CHUKA UNIVERSITY

UNIVERSITY EXAMINATIONS

EXAMINATION FOR THE AWARD OF DEGREE OF MASTER OF SCIENCE

CHEM 801: ADVANCED CHEMOMETRICS

STREAMS: MSC. **TIME: 3 HOURS**

DAY/DATE: TUESDAY 06/08/2019 **2.30 P.M. – 5.30 P.M.**

INSTRUCTIONS:

- **Answer question ONE and any other TWO questions.**

QUESTION ONE (20 MARKS)

1. (a) (i) Discuss the three methods which are most preferred for the determination of accuracy. (8 marks)

(ii) Briefly describe the acceptance criteria for accuracy. (1 mark)

(b) In spectrophotometry, the concentration of analyte is measured by its absorbance of light nine reagent blanks were also measured and gave values of 0.0006, 0.0012, 0.0022, 0.0005, 0.0016, 0.0008, 0.0017, 0.0010 and 0.0009.

(i) Calculate the minimum detectable signal and detection limit corresponding to 0.01ppb of standard having absorbance of 0.0078. Hence determine the total level reading at this level. (4 marks)

(ii) A calibration curve was conducted using a series of standard solutions. The concentrations and the absorbance of the standards are listed in the table below.

Concentration	0.01	0.10	0.50	1.00	2.50

Absorbance	0.0078	0.088	0.446	0.8980	1.877

(I) Determine the regression equation. (4 marks)

(II) Determine the concentration detection limit. (3 marks)

(c) You have received three shipments of iron ore of the following weights: 2852, 1578 and 1877Lb. There is an uncertainty in the weights of Analysis of the ores gives 36.28 and respectively. You are to pay 300 Dollar's per ton of iron.

Calculate the amount you should pay for these three shipments and the uncertainty in the payment.

{1ton = 2000lbs} (9 marks)

QUESTION TWO (20 MARKS)

2. (a) An ion-selective electrode (ISE) determination of sulphide from sulphate reducing bacteria was compared with a gravimetric determination. The results obtained were expressed in milligrams of sulphide. The results/ data obtained are given in the table below.

Sample	1	2	3	4	5	6	7	8	9	10
Sulphide (ISE) method	108	12	152	3	106	11	128	12	160	128
Sulphide (gravimetry)	105	16	113	0	108	11	141	11	182	118

(i) Comment on the suitability of the ISE method for this sulphide determination. (4 marks)

(ii) Calculate the correlation coefficient {consider in each case 95% confidence levels}. (2 marks)

(b) The gold content of a concentrated sea water sample was determined by using atomic absorption spectrometry with the method of standard addition. The results obtained were as follows:

Gold added ng per	0	10	20	30	40	50	60	70

ml of concentrated								
Absorbance	0.257	0.314	0.364	0.413	0.468	0.528	0.574	0.635

(i) Calculate the standard deviation and confidence limits of the slope and intercept of the regression line at 95% confidence levels. (6 marks)

(ii) Estimate the concentration of the gold in the concentrated sea water and obtain 95% confidence limit for this concentration. (1 marks)

(c) Briefly explain the meaning of hypothesis testing. (5 marks)

QUESTION THREE (20 MARKS)

3. (a) (i) A new procedure for the rapid determination of sulphur in kerosene was tested on a sample known from its method of preparation to contain (0.123% s. The results were %s=0.112, 0.118, 0.115 and 0.119. Evaluate whether the data indicate that there is a bias in the method at the 95%, 99% confidence level. (4 marks)

(ii) Explain why in molecular fluorescence spectrometry, signal vs concentration plots will often be approximately linear in very dilute solution but will show increasing (negative) curvature at higher concentrations.

(1 marks)

(b) Calculate the unweighted and weighted regression lines for the following calibration data. For each line calculate also the concentrations of test samples with absorbance of 0.100 and 0.600

Concentration	0	2	4	8	10	
Absorbance	0.009	0.158	0.301	0.472	0.577	0.739
Standard deviation	0.001	0.004	0.010	0.013	0.017	0.022

(8 marks)

(c) (i) Explain the purpose of experimental design in research. (1 marks)

(ii) Describe the principal component analysis as used in analytical chemistry. (4 marks)
