

CHUKA UNIVERSITY EXAMINATIONS (2021)

CHEM 315: CHEMICAL APPLICATIONS OF GROUP THEORY

STREAMS: BSc (CHEMISTRY)

TIME: 2 HRS

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) CH₃Cl (ii) XeF₄ (iii) I₃⁻ (iv) NH₂Cl

(c) The NH₃ 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 H₂O as a basis (**4 marks**)

(e) Determine the vibrational modes of BrF₃ (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:

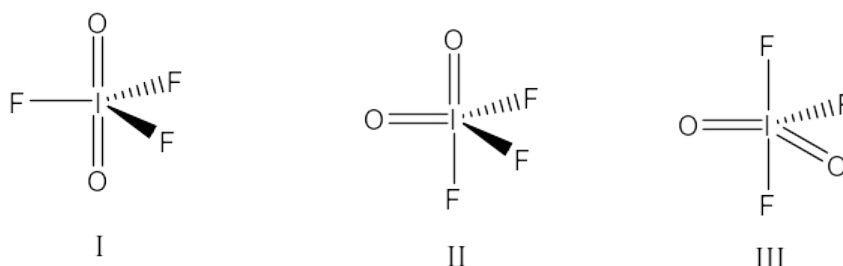
(i) Determine the atomic orbitals that the oxygen atom can use to form molecular orbitals with hydrogen atoms (4 marks)

(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)

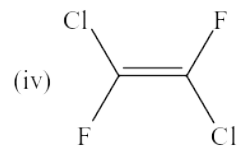
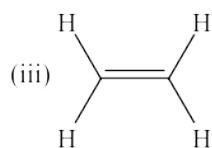
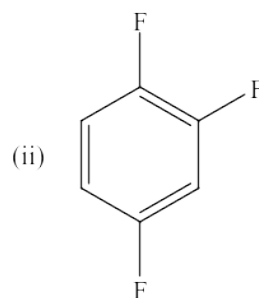
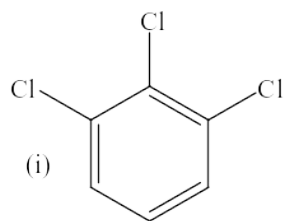


(b) Derive the characters of the irreducible representation of the C_{3v} point group using the Great Orthogonality Theorem (6 marks)

(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**)