CHUKA UNIVERSITY

UNIVERSITY EXAMINATIONS

EXAMINATION FOR THE AWARD OF DEGREE OF BACHELOR OF SCIENCE IN CHEMISTRY

CHEM 315: CHEMICAL APPLICATIONS OF GROUP THEORY

STREAMS: BSC. CHEM **TIME: 2 HOURS**

DAY/DATE: WEDNESDAY 16/04/2025 **2.30 P.M. – 4.30 P.M.**

INSTRUCTIONS

- **Answer question One (Compulsory) and any other Two questions**

QUESTION ONE [30 MARKS]

(a) Draw and label all the rotation axes and reflection planes for the trigonal planar BH_3 molecule (**4 marks**)

(b) Determine the molecular geometry, the symmetry elements and the point group of each of the following molecules (**10 marks**)

(i) BrF_4^- (ii) SeF_4 (iii) CCl_4 (iv) $Mn(CO)_5Br$ (v) *trans*-N_2F_2

(c) State the properties of a mathematical group (**4 marks**)

(d) Consider the $\mathbf{D_{4h}}$ point group (use the attached character table):

(i) Determine the direct product $E_u \cdot E_u$ and reduce to a sum of irreducible representations (**4 marks**)

(ii) Show that the irreducible representations B_{2g} and E_g are orthogonal to one another (**2 marks**)

(e) Determine whether the *cis*-$[Co(en)_2Cl_2]^+$ ion is chiral or achiral (**2 marks**)

(f) Generate a matrix representation for the $\mathbf{C_{2v}}$ point group using the three (p_x, p_y, p_z) *p*-orbitals of the oxygen atom of H_2O as the basis set (**4 marks**)

QUESTION TWO [20 MARKS]

(a) Consider the NH_3 ($\mathbf{C_{3v}}$) molecule:

(ii) Construct the group multiplication table of NH_3 (**6 marks**)

(iii) Determine the unique non-trivial subgroups of the NH_3 point group (**2 marks**)

(iv) Divide the operations of the group into classes (**3 marks**)

(b) Determine the set of specific atomic orbitals that can be combined to form hybrid orbitals for the BCl_3 ($\mathbf{D_{3h}}$) molecule (**9 marks**)

QUESTION THREE [20 MARKS]

(a) Consider the partial character table for the $\mathbf{D_{2d}}$ point group shown below. Generate the characters of the five irreducible representations of the $\mathbf{D_{2d}}$ group (**5 marks**)

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
A_1							x^2+y^2, z^2
A_2						R_z	
B_1							x^2-y^2
B_2						z	xy
E						(x,y) (R_x,R_y)	(xz,yz)

(b) Derive the irreducible representations of the $\mathbf{D_2}$ {E, C_2, C_2', C_2''} point group using the great orthogonality theorem (**5 marks**)

(c) Determine the activities of the normal vibrational modes of the BeF_3^- ($\mathbf{D_{3h}}$) ion (**10 marks**)

QUESTION FOUR [20 MARKS]

Consider the CH_4 ($\mathbf{T_d}$) molecule:

(i) Determine the atomic orbitals that carbon can use to form molecular orbitals in CH_4 (**8 marks**)

(ii) Construct the SALCs for the CH_4 molecule (**6 marks**)

(iii) Construct the molecular orbital diagram of CH_4 (**4 marks**)

(iv) Describe the EPS spectrum of CH_4, based on your MOD in (iii) above **(2 marks)**

Character Tables

D_{3h} $(\bar{6})m2$	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)	$(x^2-y^2, 2xy)$
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)	(xy, yz)

D_{4h} $(4/mmm)$	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1		x^2-y^2
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1		xy
E_g	2	0	−2	0	0	2	0	−2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1		
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1		
E_u	2	0	−2	0	0	−2	0	2	0	0	(x, y)	

T_d $(\bar{4}3m)$	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	−1	−1		
E	2	−1	2	0	0		$(2z^2-x^2-y^2,\ \sqrt{3}\ (x^2-y^2)$
T_1	3	0	−1	1	−1	(R_x, R_y, R_z)	
T_2	3	0	−1	−1	1	(x, y, z)	(xy, xz, yz)

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