

CHUKA



UNIVERSITY

UNIVERSITY EXAMINATIONS

EXAMINATION FOR THE AWARD OF DEGREE OF MASTER OF SCIENCE IN
CHEMISTRY

CHEM 811: ADVANCED GROUP THEORY

STREAMS: MSC (CHEMISTRY)

TIME: 3 HOURS

DAY/DATE: THURSDAY 8/08/2019

2.30 P.M - 5.30 P.M.

INSTRUCTIONS

Answer All Questions

QUESTION ONE [20 MARKS]

- (a) Determine the molecular point group for each of the following species; (6 marks)
- (i) XeO_4
 - (ii) CCl_3^+
 - (iii) NOF
 - (iv) I_3^-
- (b) (i) Generate a matrix representation of the C_{2h} point group using a set of x, y, and z coordinates as your basis. (2 marks)
- (ii) Show that the matrix representation satisfy the requirements of a mathematical group (2 marks)
- (c) Consider the C_{3v} point group to which the NH_3 molecule belongs:
- (i) Construct the multiplication table for the C_{3v} point group (5 marks)
 - (ii) Tabulate the non-trivial sub-groups of the C_{3v} point group (2 marks)
 - (iii) Determine the classes of the C_{3v} point group (3 marks)

QUESTION TWO [20 MARKS]

- (a) The AX_4 molecules can either be tetrahedral (T_d) or square planar (D_{4h}). Describe how group theoretical analysis of vibrational (IR and Raman) spectroscopy of an AX_4 molecule can be used to establish its molecular geometry (12 marks)

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- (b) Determine the atomic orbitals of the indium atom that can be used to form σ hybrid orbitals for the InCl_5^{2-} (C_{4v}) ion. (6 marks)

QUESTION THREE [20 MARKS]

Consider the $[\text{PtCl}_4]^{2-}$ ion which belongs to the D_{4h} point group:

- (a) Determine the atomic orbitals on platinum that are used to form σ -bonds with chlorine atoms in the $[\text{PtCl}_4]^{2-}$ ion. (12 marks)
- (b) Determine the SALCs that are required to form Pt-Cl σ -bonds in the $[\text{PtCl}_4]^{2-}$ ion. (4 marks)
- (c) Sketch the molecular orbital diagram for the $[\text{PtCl}_4]^{2-}$ ion. (4 marks)
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