



SOUTH EASTERN KENYA UNIVERSITY

UNIVERSITY EXAMINATIONS 2016/2017

SECOND SEMESTER EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE (CHEMISTRY)

SCH 205: GROUP THEORY AND ITS CHEMICAL APPLICATIONS

DATE: 12TH APRIL, 2017

TIME: 4.00-6.00 P.M

INSTRUCTIONS TO CANDIDATES

- (a) Answer question One and any other Two questions
- (b) Question 1 carries 30 marks while the other questions carry 20 marks each
- (c) Illustrate your answers with well labeled diagrams where appropriate
- (d) No written materials allowed.
- (e) Write all answers in the booklet provided.
- (f) Do not forget to write your Registration Number.
- (g) Do not write any answers on this question paper
- (h) A table of group theory operations and their contributions is provided
- (i) The Character Table is provided

QUESTION 1 (30 MARKS)

- a) Determine the symmetry elements of the following orbitals
 - i. p_x orbital,
 - ii. d_{xy} orbital

(10 marks)
- b) Determine the symmetry point groups for the following molecules
 - i. $cis\text{-Pt}(\text{NH}_3)_2\text{Cl}_2$
 - ii. $trans\text{-Pt}(\text{NH}_3)_2\text{Br}_2$
 - iii. CF_2CH_2
 - iv. SO_4^{2-}
 - v. SO_3

vi. tetrachloroallene

(10 marks)

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

- i. List all symmetry operations for the molecule
- ii. Write a set of transformation matrices that describe the effect of each symmetry operation in C_{2h} point group on the set of co-ordinates x, y, z for a point
- iii. Using the terms along the diagonal, obtain as many irreducible representations as possible from the transformation matrices.

(10 marks)

QUESTION 2 (20 MARKS)

What are s , p , and d orbitals of a central atom can be used to form δ hybrid orbitals for an AB_8 molecule having a square antiprism structure. (20 marks)

QUESTION 3 (20 MARKS)

Set up the correlation diagram for the CH_4 molecule. Consider the $2s$ and $2p$ orbitals of carbon and the $1s$ orbital of each hydrogen atom. (20 marks)

QUESTION 4 (20 MARKS)

Find the hybrid orbitals of a central atom in ammonia suitable for forming a set of δ bonds.

(20 marks)

QUESTION 5 (20 MARKS)

The molecule with simple formula N_2F_2 has several isomers; two of these isomers have central nitrogen's, with terminal fluorine on each nitrogen.

- a) Draw the isomers clearly using the Lewis dot diagram.
- b) Determine the symmetry point group of each of the isomers.
- c) For the *cis* isomer determine the number and symmetry species of the Raman and infrared active vibrations. (20 marks)

GROUP THEORY OPERATIONS AND THEIR CONTRIBUTIONS

| OPERATION | E | δ | i | C ₂ | C ₃ | C ₄ | C ₅ | C ₆ | S ₃ | S ₄ | S ₅ | S ₆ | S ₈ |
|-----------|---|----------|----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| F(R) | 3 | 1 | -3 | -1 | 0 | 1 | 1.618 | 2 | -2 | -1 | 0.382 | 0 | 0.414 |

For any C_n, $f(R) = 1 + 2 \cos \frac{2\pi}{n}$

For any S_n, $f(R) = -1 + 2 \cos \frac{2\pi}{n}$

