# MERU UNIVERSITY OF SCIENCE AND TECHNOLOGY

**P.O. Box 972-60200 – Meru-Kenya.**
**Tel: +254 (0)799529958, +254 (0)799529959, +254 (0)712524293**
**Website: www.must.ac.ke Email: info@must.ac.ke**


**University Examinations 2023/2024**

FIRST YEAR, FIRST SEMESTER EXAMINATION FOR THE DEGREE OF MASTER OF SCIENCE IN CHEMISTRY

## SCH 7114: ADVANCED GROUP THEORY

**DATE: DECEMBER 2023** **TIME:3 HOURS**

**INSTRUCTIONS:** *answer question one and any other two questions*

NB: relevant character tables are attached

**QUESTION ONE 30 MARK**

a. Identify the symmetry elements in each of the following molecules and hence assign the appropriate point group to which each of the molecules belongs. (use VSEPR model to draw the molecules in three-dimensions) (9 marks)

(i) $NH_3$

(ii) $CH_2Cl_2$

(iii) $PF_5$ (trigonal bipyramidal)

b. Explain the following terms as used in infrared spectroscopy (4 marks)

(i) Fundamental band

(ii) Overtone

c. Microwave rotational spectroscopy uses microwave radiation to measure the energies of rotational transitions for molecules in the gas phase.

(i) Explain why the sample must be in gas phase (2 marks)

(ii) Explain whether or not HCl is microwave active. (2 marks)

d. With reasons classify each of the following molecules as chiral or achiral (6 marks)

(i) $Fe(CO)_5$

(ii) CHFClBr

(iii) $CH_2Cl_2$

e. Using the $D_2d$ character table, verify that E irreducible representation is orthogonal to each of the other irreducible representations (4 marks)

f. The ferrocene molecule (Fig 1) is a pentagon prism with Fe atom sandwiched between two $C_5H_5$ rings. Use group theory to predict whether it is polar or non polar. (3 marks)

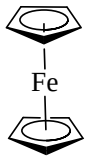


Fig1. Structure of ferrocene

**QUESTION TWO 15 MARKS**

a. (i) Determine the point group of $NO_3^-$ ion. (3 marks)

( (i) How many vibration modes does an $NO_3^-$ ion have? (8 marks)

(ii) Which of these vibration modes are IR active and which modes are Raman active? (4 marks)

**QUESTION THREE 15 MARKS**

a. Derive the multiplication table for $C_3v$ using s-orbitals of Nitrogen and Hydrogen in ammonia molecules as the basis (5 marks)

b. Show that $C_3v$ satisfies each of the rules that defines a mathematical group. (4 marks)

c. What conditions a molecule should meet for elucidation using

(i) Microwave spectroscopy (2 marks)

(ii) Infrared spectroscopy (2 marks)

(iii) Raman spectroscopy (2 marks)

**QUESTION FOUR 20 MARKS**

a. Determine the hybridization of boron in $BH_3$ (7 marks)

b. Normal modes of vibration are generally classified into stretching vibration and bending vibration. Discuss these two modes in details. (8 marks)