UNIVERSITY OF EMBU

2017/2018 ACADEMIC YEAR

SECOND SEMESTER EXAMINATIONS

SECOND YEAR EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE

SCH 205: GROUP THEORY AND ITS CHEMICAL APPLICATIONS

DATE:APRIL 4, 2018 **TIME: 2:00-4:00PM**

INSTRUCTIONS:

Answer Question ONE and any other TWO Questions
The periodic table of elements, a table of symmetry-adapted orbitals and selected character table are provided at the last page

QUESTION ONE (30 MARKS)

a) Using examples, briefly differentiate between symmetry element and symmetry operation. (4 marks)

b) Determine all the symmetry elements in the following molecules: (6 marks)

i) H_2O

ii) *p*-Dichlorobenzene

c) Explain the symmetry criteria that allow a molecule to be optically active? (3 marks)

d) Using diagrams as necessary, show that $S_2 \equiv i$. (4 marks)

e) The CCl_4 molecule belongs to the point group T_d. List the symmetry elements of the group and locate them in the molecule. (3 marks)

f) For cis-1,3-butadiene, of C_{2v} symmetry,

i) List all the symmetry operations for this molecule (2 marks)

ii) Write a set of transformation matrices that describe the effect of each symmetry operation in the C_{2v} group on a set of coordinates x, y, z for a point. (4 marks)

g) List all the fundamental properties that a group must satisfy. (4 marks)

QUESTION TWO (20 MARKS)

a) Determine the symmetry elements that are lost in going from NH_3 to NH_2Cl? (5 marks)

b) List the symmetry operations and the corresponding symmetry elements of the point groups. (10 marks)

c) Explain the structure and content of a character table. (5 marks)

QUESTION THREE (20 MARKS)

a) Show that BF_3 belongs to the D_{3h} point group. (7 marks)

b) Using a diagram of boron trifluoride, show that three operations generated by C_3 axis are C_3, C_3^2 and E. (6 marks)

c) Find out the symmetry species of the normal modes of vibration of *cis*-planar H_2O_2. (7 marks)

QUESTION FOUR (20 MARKS)

a) Explain the term "Group" as relates to group theory. (2 marks)

b) Analysis of the x, y, and z coordinates of each atom in NH_3 gives the following representation:

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ	12	0	2

i) Reduce Γ to its irreducible representations. (7 marks)

ii) Classify the irreducible representations into translational, rotational, and vibrational modes. (6 marks)

c) Molecules belonging to the point groups T_h or T_d cannot be chiral. Which elements of these groups rule out chirality? (5 marks)

QUESTION FIVE (20 MARKS)

a) Prove that C_2^z σ_{xz} and σ_{xz} C_2^z commute. (6 marks)

b) Use the symmetry of the atomic orbitals of the central atom to construct (using appropriate combinations of group orbitals peripheral atoms) the molecular orbital diagrams for H_2O.

(14 marks)

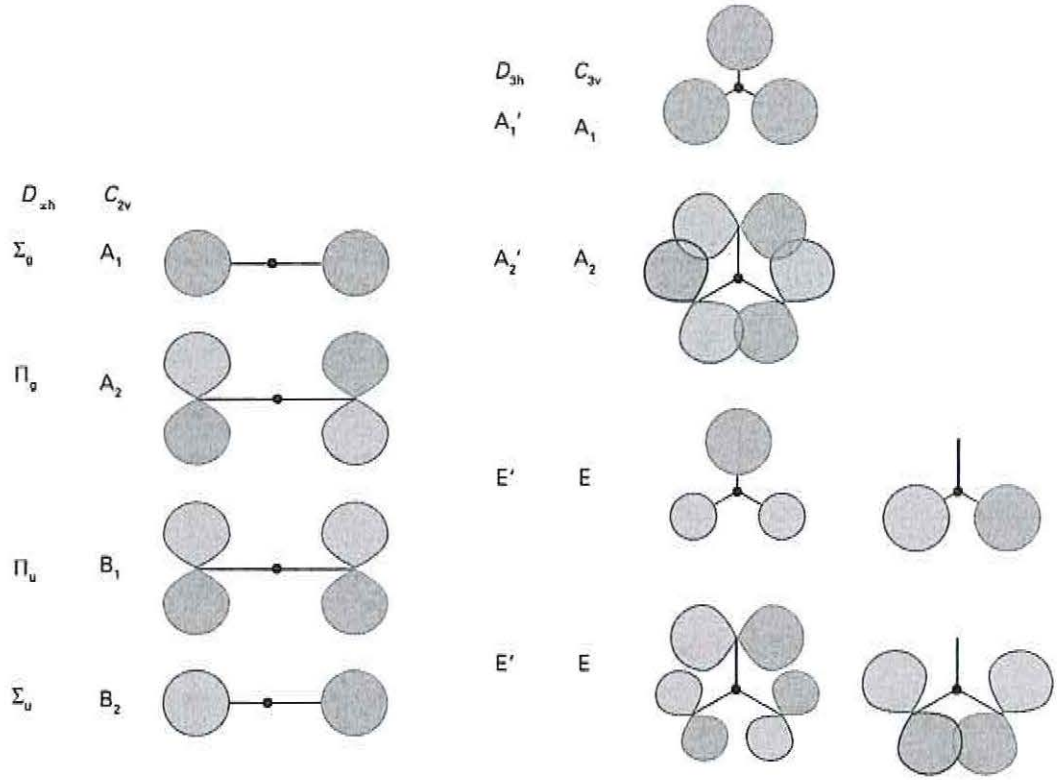
Information you may require

Symmetry-adapted orbitals

Table 1 gives the symmetry classes of the s, p, and d orbitals of the central atom of an AB_n molecule of the specified point group. In most cases, the z-axis is the principal axis of the molecule; in C_{2v} the x-axis lies perpendicular to the molecular plane.

Table 1 Symmetry species of orbitals on the central atom

	$D_{\infty h}$	C_{2v}	D_{3h}	C_{3v}	D_{4h}	C_{4v}	D_{5h}	C_{5v}	D_{6h}	C_{6v}	T_d	O_h
s	Σ	A_1	A_1'	A_1	A_{1g}	A_1	A_1'	A_1	A_{1g}	A_1	A_1	A_{1g}
p_x	Π	B_1	E'	E	E_u	E	E_1'	E_1	E_{1u}	E_1	T_2	T_{1u}
p_y	Π	B_2	E'	E	E_u	E	E_1'	E_1	E_{1u}	E_1	T_2	T_{1u}
p_z	Σ	A_1	A_2''	A_1	A_{2u}	A_1	A_2''	A_1	A_{2u}	A_1	T_2	T_{1u}
d_{z^2}	Σ	A_1	A_1'	A_1	A_{1g}	A_1	A_1'	A_1	A_{1g}	A_1	E	E_g
$d_{x^2-y^2}$	Δ	A_1	E'	E	B_{1g}	B_1	E_2'	E_2	E_{2g}	E_2	E	E_g
d_{xy}	Δ	A_2	E'	E	B_{2g}	B_2	E_2'	E_2	E_{2g}	E_2	T_2	T_{2g}
d_{yz}	Π	B_2	E''	E	E_g	E	E_1''	E_1	E_{1g}	E_1	T_2	T_{2g}
d_{zx}	Π	B_1	E''	E	E_g	E	E_1''	E_1	E_{1g}	E_1	T_2	T_{2g}



Selected Character Table

C_{2v} ($2mm$)	E	C_2	$\sigma_v(xz)$	σ'_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

C_{3v} ($3m$)	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, 2xy)(xz, yz)$

C_{4v} ($4mm$)	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)

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