CHUKA  **UNIVERSITY**

UNIVERSITY EXAMINATIONS

EXAMINATION FOR THE AWARD OF DEGREE OF BACHELOR OF SCIENCE AND EDUCATION

CHEM 437: ORGANIC SPECTROSCOPY

STREAMS: **TIME: 2 HOURS**

DAY/DATE: TUESDAY 17/04/2018 **11.30 A.M – 1.30 P.M**

INSTRUCTION:

- **Answer question one and any other two questions**

QUESTION ONE

(a) The Infra- red spectroscopy is one of the physical methods (techniques) used in the elucidation of structures of molecules.

(i) What are the requirements for the molecule to be infrared active?

(ii) State clearly the major difference between the simple (harmonic) molecule and a real (anharmonic) molecule.

(iii) Show the major difference in the unfrared spectra resulting from the simple (harmonic) molecule and real (anharmonic) molecule.

(b) The number of total vibrations of a complex of N atoms can be predicted depending whether it is linear or nonlinear (3N-5 or 3N-6) respectively.

(i) For n=3, determine the number of stretching and bending vibrations in linear and non linear molecule respectively.

(ii) Explain the discrepancy in the number of total vibrations observed and that calculated from equation (b) above for linear triatomic molecule.

(iii) Briefly explain what are fundamental, overtone, combination and difference vibrations in a real molecule.

(c) Briefly explain two major differences between the dispersive infrared spectrometer and the fourier transform infrared sprectrometer.

(d) A particular sample of solution of a coloured substance, known to follow beer Lambert law, shows 80% transmittance when measured in a cuvet 1.00 cm in length.

(i) Calculate the % transmittance for a solution of twice the concentration in the same cuvet.

(ii) What must be the path length in the cuvet to give the same transmittance (80%) for a solution of twice the original concentration?

(iii) Calculate the % transmittance of the original solution contained in a cuvet with 0.5 cm path length.

QUESTION TWO

The simultaneous determination of titanium and vanadium, each as their peroxide complex, can be done in steel. When 1.000-g samples of steel were dissolved, colours developed, and diluted to 50ml exactly, the presence of 1.00 mg of Ti gave an absorbance of 0.269 at 400nm, and 0.134 at 460nm. Under similar conditions 1.00mg of V gave an absorbance of 0.057 at 400nm and 0.091 at 460 nm. For each of the following samples, 1.000g in weight and ultimately diluted to 50ml, calculate the % titanium and vanadium from these absorbance readings;

Sample	A_{400}	A_{460}	Sample	A_{400}	A_{460}
1	0.0172	0.116	5	0.902	0.570
2	0.366	0.430	6	0.600	0.660
3	0.370	0.298	7	0.393	0.215
4	0.640	0.436	8	0.206	0.130
			9	0.323	0.177

QUESTION THREE

(a) The nuclear magnetic resonance (NMR) spectra arise from the interaction of the magnetic dipoles of the nuclei and the external magnetic field.

(i) Explain three ways by which the presence of the nuclear spins can be explained in different nuclei of isotopes.

(ii) Briefly explain how the NMR spectra of a compound can be generated.

(b) (i) In NMR techniques, suggest a method for obtaining the resonance of ^{11}B (19.3 MHz) on an NMR spectrometer equipped with a 5-MHz crystal ascillator when H0 = 14.09 Kg.

(ii)In the double resonance procedures, why cannot sweep of the static magnetic field be used to generate the spectrum?

(iii) Estimate the nuclear overhauser effect sensitivity enhancement for (a) decoupling protons from ^{13}C NMR spectra, and (b) decoupling ^{13}C from ^{1}H spectra.

QUESTION FOUR (20MARKS)

(a) Explain in details how mass spectrum of a molecule is generated.

(b) A material containing only C,H and O, in the form leaflets melting at 40°C, possesses a rather simple mass spectrum with the parent peak at m/e 122 (35%) plus peaks at m/e 92 (65%) m/e 91 and small peaks at m/e 77 and 65. Metastable peaks appear at m/e 45.0 and 46.5. Deduce the structure of the compound.

C = 12.000, H = 1.000, O = 16.000
