

CHUKA



UNIVERSITY

UNIVERSITY EXAMINATIONS

EXAMINATION FOR THE AWARD DEGREE OF
MASTER OF SCIENCE IN CHEMISTRY

CHEM 825: ADVANCED GROUP THEORY

STREAM: MSC (CHEMISTRY)

TIME: 3 HOURS

DAY/DATE: THURSDAY 9/04/2020

11.30 A.M - 2.30 P.M.

INSTRUCTIONS:

Answer All Questions

QUESTION ONE [20 MARKS]

(a) Determine the point group of each of the following species [12 Marks]

(i) SiF_4 (ii) NH_2Cl (iii) SF_5Cl (iv) KrF_2 (v) SeCl_4 (vi) IF_4^-

(b) Determine the matrix representation of the C_{2v} point group using the p_y -orbitals of carbon in the allyl radical as a basis [4 Marks]

(c) Show that the matrix representation in (b) above satisfy the axioms of group theory

[2 Marks]

(d) Construct the group multiplication table for the C_{2h} point group. The *trans*-1,2-dichloroethene molecule belong to the C_{2h} point group. [2 Marks]

QUESTION TWO [20 MARKS]

- (a) Determine the vibrational modes of CO_3^{2-} that are Infra-red and Raman active. [10 Marks]
- (b) Determine the atomic orbitals of the central atom that the IF_5 molecule use to form hybrid orbitals for σ -bonding. [10 Marks]

QUESTION THREE [20 MARKS]

- (a) Consider the C_{3v} point group:
- (i) Construct the group multiplication table. [5 Marks]
- (ii) Determine the classes in the group. [3 Marks]
- (iii) Determine the subgroups in the group. [2 Marks]
- (b) (i) Determine the atomic orbitals of the central atom and the normalized SALCs that are required to form σ bonds in BF_3 (D_{3h}) molecule. [7 Marks]
- (ii) Sketch the molecular orbital diagram for the BF_3 molecule. [3 Marks]
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