



# MACHAKOS UNIVERSITY

University Examinations 2021/2022

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

SECOND YEAR SUPPLEMENTARY/SPECIAL EXAMINATION FOR

BACHELOR OF SCIENCE IN ANALYTICAL CHEMISTRY

SAN 204: CHEMOMETRICS

DATE: 16/03/2022

TIME: 8:30-10:30 AM

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## INSTRUCTIONS:

- The paper consists of **two** sections.
- Section **A** is **compulsory** (30 marks).
- Answer any **two** questions from section **B** (each 20 marks).

## SECTION A

### QUESTION ONE (30 MARKS)

- a) Define the following terms;
- (i) Confidence limit
  - (ii) Random error
  - (iii) Chemometrics
  - (iv) Line of best fit
  - (v) Multivariate data (10 marks)
- b) Briefly describe the formula used in chi-square distribution analysis. (3 marks)
- c) A new method B for the determination of the chemical oxygen demand of wastewater was compared with the standard method A. The following results were obtained for a sewage effluent sample: Both samples had 7 values, thus degree of freedom is 6 at 5 % significance level.

Methods	Average (mol/L)	Standard deviations (mol/L)
A	0.467	0.0229
B	0.503	0.0182

Is the precision of method B significantly greater than that of the method A? (6 marks)

- d) State any **THREE** statistical softwares for data analysis commonly used. (3 marks)
- e) Briefly discuss any **TWO** differences between;
- (i) LOD and LOQ. (4 marks)
  - (ii) Type I error and Type II error (4 marks)

## SECTION B

### QUESTION TWO (20 MARKS)

- a) Describe any **FOUR** types of errors encountered in the laboratory measurements. (8 marks)
- b) For a particular determination, the slope of the calibration curve was 0.153 L/mg. The standard deviation of the noise level for a blank sample was measured to be 0.022. What is the detection limit in concentration units for this technique? (4 marks)
- c) Using examples, describe how a calibration curve is obtained? (4 marks)
- d) The number of binding sites per molecule in a sample of monoclonal antibody is determined five times, with results of 1.95, 1.95, 1.92, 1.93 and 1.97. Comment on the precision and accuracy of these results. (4 marks)

### QUESTION THREE (20 MARKS)

- a) Briefly describe how Dixon's test is applied in statistics. (4 marks)
- b) Differentiate between gross and systematic errors. (4 marks)
- c) In statistical analysis, when is the F-test considered for use? (3 marks)
- d) The following results were obtained in the determination of  $Al^{3+}$  in water samples at 5 % confidence level. 53.1 ppb 50.7 ppb 49.1 ppb 49.0 ppb 51.1 ppb  
Is there a need to reject or accept the outlier using the Grubb's tests? (4 marks)
- e) The following figures refer to the glucose levels in  $gL^{-1}$ , in the blood sera of 14 healthy adults: 37, 39, 37, 42, 39, 45, 42, 39, 44, 40, 39, 45, 43, 41  
The first seven figures are for men and the second seven for women. Test whether the mean concentrations for men and women differ significantly. (5 marks)

#### QUESTION FOUR (20 MARKS)

- a) ) Briefly differentiate between a Q test and Grubb's test as test for outliers. (4 marks)
- b) The caffeine levels (%) of six batches of seized port containers were determined, with the following results: 15.1, 21.2, 18.5, 19.2, 16.0, and 17.8. Calculate the;
- i) 99 % and
  - ii) 95 % confidence limits for these measurements. (6 marks)
- c) Briefly discuss **THREE** advantages of chemometrics. (6 marks)
- d) Measurements in chemistry come in different forms. State any **FOUR** forms. (4 marks)

#### QUESTION FIVE (20 MARKS)

- a) For most of data analysis steps, Input stage normally comes first. What are the other **FOUR** steps commonly followed? (4 marks)
- b) Briefly describe how sampling is conducted in a normal research set up. (4 marks)
- c) 10 workers are selected at random from a large number of workers in a factory. The number of times they are affected by asthmatic complaint due to asbestos in a year are found to be 51, 52, 53, 55, 56, 57, 58, 59, 59, and 60. In the light of these data would it be appropriate to suggest that the mean of the number times they are affected is 58? (4 marks)
- d) Briefly state the factors that affect Type II error. (4 marks)
- e) Differentiate between qualitative and quantitative analysis as part of data output. (4 marks)



## Tables

**Table A.5** Critical values of  $G$  ( $P = 0.05$ ) for a two-sided test

Sample size	Critical value
3	1.155
4	1.481
5	1.715
6	1.887
7	2.020
8	2.126
9	2.215
10	2.290

Taken from Barnett, V. and Lewis, T., 1984, *Outliers in Statistical Data*, 2nd edn, John Wiley & Sons Limited.

**Table A.6** Critical values of  $G$  ( $P = 0.05$ ) for a two-sided test

Sample size	Critical value
4	0.829
5	0.710
6	0.625
7	0.568

Adapted with permission from Statistical treatment for rejection of deviant values: critical values of Dixon's "Q" parameter and related subrange ratios at the 95% confidence level, *Analytical Chemistry*, 63(2), pp. 139–46 (Rorabacher, D.B. 1991), American Chemical Society. Copyright 1991 American Chemical Society.

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