

CHUKA



UNIVERSITY

UNIVERSITY EXAMINATIONS

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

CHEM 315: CHEMICAL APPLICATION OF GROUP THEORY

STREAMS: BSC CHEMISTRY

TIME: 2 HOURS

DAY/DATE: MONDAY 05/07/2021

5.00 P.M. – 7.00 P.M.

INSTRUCTIONS:

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

QUESTION ONE [30 MARKS](a) Define each of the following terms (4 marks)

- | | |
|--------------------------|-----------------------------|
| (i) rotational axis | (ii) plane of symmetry |
| (iii) center of symmetry | (iv) improper rotation axis |

(b) Determine the Lewis structure, the molecular geometry, the symmetry elements and the point group of each of the following species. (8 marks)

- | | | | |
|----------------------------|---------------------|----------------------|-----------------------------|
| (i) CH_3Cl | (ii) XeF_4 | (iii) I_3^- | (iv) NH_2Cl |
|----------------------------|---------------------|----------------------|-----------------------------|

(c) The NH_3 molecule belong to the C_{3v} point group. Construct the multiplication table for the C_{3v} point group. (6 marks)(d) Construct a matrix representation of the C_{2v} point group using the s-orbitals of the hydrogen and oxygen atoms of H_2O as a basis. (4 marks)(e) Determine the vibrational modes of BrF_3 (C_{2v}) that are Infrared and Raman active. (8 marks)

QUESTION TWO [20 MARKS]

(a) Consider the multiplication table for the C_{3h} point group:

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5
E	E	C_3	C_3^2	σ_h	S_3	S_3^5
C_3	C_3	C_3^2	E	S_3	S_3^5	σ_h
C_3^2	C_3^2	E	C_3	S_3^5	σ_h	S_3
σ_h	σ_h	S_3	S_3^5	E	C_3	C_3^2
S_3	S_3	S_3^5	σ_h	C_3	C_3^2	E
S_3^5	S_3^5	σ_h	S_3	C_3^2	E	C_3

(i) Construct a multiplication table for each of the non-trivial sub-group(s) of the C_{3h} point group. **(2 marks)**

(ii) Determine the classes of the C_{3h} point groups. **(6 marks)**

(b) The H_2O molecule belong to the C_{2v} point group:

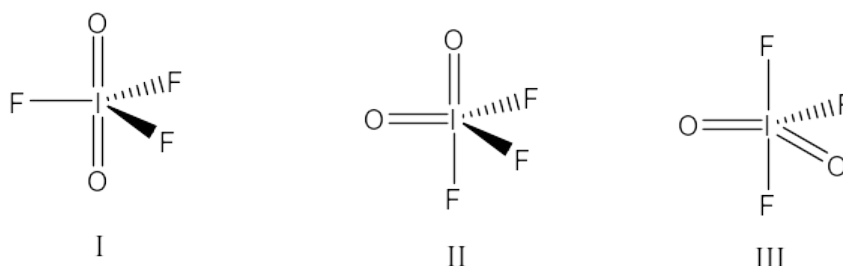
(i) Determine the atomic orbitals that the oxygen atom can use to form molecular orbitals with hydrogen atoms. **(4 marks)**

(ii) Construct normalized SALCs for the H_2O molecule using the projector operator. **(2 marks)**

(iii) Draw a well labelled molecular orbital diagram for H_2O . **(6 marks)**

QUESTION THREE [20 MARKS]

(a) Consider the structures of the three isomers of IF_3O_2 . Determine the symmetry elements and the point group of each isomer. **(6 marks)**



(b) Derive the characters of the irreducible representation of the C_{3v} point group using the Great Orthogonality Theorem. **(6 marks)**

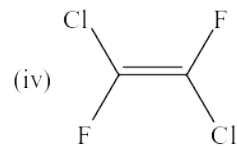
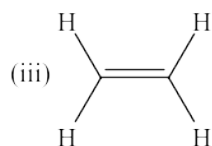
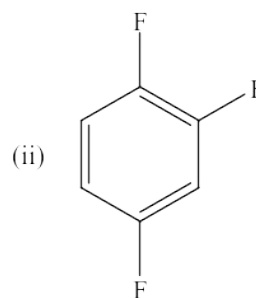
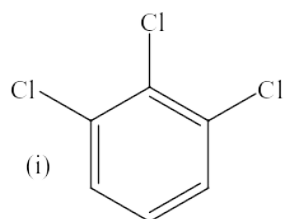
(c) Determine the possible hybridization(s) of the boron atom in the BH_3 (D_{3h}) molecule.

(8 marks)

QUESTION FOUR [20 MARKS]

(a) Determine the symmetry elements and the point group of each of the following compounds.

(8 marks)



(b) The molecular geometry of PF_3 can either be trigonal planar or trigonal pyramidal.

Describe how group-theoretical analysis of its fundamental vibrational modes can be used to establish the correct geometry.

(12 marks)
