KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2021/2022 ACADEMIC YEAR

THIRD YEAR SECOND SEMESTER
MAIN EXAMINATIONS

FOR THE DEGREE OF BACHELOR OF CHEMISTRY

COURSE CODE: SCH 327

COURSE TITLE: SYMMETRY, MOLECULAR STRUCTURE AND PROPERTIES

DURATION: 2 HOURS

DATE: 02/09/2022 **TIME:** 9:00aM-11:00aM

INSTRUCTIONS TO CANDIDATES

- Answer **QUESTION ONE** (Compulsory) and any other two (2) Questions.
- Indicate **answered questions** on the front cover.
- Start every question on a new page and make sure question's number is written on each page.

This paper consists of **5** printed pages. Please Turn Over

QUESTION ONE.COMPULSORY (30MARKS)

(a) Define the term molecular degrees of freedom (4marks)
(b) Differentiate between a symmetry operation and a symmetry element (4marks)
(c) Calculate the number of vibrational modes in CO_2 and CH_4 (4 marks)
(d) List the selection rules for Raman and IR active vibrations (2marks)
(e) Define the term vibrational spectroscopy and hence differentiate between translational and rotational modes (4marks)
(f) When radiation of a particular frequency fall on a molecule, some radiation is scattered. Name the two types of scattered radiation (2marks)
(g) Explain how an indistinguishable configuration comes about as a result of rotation and reflection in symmetry (3 marks)

(h) Draw the structures of PCl, NH_3 and BCl_3 according to VSEPR theory. (5 marks)
(i) Explain the symmetry criteria that allow a molecule to be optically active (2marks)

QUESTION TWO

(a) Explain how a molecule is assigned a point group (2marks)
(b) List the symmetry operations and the corresponding symmetry elements of the point groups (3marks)
(c) How do the rotation axes and planes of symmetry in cis- and trans-N_2F_2 differ? (5 marks).
(d) Draw the structures of each of the following species and confirm that each possesses a center of symmetry: CS_2, $[PF_6]^-$, XeF_4, I_2, $[ICl_2]^-$ (10 marks)

QUESTION THREE

(a) Assign a point group to each member in the series (i) CCl_4, (ii) CCl_3F, (iii) CCl_2F_2, (iv) $CClF_3$ and (v) CF_4. (5 marks)
(b) Determine the number of degrees of vibrational freedom for each of the following: (i) SO_2; (ii) SiH_4; (iii) HCN; (iv) H_2O; (v) BF_3 (5 marks)
(c) Explain what is meant by (i) Chiral (ii) Enantiomer (iii) Helical Chain (3 marks)
(d) How many normal modes of vibration are IR active for (i) H_2O, (ii) SiF_4, (iii) PCl_3, (iv) $AlCl_3$, (v) CS_2 and (vi) HCN? (6 marks)
(a) The point group of $[AuCl_2]^-$ is D∞h. What shape is this ion? (1 mark)

QUESTION FOUR

(a) Using VSEPR theory, draw the structures of CF_4, XeF_4 and SF_4. Assign a point group to each molecule. Show that the number of degrees of vibrational freedom is independent of the molecular symmetry. (10 marks)

(b) How many degrees of freedom do each of the following possess: $SiCl_4$, BrF_3, $POCl_3$ (3 marks)

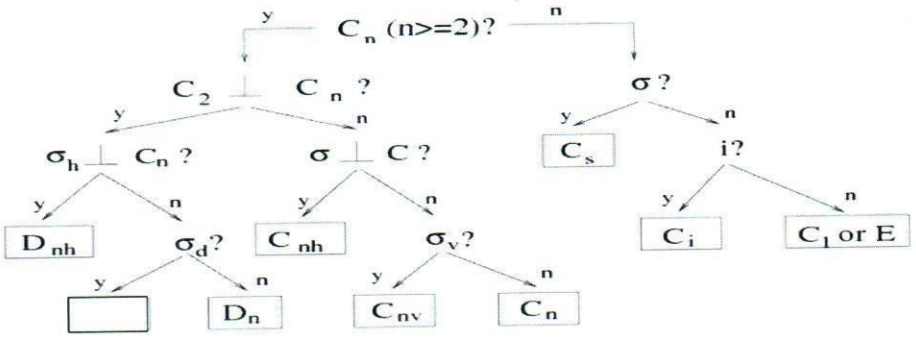
(c) The IR spectrum of SF_2 has absorption at 838, 813 and 357cm^{-1}. Explain why these data are consistent with SF_2 belonging to the C_{2v} rather than D∞h point group. (3 marks)

(d) The vibrational modes of XeF_2 are at 555, 515 and 213cm^{-1} but only two are IR active. Explain why this is consistent with XeF_2 having a linear structure. (4 marks)

QUESTION FIVE

(a) Use the flow chart below to assign the point groups to the following molecules (10 marks)

(i)Ammonia, (ii) acetone, (iii) dimethylcyclopentane, (iv) ethanediol, (v) propanediene



(b) The $[PdCl_4]^{2-}$ ion gives rise to three absorptions in its IR spectrum (150, 321 and 161 cm^{-1}. Rationalize why this provides evidence for a D_{4h} rather than a T_4 structure. (5 marks)

(c) The IR spectrum of gaseous ZrI_4 shows absorption at 55 and 254 cm^{-1}. Explain why this observation is consistent with molecules of ZrI_4 having T_4 symmetry. (5 marks)

Additional data for use