



DEDAN KIMATHI UNIVERSITY OF TECHNOLOGY

UNIVERSITY EXAMINATIONS 2021/2022

EXAMINATION FOR DEGREE OF MASTERS OF SCIENCE – IN CHEMISTRY

SCH 6115 GROUP THEORY

DATE: DECEMBER 2021

TIME: 3 Hours

INSTRUCTIONS: Answer ALL Questions

Question One (15 Marks)

- a) List and describe five symmetry elements [3mks]
- b) Using matrix method show that the line of intersection of two perpendicular planes of symmetry must be a twofold axis of symmetry [2mks]
- c) Benzene is a molecule with high symmetry (D_{6h}) determine the symmetry types of genuine vibrations and the respective activities of each type of vibrations [5mks]
- d) Write a matrix that converts an (incorrectly) C-centered monoclinic lattice to the proper primitive one. [2mks]
- e) How will the d orbitals split in a trigonal bipyramidal environment? Using a crystal field (pure point charge) model, determine what the relative energies of the orbitals will be [3mks]

Question Two (15 Marks)

- a) What are the highest order pure rotational subgroups of C_{8h} , D_{2d} , C_{5v} ? [3mks]
- b) What is the conventional designation for the group operations generated by an S_n axis when n is odd? [2mks]
- c) Determine group obtained by adding to or deleting from each of the following groups the indicated symmetry operations [5mks]
 - i. C_3 plus i -----
 - ii. C_{5v} plus σ_h -----
 - iii. S_6 minus i -----
 - iv. T_d plus i -----
 - v. D_{3d} minus S_6 -----
- d) Write out all the operations generated S_8 axis and express it in conventional notation [5mks]

Question Three (15 Marks)

- i. Consider a regular pentagonal dodecahedral molecule, $C_{20}H_{20}$. What irreducible representations are spanned by the set of C-H bonding orbitals? By the set of (30) C-C bonding orbitals? [5mks]
- ii. What s, p, and d orbitals of a central atom can be used to form a hybrid orbitals of an AB_8 molecule having a square antiprism structure? [5mks]
- iii. Investigate the symmetry restrictions on the reaction of the allyl anion with the ethylene molecule to form the cyclopentadienyl anion. If the reaction is not thermally allowed, which reactant should be singly excited for an allowed photochemical reaction? [5mks]

Question Four (15 Marks)

- a) Describe what you understand by the phrase symmetry operation [2mks]
- b) Prove that in any Abelian group, each element is in a class by itself [3mks]
- c) Write down the multiplication table for a the cyclic group of order 5. Show by trial and error that no other one is possible. [5mks]
- d) Define the term “chemical group” and describe conditions that must be satisfied to establish a mathematical group [5mks]

=====End =====Good=====Luck=====