



KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2020/2021 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: 7/10/2021

TIME: 8:00-10:00AM

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.

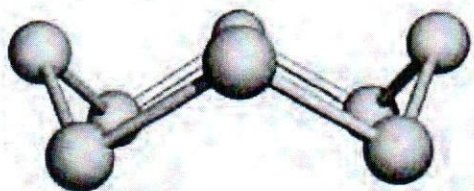
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QUESTION ONE. COMPULSORY

- (a) Define the following terms; (4 marks)
- Symmetry element
 - Symmetry operation
- (b) Calculate the number of vibrational modes in CO_2 and CH_4 (4 marks)
- (c) The symmetry operators for NH_3 are E , C_3 and $3\sigma_v$. (2 marks)
- Draw the structure of NH_3 . (2 marks)
 - What is the meaning of the E operator? (2 marks)
 - Draw a diagram to show the rotation and reflection symmetry operations. (2 marks)
- (d) What symmetry elements do BCl_3 and PCl_3 (2 marks)
- have in common and (2 marks)
 - Not have in common? (3 marks)
- (e) Determine the point group of PF_5 . (3 marks)
- (f) To what point group does POCl_3 belong? (3 marks)
- (g) Three projections of the cyclic structure of S_8 are shown below all S-S bond distances are equivalent, as are all S-S-S bond angles. To what point group does S_8 belong? (5 marks)



- (h) The IR spectrum of SnCl_2 exhibits absorptions at 352 , 334 and 120 cm^{-1} . What shape do these data suggest for the molecule, and is this result consistent with VSEPR theory? (5 marks)
- (i) Determine the point group of $\text{trans-N}_2\text{F}_2$. (2 marks)

QUESTION TWO

- (a) The oxalate ligand, $[\text{C}_2\text{O}_4]^{2-}$, is a bidentate ligand and the structure of the complex ion $[\text{Fe}(\text{ox})_3]^{3-}$ is shown below. Confirm that the point group to which the ion belongs is D_3 and that members of this point group are chiral. (5 marks)
- (b) How do the rotation axes and planes of symmetry in cis- and $\text{trans-N}_2\text{F}_2$ differ? (5 marks)
- (c) Draw the structures of each of the following species and confirm that each possesses a center of symmetry: CS_2 , $[\text{PF}_6]^-$, XeF_4 , I_2 , $[\text{ICl}_2]^-$ (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)

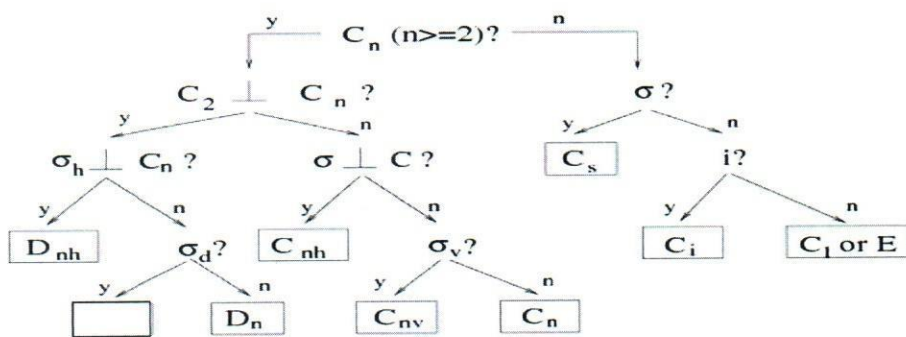
- (b) Determine the number of degrees of vibrational freedom for each of the following: (i) SO_2 ; (ii) SiH_4 ; (iii) HCN ; (iv) H_2O ; (v) BF_3 (5 marks)
- (c) Explain what is meant by (i) Chiral (ii) Enantiomer (iii) Helical Chain (3 marks)
- (d) How many normal modes of vibration are IR active for (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 $[\text{AuCl}_2]^-$ is $D_{\infty h}$. 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 $D_{\infty h}$ 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 $[\text{PdCl}_4]^{2-}$ 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_d 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_d symmetry. (5 marks)

Additional data for use

