EMBU UNIVERSITY COLLEGE

(A CONSTITUENT COLLEGE OF THE UNIVERSITY OF NAIROBI)

TRIMESTER EXAMINATIONS 2013/2014

SECOND YEAR EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE

SCH 205: GROUP THEORY AND ITS CHEMICAL APPLICATIONS

DATE: AUGUST 12, 2014 **TIME: 11.00AM – 1.00PM**

INSTRUCTIONS:

Character tables are attached

Answer Question ONE and ANY Other TWO Questions

QUESTION ONE:

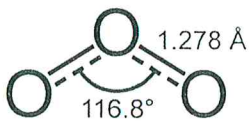
a) Briefly explain the following terms as used in group theory

i.) Symmetry operation

ii.) Principal axis (4 marks)

b) List the four conditions that must be met by a group (4 marks)

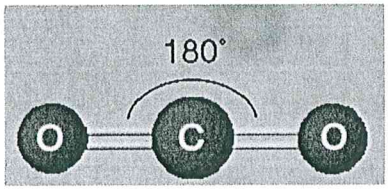
c) Identify four symmetry elements present in ozone molecule shown below



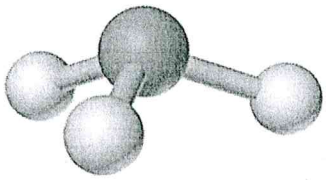
(4 marks)

d) Identify the point groups of the following molecules

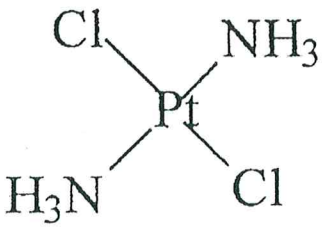
i.)



ii.)



iii.)



(6 marks)

e) Use the character table of C_{2v} provided below to answer the questions that follow

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

S

W

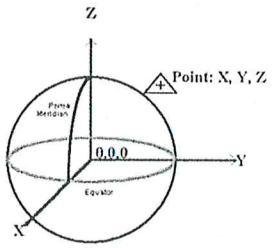
i.) What do items enclosed in S and W represent (4 marks)

ii.) Which representation is totally symmetric and why? (2 mark)

iii.) What is the order of the group (2 mark)

f) Generate a reducible representation that shows how x, y and z axis transform under the operations of C_{2h} by completing the table provided below

C_{2h}	E	C_2	i	σ_h
$\Gamma_{x,y,z}$				



(4 marks)

QUESTION TWO

a) SO_3 is a triagonal planar molecule belonging to point group D_{3h}. The point group is provided below. Use it to answer the questions that follow

i.) Distinguish between a π- bond and a σ-bond (2 marks)

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)	$(x^2-y^2, 2xy)$
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)

ii.) Generate a reducible representation that shows how the σ-bonds in SO_3 transform under the symmetry operations of D_{3h}. (6 marks)

iii.) Reduce the representation generated to the respective irreducible representations and use them to identify the atomic orbitals of central atom involved σ-bond formation (6 marks)

iv.) Generate a reducible representation that shows how the π-bonds in SO_3 transform under the symmetry operations of D_{3h}. (6 marks)

QUESTION THREE

a) NH_3 is a triagonal pyramid molecule belonging to point group C_{3v}. The point group is provided below. Use it to answer the questions that follow

C_{3v}	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	$(x, y)(R_x, R_y)$	$(x^2-y^2, 2xy)(xz, yz)$

i.) Generate a reducible representation that shows how the σ-bonds in NH_3 transform under the symmetry operations of C_{3v}. (3 marks)

ii.) Reduce the representation generated to the respective irreducible representations and use them to identify the atomic orbitals of central atom involved σ-bond formation (3 marks)

iii.) Generate SALCs (Symmetry-adapted linear Combination of the three 1s orbitals for NH_3 (6 marks)

iv.) List the bonding and antibonding resulting LCAO-MOs for NH_3 molecule and sketch their molecular orbital diagram that show their relative energy profile (8 marks)

QUESTION FOUR

a) SO_2 molecule has a bent geometry and belongs to point group C_{2v}. The point group is provided below. Use it to answer the questions that follow

C_{2v} (2mm)	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

i.) Calculate and sketch the number of normal modes of vibration for SO_2 molecule (4 marks)

ii.) Generate a reducible representation that shows how the three degree of freedom per atom transforms under the symmetry operations of C_{2v}. (4 marks)

iii.) Reduce the representation generated to the respective irreducible representations and use them to identify the normal vibration modes of SO_2 (10 marks)

iv.) Out of the normal modes identified in ii above, state which are Raman and IR active

(2 marks)

QUESTION FIVE

a) CO_2 is a linear molecule belonging to point group $D_{\infty h}$. Use the point group D_{2h} is provided below to answer the questions that follow

D_{2h} (*mmm*)	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	

i.) Generate a reducible representation that shows how the σ and π-bonds in CO_2 transform under the symmetry operations of D_{2h}.

(4 marks)

ii.) Reduce the representation generated to the respective irreducible representations and use them to identify the atomic orbitals of central atom involved in σ and π-bond formation

(6 marks)

iii.) Use the correlation table given below to correlate the irreducible representation obtained in iii above with those of the $D_{\infty h}$ point group (4 marks)

iv.) Generate SALCs (Symmetry-adapted linear Combination) of the orbitals with ability to form π-bond (6 marks)

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