

CHUKA



UNIVERSITY

UNIVERSITY EXAMINATIONS

**EXAMINATION FOR THE AWARD OF DEGREE OF BACHELOR OF SCIENCE IN
CHEMISTRY**

CHEM 315: CHEMICAL APPLICATIONS OF GROUP THEORY

STREAMS: BSc (CHEMISTRY)

TIME: 2 HOURS

DAY/DATE: TUESDAY 16/04/2019

8.30 A.M. – 10.30 A.M.

INSTRUCTIONS:

- **Answer question One (Compulsory) and any other Two questions**

QUESTION ONE [30 MARKS]

(a) Define each of the following terms: (6 marks)

- (i) symmetry operation (ii) symmetry element (iii) rotational axis
(iv) plane of symmetry (v) center of symmetry (vi) improper rotation axis

(b) Determine the molecular geometry, the symmetry elements and the point group of each of the following molecules (9 marks)

- (i) XeO_3 (ii) BH_3 (iii) KrF_2

(c) Consider the following multiplication table for the C_{2h} point group:

C_{2h}	E	C_2	i	σ_h
E	E	C_2	i	σ_h
C_2	C_2	E	σ_h	i
i	i	σ_h	E	C_2
σ_h	σ_h	i	C_2	E

- (i) Determine the non-trivial sub-groups of the C_{2h} point group (1 mark)
- (ii) Determine the classes of the C_{2h} point group (4 marks)
- (d) The water molecule belong to the C_{2v} point group. Derive a matrix representation for the C_{2v} point group using a vector $(x \ y \ z)$ in the normal coordinate system as the basis of the representation (4 marks)
- (e) Discuss the composition of a character table (6 marks)

QUESTION TWO [20 MARKS]

- (a) Determine the symmetry elements and the point group of each of the following molecule (8 Marks)

(b) Determine the hybrid orbitals that the phosphorous atom can use to form σ -bonds to the five fluorine atoms in the PF_5 (D_{3h}) molecule (12 Marks)

QUESTION THREE [20 MARKS]

(a) The water molecule belong to the C_{2v} point group:

(i) Construct the multiplication table for the C_{2v} point group (4½ marks)

(ii) Determine the non-trivial sub-groups of the C_{2v} point group (1½ marks)

(iii) Determine the classes of the C_{2v} point group (4 marks)

(b) Determine the fundamental vibrational modes of IF_5 (C_{4v}) that are infra-red and Raman active (10 marks)

QUESTION FOUR [20 MARKS]

(a) Determine the polarity of the following species (4 marks)

(i) NH_3 (ii) BF_3 (iii) SF_4 (iv) CO_2

(b) Determine the chirality of the following species (3 Marks)

(i) CHClFBr (ii) $\text{Mn}(\text{acac})_3$

(c) The SO_3 molecule belong to the D_{3h} point group:

(i) Determine the atomic orbitals that the sulphur atom can use to form molecular orbitals with the oxygen atoms (7 marks)

(ii) Construct the normalized symmetry adapted linear combinations (SALCs) formed by the oxygen atoms (6 marks)

