UNIVERSITY OF EMBU

2016/2017 ACADEMIC YEAR

SECOND SEMESTER EXAMINATION

SECOND YEAR EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE

SCH 205: GROUP THEORY AND ITS CHEMICAL APPLICATIONS

DATE: APRIL 5, 2017 **TIME: 2:00-4:00PM**

INSTRUCTIONS:

Answer Question ONE and ANY Other TWO Questions

The periodic table of elements 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) In group theory, what is meant by the symbols E, σ, C_n and S_n? (4 marks)

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

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

ii) What is the order of the point group C_{2V}? (1 mark)

iii) 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)

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

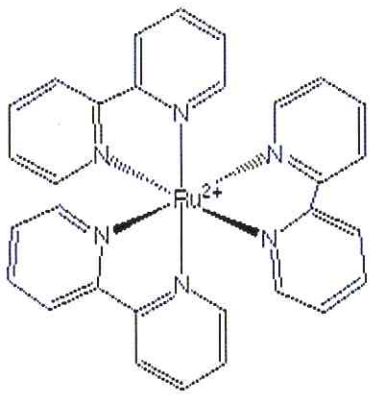
f) List all the fundamental properties that a group must satisfy. (4 marks)

g) Find the principal and the subsidiary axes of symmetry in benzene. (3 marks)

QUESTION TWO (20 MARKS)

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

b) Determine the point group of $Ru(bipy)_3^{2+}$ (shown below). (5 marks)



$Ru(bipy)_3^{2+}$

c) Aluminum (III) hexafluoride anion, AlF_6^{3-}, has an octahedral structure in which the Al^{3+} cation is located at the center and the six F- anions are located at the mid points of the six faces of a cube. Fill in the following table with information about the structure of AlF_6^{3-}.

(8 marks)

Symmetry element	**How many?**
C_2 axes	
C_3 axes	
C_4 axes	
C_6 axes	
S_3 axes	
S_4 axes	
S_6 axes	
inversion center?	

d) Is this molecule polar? Chiral? (2 marks)

QUESTION THREE (20 MARKS)

a) Draw the structure of $[XeF_5]^-$. On the diagram, mark the C_5 axis. The ion contains five C_2 axes. Show these axes. (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) 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)

b) Show that the total number of degrees of freedom = $3N$. (5 marks)

c) Which vibrational modes are infrared active? (2 marks)

QUESTION FIVE (20 MARKS)

a) For trans-1,2-dichloroethylene, of C_{2h} symmetry,

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

ii) Write a transformation matrix for each symmetry operation that describes the effect of that operation on the coordination of a point x, y, z. (Your answer should consist of four 3x3 transformation matrices.) (6 marks)

b) Using the terms along the diagonal, obtain as many irreducible representations as possible from the transformation matrices. (7 marks)

c) Using the C_{2h} character table, verify that the irreducible representations are mutually orthogonal. (3 marks)

PERIODIC TABLE

1																	18
1 H 1.008	2											13	14	15	16	17	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31	3	4	5	6	7	8	9	10	11	12	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57* La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89** Ac (227)	104 Db (261)	105 Jl (262)	106 Rf (263)	107 Bh (262)	108 Hn (?)	109 Mt (?)									

* Lanthanides	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.2	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
** Actinides	90 Th (232)	91 Pa (231)	92 U (238)	93 Np (237)	94 Pu (239)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (252)	99 Es (252)	100 Fm (257)	101 Md (256)	102 No (259)	103 Lr (260)

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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