates in the case of H_2O. [5]

Q.2(a) Show the SALC of π-orbitals of ethylene. [5]

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	

Q.2(b) Using HMO approach form the secular determinant of π-orbitals of ethylene and calculate the energy of π-bonding and anti-bonding orbitals. [5]

Q.3(a) Show that the symmetry representation of σ-MOs in H_2O. [5]

Q.3(b) Determine the symmetry representation of hybrid orbitals in boron in BF_3. [5]

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)

Q.4(a) Explain the concept of vibronic coupling. [5]

Q.4(b) Explain how and why splitting of d orbital energy levels happen in the presence of an Octahedral crystal field. [5]

Q.5(a) Draw all the seven three-dimensional unit cell with the lattice parameters. [5]
Q.5(b) Why is 5-fold rotational axis not observed in crystal symmetry? [5]

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