UNIVERSITY OF SWAZILAND

DEPARTMENT OF CHEMISTRY

Course Name: Evaluation of Analytical Data

Course Code: C518

Examination: MAIN

Examination Date: May 2006

Time: 3 Hours

Instructions:

1. **Do not open this script unless authorized to do so by the Chief Invigilator.**
2. **This paper consists of five (5) questions, each worth 25 marks. Answer four (4) of these.**
3. **Candidates who show all procedural calculations will be rewarded.**
4. **Diagrams must be large and labeled correctly.**
5. **Some useful physical contents: $c = 2.908 \times 10^{8}$ $msec^{-1}$; $h = 6.626 \times 10^{-34}$; Jsec; $N = 6.626 \times 10^{23}$**
6. **This exam paper has 5 pages, including this page. Check to make sure.**

Special Requirements: **GRAPH PAPER**

DATA SHEET

QUESTION 1 **[25]**

a) Write down the equation that relates the total error in chemical analysis to its individual error components assuming a Gaussian distribution of the errors. [2]

b) For the following approaches to sampling, state how samples are collected, the equation (s) used to calculat sampling weights and numbers, and the merits and demerits of each approach.

i) Benedetti-Pichler. [3]
ii) Student's t. [3]

c) Following sampling, a spatial distribution may reveal a non-Gaussian population with "hot spots" and "col spots". Describe what is meant by "hot spots" and "cold spots" in analytical sampling, and suggest how this ca be statistically treated if Gaussian statistics are to be applied to the population. [3]

d) Briefly explain how you would test for normality in a data set using the Kolmogorov-Sminoff non-parametric tes [3]

e) The following data is obtained in an analysis of Cu and Zn in soil samples taken from a field in a random pattern.

Analyte	Sample #1	Sample #2	Sample #3	Sample #4	Sample #5	Sample #6	Sample #7	Sample #
Cu (ppm)	125	126	124	128	147	123	128	126
Zn (ppm)	85	23	90	35	72	125	40	35

i) Should the value "147" be considered part of the Cu data set at the 90% confidence level? [2]
ii) On the basis of your answer in (i) above, state if the analysis produces a result that is different from th true value of 136 at the 95% confidence level. [3]
iii) Using an alternative uv-visible method for Cu, the values obtained on six (6) samples of the same fie are as follows:

165ppm   124 ppm   173 ppm   142 ppm   126 ppm   115 ppm

- Calculate the number of samples required to hold the precision of copper to the same level as t population standard deviation. [4]

- How would this number of samples affect the sampling error of the zinc result? [2]

QUESTION 2 **[25]**

a) The concept of signal – to – noise ratio is a useful figure of merit in describing output quality in analyti instrumentation, and also in the determination of detection limits.

i) What is meant by "signal – to – noise" in analytical measurements? [3]

ii) With due regards to signal –to – noise ratio, define "detection limits" as applied to analyti spectroscopy. [3]

b) In analytical data acquisition, noise is unwanted because it degrades the quality of signals.

i) Describe Johnson noise, and state the equation which gives a relationship of the magnitude of this no to the bandwidth. [4]

ii) Describe Flicker noise, and state the equation which gives a relationship of the magnitude of this noise the band width. [4]

iii) Noise can be removed from analytical signals by means of an electrical filter. Draw and label a circ diagram of an electrical filter. [3]

c) A major source of error in analytical data acquisition is aliasing.

i) What is meant by "aliasing" (use diagrams to illustrate) [2]

ii) State the "Nyquist Theorem", and explain how it solves aliasing problems in analytical data acquisitio [2]

d) Operational amplifiers (OP Amps) are widely used in analytical instrumentation to process analog signals. Dr the electronic circuit and state the output of Summing Amplifier. [2]

e) Draw the symbolic circuit and construct a truth table for an AND function. [2]

QUESTION 3 **[25]**

a) During measurement, uncertainties in the analytical data obtained need to be carefully scrutinized and quantifi Although these errors have been greatly reduced with the advent of digital electronics, it is important to quan them in an analysis.

For the following triplicate calibration of Fe measured in tap water by spectrophotometry after complexation v bipyridine:

Solution	Concentration	Absorbance
Standard # 1	1.16 1.16 1.16	0.120 0.125 0.130
Standard # 2	2.32 2.32 2.32	0.248 0.255 0.252
Standard # 3	3.48 3.48 3.48	0.382 0.385 0.384
Standard # 4	4.65 4.65 4.65	0.504 0.506 0.502
Unknown Sample	Aliquot # 1 Aliquot # 2 Aliquot # 3	0.337 0.335 0.340

i) Use the Least Squares Method to calculate the equation of the calibration curve. [5]

ii) Calculate the uncertainty in the Least Squares value obtained in a (i) above in μg/ml. [3]

b) In an analysis, the reliability and validity of the results obtained need to be evaluated, usually through the us certified reference materials, quality control charts, and interlaboratory comparisons.

i) What is meant by a "certified reference material" in so far as analysis of agricultural soils is concerned? [3

ii) How is a certified reference material for agricultural soils produced? [3]

iii) Explain how the material is "certified" [3]

iv) Explain how the material is used to test the validity and reliability of data in an analysis of Cu, Zn and I soils. [3]

v) Draw a control chart for analytical measurements and explain why such charts are useful and how the used. [3]

vi) Explain how interlaboratory comparisons are used to evaluate reliability and validity of analytical data.[2

Question 4 [25 Marks]

a) Briefly define the term Principal Component Analysis. In your description include possible applications of principal component analysis using any example of your choice. You may use diagrams and equations to illustrate your answer. [6]

b) In Principal Component Analysis it is essential that data must be standardized. Give reasons. [2]

c) Five samples were taken for analysis of Cadmium and Lead from a contaminated sample site, see data below:

Samples sites	S1	S2	S3	S4	S5
Variables					
Cd	4	4	5	1.5	2
Pb	1.5	6	2.5	2	8

Calculate:

i) the eigen values and eigen vectors [2]

ii) the loadings and the score factors [2]

Show your working. You may use Unscrambler software on the PC provided to confirm your working.

d) Using the answers from (c) above give a plot of both the loadings and score factors. Briefly discuss the two plots highlighting any observed groupings and correlations. [2]

e) Using the Unscrambler software on the computer provided open the data " GEO " and perform the following tasks excluding the last columns, latitude and longitude in all the analysis below.

i) Using basic univariate statistics determine the dominant variables of the data given. Give justifications for your answer. [1]

ii) Perform a Principal Component Analysis using the default values given below:

Weighting : 1/Sdev.
Validation : Leverage
Centering : Mean Centering
PC's : 10

Show the score, loadings, residual and explained variance plots. [2]

iii) Briefly discuss your findings in your Principal Component Analysis above (e(ii)). In your discussion include comments on samples groups, variable correlations, dominant pollutants and their likely sources, outliers, percentage explained variance and0 any vital observations in your result output. [8]

Question 5 [25 Marks]

a) Briefly define the term Cluster Analysis. In your description include possible applications of principal component analysis using any example of your choice. You may use diagrams and equations to illustrate your answer. [6]

b) Five samples were taken for analysis of Cadmium and Lead from a contaminated sample site, see data below:

Samples sites / Variables	S1	S2	S3	S4	S5
Cd	4	4	5	1.5	2
Pb	1.5	6	2.5	2	8

Calculate the distance matrix. [4]

c) Using the answers from (c) above give a plot of the dendograms for both the samples and variables. [4]

e) Using statistica perform a Cluster Analysis of the data given below.

i) Show sample and variable dendograms [5]

iii) Briefly discuss your findings in your Cluster Analysis above (e(i)). [6]

Code	Si	Al	Fe	Ti	Na	Mg	Ca
A1	53.3	12.4	10.3	1.2	0.3	2.8	13.9
A2	52.8	12.3	10.2	1.2	0.2	2.7	13.8
A3	52.9	12.3	10.2	1.2	0.2	2.7	13.9
B1	69	11.34	9.01	1	0.2	2.8	14.1
B2	57	10.35	8.37	1	0.2	2.5	13.7
B3	61	10.39	8.44	1	0.2	2.6	14
C1	53.3	12.25	10.63	1.2	0.2	2.5	13.6
C2	53.4	12.47	10.69	1.3	0.4	2.5	13.7
C3	53.2	12.18	9.85	1.2	0.2	2.3	13.5
D1	55.3	12.8	10	1.17	0.13	3	14.22
D2	54.7	12.4	9.9	1.17	0.13	2.7	13.92
D3	54.8	12.5	10	1.17	0.13	2.81	13.95
E1	53.9	12.6	9.6	1.4	0.18	3.4	13
E2	54.1	12.8	9.7	1.4	0.19	3.5	13.3
E3	53.8	12.3	9.5	1.3	0.17	3.3	12.9

11. ACID-BASE INDICATORS AT 25°C

Indicator	pH range	pKin	Acid	Base
Thymol blue	1.2 – 2.8	1.6	red	yellow
Methyl yellow	2.9 – 4.0	3.3	red	yellow
Methyl orange	3.1 – 4.4	4.2	red	yellow
Bromocresol green	3.8 – 5.4	4.7	yellow	blue
Methyl red	4.2 – 6.2	5.0	red	yellow
Chlorophenol red	4.8 – 6.4	6.0	yellow	red
Bromothymol blue	6.0 – 7.6	7.1	yellow	blue
Phenol red	6.4 – 8.0	7.4	yellow	red
Cresol purple	7.4 – 9.0	8.3	yellow	purple
Thymol blue	8.0 – 9.6	8.9	yellow	blue
Phenolphthalein	8.0 – 9.8	9.7	colorless	red
Thymolphthalein	9.3 – 10.5	9.9	colorless	blue

14. DATA REJECTION—Q TABLE

n	Q_{90}	n	Q_{90}	n	Q_{90}
3	0.94	6	0.56	9	0.44
4	0.76	7	0.51	10	0.41
5	0.64	8	0.47		

15. Bond Enthalpies

kJ mol^{-1} at 25°C (i.e. Bond Energies)

Single	O	N	C	S	F	Cl
H	463	391	413	368	563	432
C	358	305	346	272	489	328
N	222	163	MISC.		275	192

S—S 251	H—H 436	C=C 615
S—F 327	N≡N 946	C≡C 812
S—Cl 271	N=O 607	C=O 749

19. t TABLE

D.F.	t_{50}	t_{90}	t_{95}
1	1.0	6.3	13
2	0.82	2.9	4.3
3	0.76	2.35	3.2
4	0.74	2.13	2.8
5	0.73	2.02	2.57
6	0.72	1.94	2.45
7	0.71	1.90	2.36
8	0.71	1.86	2.31
9	0.70	1.83	2.26
10	0.70	1.81	2.23
20	0.69	1.72	2.09
30	0.68	1.70	2.04
∞	0.67	1.64	1.96

12. ELECTRODE POTENTIALS, $\mathcal{E}°$

$Na^+ + e \rightleftarrows Na$	– 2.713
$Mg^{++} + 2e \leftrightarrows Mg$	– 2.37
$Al^{+++} + 3e \leftrightarrows Al$	– 1.66
$Zn^{++} + 2e \leftrightarrows Zn$	– 0.763
$Fe^{++} + 2e \leftrightarrows Fe$	– 0.44
$Cd^{++} + 2e \leftrightarrows Cd$	– 0.403
$Cr^{+++} + e \leftrightarrows Cr^{++}$	– 0.38
$Tl^+ + e \rightleftarrows Tl$	– 0.336
$V^{+++} + e \rightleftarrows V^{++}$	– 0.255
$Sn^{++} + 2e \leftrightarrows Sn$	– 0.14
$Pb^{++} + 2e \leftrightarrows Pb$	– 0.126
$2H^+ + 2e \leftrightarrows H_2$	0.000
$S_4O_6^= + 2e \leftrightarrows 2S_2O_3^=$	0.09
$TiO^{++} + 2H^+ + e \leftrightarrows Ti^{+++} + H_2O$	0.10
$S + 2H^+ + 2e \leftrightarrows H_2S$	0.14
$Sn^{+4} + 2e \leftrightarrows Sn^{++}$	0.14
$Cu^{++} + e \leftrightarrows Cu^+$	0.17
$SO_4^= + 4H^+ + 2e \leftrightarrows H_2O + H_2SO_3$	0.17
$AgCl + e \leftrightarrows Cl^- + Ag$	0.222
Saturated calomel	(0.244)
$Hg_2Cl_2 + 2e \leftrightarrows 2Cl^- + 2Hg$	0.268
$Bi^{+++} + 3e \leftrightarrows Bi$	0.293
$UO_2^{++} + 4H^+ + 2e \leftrightarrows U^{+4} + 2H_2O$	0.33
$VO^{++} + 2H^+ + e \leftrightarrows V^{+++} + H_2O$	0.34
$Cu^{++} + 2e \leftrightarrows Cu$	0.34
$Fe(CN)_6^{-3} + e \leftrightarrows Fe(CN)_6^{-4}$	0.355
$Cu^+ + e \leftrightarrows Cu$	0.52
$I_3^- + 2e \rightleftarrows 3I^-$	0.545
$H_3AsO_4 + 2H^+ + 2e \rightleftarrows H_3AsO_3 + H_2O$	0.56
$I_2 + 2e \rightleftarrows 2I^-$	0.621
$2HgCl_2 + 2e \rightleftarrows Hg_2Cl_2 + 2Cl^-$	0.63
$O_2 + 2H^+ + 2e \rightleftarrows H_2O_2$	0.69
Quinone + $2H^+ + 2e \rightleftarrows$ Hydroquinone	0.70
$Fe^{+++} + e \rightleftarrows Fe^{++}$	0.771
$Hg_2^{++} + 2e \rightleftarrows 2Hg$	0.792
$Ag^+ + e \leftrightarrows Ag$	0.799
$Hg^{++} + 2e \leftrightarrows Hg$	0.851
$2Hg^{++} + 2e \leftrightarrows Hg_2^{++}$	0.907
$NO_3^- + 3H^+ + 2e \leftrightarrows HNO_2 + H_2O$	0.94
$HNO_2 + H^+ + e \leftrightarrows NO + H_2O$	0.98
$VO_2^+ + 2H^+ + e \leftrightarrows VO^{++} + H_2O$	0.999
$Br_2 + 2e \leftrightarrows 2Br^-$	1.08
$2IO_3^- + 12H^+ + 10e \leftrightarrows 6H_2O + I_2$	1.19
$O_2 + 4H^+ + 4e \leftrightarrows 2H_2O$	1.229
$MnO_2 + 4H^+ + 2e \leftrightarrows Mn^{++} + 2H_2O$	1.23
$Cr_2O_7^= + 14H^+ + 6e \leftrightarrows 7H_2O + 2Cr^{+++}$	1.33
$Cl_2 + 2e \leftrightarrows 2Cl^-$	1.358
$2BrO_3^- + 12H^+ + 10e \leftrightarrows 6H_2O + Br_2$	1.50
$MnO_4^- + 8H^+ + 5e \leftrightarrows 4H_2O + Mn^{++}$	1.51
$Ce^{+4} + e \leftrightarrows Ce^{+3}$	1.61

13. MEAN ACTIVITY COEFFICIENTS

M	KCl	Na_2SO_4	$ZnSO_4$
0.001	0.965	0.89	0.70
0.01	0.901	0.72	0.39
0.1	0.769	0.45	0.15

16. HEATS OF FORMATION

$\Delta H°$ in kJ mol^{-1} at 25°C
All ions in H_2O solution except as noted
All Elements = 0

H_g	218	H^+	0.0	H_2O_g	–242
O_g	249	Na^+	–240	H_2O_l	–286
C_g	717	Ag^+	106	CO_g	–111
N_g	473	NH_4^+	–133	CO_{2g}	–394
F_g	79	OH^-	–230	NH_{3g}	–46
Cl_g	122	F^-	–333	NO_g	90
Br_g	112	Cl^-	–167	NO_{2g}	33
I_g	107	Br^-	–122	N_2O_{4g}	9
S_g	279	I^-	–55	SO_{2g}	–297
P_g	315	$S^=$	33	SO_{3g}	–396
Na_g	107	$SO_4^=$	–909	H_2S_g	–21
K_g	88	$CO_3^=$	–677	NaF_s	–574
Na^+_g	609	HF_g	–271	$NaCl_s$	–411
K^+_g	514	HCl_g	–92	KF_s	–567
F^-_g	–255	HBr_g	–36	KCl_s	–437
Cl^-_g	–233	HI_g	26	$AgCl_s$	–127
CH_{4g}	–75	HCN_g	135	$AgBr_s$	–100
C_2H_{2g}	227	PH_{3g}	5	PCl_{3g}	–287
C_2H_{4g}	52	C_6H_{6l}	49	PCl_{5g}	–375
		C_2H_{6g}	–85	CH_3OH_l	–238
		C_3H_{8g}	–105	$C_2H_5OH_g$	–235
		nC_4H_{10g}	–127	$C_2H_5OH_l$	–278
		nC_8H_{18g}	–209	$COCl_{2g}$	–219
		CCl_{4l}	–135	CH_3Cl_g	–81

17. ABS. ENTROPY S°

J mol^{-1} K^{-1}, at 25°C

H_{2g}	131	P_{4wh}	164	SF_{6g}	292
N_{2g}	192	HF_g	174	NO_g	211
O_{2g}	205	HCl_g	187	NO_{2g}	240
Cl_{2g}	223	H_2O_g	189	N_2O_{4g}	304
F_{2g}	203	CO_g	198	NH_{3g}	192
C_{gra}	5.7	CO_{2g}	214	PCl_{3g}	312
S_{8r}	254	SO_{2g}	248	PCl_{5g}	365
CH_{4g}	186	SO_{3g}	256	BF_{3g}	254
		C_2H_{6g}	229	CH_3OH_l	127
		C_3H_{8g}	270	$C_2H_5OH_g$	283
		C_2H_{2g}	201	$C_2H_5OH_l$	161
		C_2H_{4g}	219	$(CH_3)_2O_g$	266
		C_6H_{6g}	269	CH_3COOH_g	282

18. $\Delta G°$ FORMATION

kJ mol^{-1} at 25°C

H_g	203	HF_g	–273	H_2O_g	–229
F_g	62	HCl_g	–95	H_2O_l	–237
Cl_g	106	HBr_g	–54	SO_{2g}	–300
O_g	232	HI_g	1.7	SO_{3g}	–371
NO_g	87	NH_{3g}	–16	PCl_{3g}	–268
NO_{2g}	51	CO_g	–137	PCl_{5g}	–305
N_2O_{4g}	98	CO_{2g}	–394	CH_{4g}	–51
C_2H_{4g}	68	C_2H_{2g}	209	C_2H_{6g}	–33
C_6H_{6l}	125	CH_3OH_l	–162		
CCl_{4l}	–65	$C_2H_5OH_l$	–175		
BF_{3g}	–1120	$CHCl_{3g}$	–70		

20. CONC. ACIDS AND B

	M.W.	Density	Wt. %	M
Acetic	60.05	1.05	99.5	
H_2SO_4	98.07	1.83	94	
HF	20.01	1.14	45	
HCl	36.46	1.19	38	
HBr	80.91	1.52	48	
HNO_3	63.01	1.41	69	
$HClO_4$	100.46	1.67	70	
H_3PO_4	98.00	1.69	85	
NaOH	40.00	1.53	50	
NH_3	17.03	0.90	28	

21. DENSITIES (g cm^{-3}

Water at			
0°C	0.9168	Air (70 cm)	0
10°	0.9997	Glass	2
20°	0.9982	Na_2CO_3	2
22°	0.9978	NaCl	2
24°	0.9973	$BaSO_4$	4
26°	0.9968	AgCl	5
28°	0.9963	Aluminum	2
30°	0.9956	Iron	7
90°	0.9653	Brass	8
100°g	0.0006	Mercury	13
		Platinum	21

22. MOBILITIES ($m^2V^{-1}s^{-1}$ ×

Li^+	39	H_3O^+	350	$\frac{1}{2}Ba^{++}$
Na^+	50	NH_4^+	73	$\frac{1}{3}La^{+3}$
K^+	74	Ag^+	62	$\frac{1}{2}SO_4$
Cl^-	76	OH^-	198	$\frac{1}{3}PO_4$
Br^-	78	I^-	77	NO_3^-

23. WATER V.P. (torr)

0°C	4.6	25°
15°	12.8	30°
20°	17.5	50°

24. MISCELLANEOUS

Std. dev. = $\sqrt{\Sigma (X_i - \bar{X})^2/(n-1)}$

Conf. limits = $\bar{X} \pm ts/\sqrt{n}$

$E = E° - (0.0592/n)\log([Red]/[Ox])$

$\log I_o/I_t = abc = A = \log 1/T$

$\log N_T = \log N_o - 0.301T/T_{\frac{1}{2}}$

$x = (-b \pm \sqrt{b^2 - 4ac})/2a$

$n\lambda = 2d \sin \theta$

$2.303 \log_{10} a = \log_e a$

$h = 6.626 \times 10^{-34}$ J s

$e = 1.602 \times 10^{-19}$ C

$N_A = 6.022 \times 10^{23}$ mol^{-1}

F = 96487 C

g = 9.807 m s^{-2}

$c = 2.998 \times 10^8$ m s^{-1}

1 amu = 1.661×10^{-27} kg

R = 1.987 cals mol^{-1} K^{-1}

= 0.08206 litre atm mol^{-1} K^{-1}

= 8.314 J mol^{-1} K^{-1}

= 8.314 kPa dm^3 mol^{-1} K^{-1}

0 °C = 273.15 K

1 eV = 1.602×10^{-19} J

$k = 1.381 \times 10^{-23}$ JK^{-1}

		Rb	Sr	Y	Zr	Nb	U	K	Ca	Ti	V
		1	2	3	4	5	6	7	8	9	10
W=2	1	58.000	248.000	22.000	412.000	6.000	6.300	1.390	3.050	0.352	30.000
W=2	2	91.000	212.000	20.000	236.000	10.000	9.850	1.430	3.320	0.433	44.000
W=14	3	57.000	225.000	31.000	308.000	10.000	8.260	1.340	3.760	0.484	0.000
W=42	4	64.000	231.000	19.000	266.000	9.000	10.700	1.350	4.390	0.358	30.000
W=14	5	85.000	219.000	31.000	294.000	14.000	111.000	1.620	2.540	0.352	15.000
W=26	6	61.000	212.000	26.000	331.000	13.000	5.430	1.410	3.400	0.799	135.000
W=1	7	71.000	245.000	19.000	351.000	9.000	16.600	1.580	2.520	0.277	17.000
W=0	8	109.000	255.000	28.000	424.000	10.000	21.000	1.620	2.940	0.357	0.000
W=0	9	111.000	240.000	21.000	297.000	11.000	44.100	1.800	2.450	0.380	9.000
W=1	10	228.000	193.000	36.000	292.000	19.000	12.400	2.750	2.240	0.327	0.000
W=0	11	169.000	215.000	28.000	323.000	12.000	22.500	2.560	2.430	0.313	9.000
W=15	12	53.000	259.000	14.000	216.000	6.000	2.530	1.440	3.400	0.302	47.000
W=14	13	98.000	220.000	16.000	201.000	11.000	11.500	1.150	3.700	0.357	25.000
W=12	14	133.000	98.000	19.000	165.000	14.000	6.510	2.040	1.900	0.554	26.000
W=0	15	135.000	214.000	17.000	271.000	10.000	14.400	2.100	2.550	0.315	17.000
W=0	16	81.000	176.000	31.000	399.000	10.000	12.600	1.360	3.530	0.400	47.000
W=0	17	144.000	223.000	21.000	341.000	11.000	8.330	1.590	2.340	0.389	2.000
W=0	18	245.000	120.000	31.000	362.000	13.000	6.590	2.950	1.740	0.246	4.000
W=2	19	63.000	163.000	18.000	251.000	5.000	16.000	0.920	3.290	0.335	0.000
W=2	20	84.000	169.000	17.000	180.000	15.000	19.600	1.320	2.720	0.457	89.000
W=2	21	85.000	204.000	19.000	250.000	8.000	12.200	1.380	3.350	0.381	0.000
W=14	22	141.000	182.000	37.000	290.000	23.000	268.000	1.460	2.390	0.370	24.000
W=0	23	55.000	249.000	28.000	363.000	9.000	2.800	1.260	3.520	0.466	50.000
263127	24	282.000	143.000	33.000	203.000	17.000	29.600	3.330	1.910	0.276	0.000
263129	25	315.000	133.000	26.000	202.000	23.000	15.300	2.960	2.170	0.466	7.000
263152	26	60.000	256.000	16.000	272.000	5.000	5.900	1.550	2.400	0.294	0.000
263154	27	67.000	211.000	22.000	269.000	6.000	9.240	1.210	2.690	0.337	22.000
263156	28	71.000	200.000	27.000	317.000	13.000	15.500	1.150	3.320	0.440	80.000
263162	29	73.000	199.000	16.000	242.000	9.000	22.900	1.470	3.130	0.319	0.000
263166	30	75.000	193.000	18.000	222.000	7.000	12.100	1.270	3.250	0.383	52.000
263168	31	79.000	201.000	46.000	313.000	12.000	10.900	1.460	4.310	0.541	12.000
263170	32	95.000	179.000	43.000	266.000	13.000	21.500	1.420	4.120	0.581	49.000
263174	33	25.000	206.000	21.000	173.000	7.000	8.740	0.850	4.550	0.478	42.000
263180	34	49.000	188.000	50.000	273.000	14.000	12.700	0.920	3.460	0.536	65.000
263192	35	86.000	258.000	17.000	351.000	9.000	13.000	1.910	2.480	0.329	56.000
263200	36	115.000	229.000	25.000	275.000	11.000	50.900	1.460	2.500	0.350	0.000
263230	37	82.000	301.000	18.000	309.000	7.000	2.410	1.980	2.770	0.328	46.000
263236	38	77.000	310.000	24.000	323.000	7.000	1.630	1.900	3.160	0.274	38.000
263240	39	263.000	162.000	30.000	328.000	19.000	5.570	3.400	1.730	0.320	24.000
263248	40	69.000	275.000	19.000	350.000	8.000	12.500	1.750	2.640	0.266	28.000
263274	41	61.000	275.000	19.000	440.000	9.000	4.010	1.520	3.030	0.378	72.000
263276	42	63.000	251.000	10.000	262.000	6.000	4.290	1.470	2.440	0.298	0.000
263278	43	79.000	226.000	24.000	180.000	9.000	6.860	1.120	5.550	0.312	0.000
263282	44	94.000	210.000	18.000	212.000	11.000	8.110	1.550	3.890	0.374	0.000
263284	45	65.000	218.000	17.000	200.000	5.000	13.200	1.380	3.310	0.313	10.000
263290	46	44.000	163.000	10.000	166.000	8.000	7.770	0.880	2.520	0.376	2.000
263292	47	39.000	250.000	14.000	295.000	6.000	3.930	0.930	3.050	0.335	25.000
263320	48	83.000	247.000	18.000	247.000	9.000	29.500	1.350	2.600	0.345	6.000
263322	49	119.000	220.000	19.000	200.000	11.000	10.500	1.640	4.010	0.364	0.000
263324	50	85.000	232.000	19.000	269.000	10.000	30.400	1.100	3.120	0.280	0.000
263326	51	118.000	215.000	14.000	218.000	13.000	17.300	1.280	3.540	0.385	69.000
263330	52	150.000	193.000	22.000	134.000	11.000	38.500	1.890	2.790	0.263	0.000
263332	53	91.000	232.000	20.000	244.000	8.000	13.100	1.220	3.810	0.389	61.000
263334	54	52.000	210.000	22.000	295.000	7.000	28.200	1.140	3.040	0.284	0.000

		Cr	Mn	Fe	Ni	Cu	Zr	Ga	heelite gr	ATITUD	ONGI
		11	12	13	14	15	16	17	18	19	20
W=2	1	120.000	515.000	3.090	134.000	21.000	58.000	14.000	2.000		
W=2	2	405.000	696.000	4.190	239.000	44.000	104.000	19.000	2.000		
W=14	3	178.000	680.000	4.390	94.000	76.000	76.000	14.000	14.000		
W=42	4	169.000	692.000	4.460	174.000	151.000	76.000	14.000	42.000		
W=14	5	5.000	419.000	2.760	32.000	26.000	73.000	17.000	14.000		
W=26	6	9.000	664.000	4.160	72.000	56.000	82.000	16.000	26.000		
W=1	7	0.000	380.000	2.330	51.000	21.000	44.000	14.000	1.000		
W=0	8	156.000	574.000	3.250	112.000	51.000	65.000	14.000	0.000		
W=0	9	117.000	566.000	3.110	125.000	69.000	83.000	15.000	0.000		
W=1	10	0.000	434.000	2.620	38.000	36.000	63.000	19.000	1.000		
W=0	11	0.000	481.000	2.930	56.000	43.000	67.000	21.000	0.000		
W=15	12	265.000	533.000	3.160	177.000	26.000	49.000	17.000	15.000		
W=14	13	27.000	609.000	3.810	41.000	53.000	69.000	18.000	14.000		
W=12	14	318.000	657.000	5.200	105.000	84.000	100.000	19.000	12.000		
W=0	15	133.000	492.000	3.290	113.000	32.000	71.000	16.000	0.000		
W=0	16	517.000	819.000	4.930	214.000	60.000	91.000	24.000	0.000		
W=0	17	89.000	578.000	3.390	117.000	21.000	73.000	16.000	0.000		
W=0	18	0.000	307.000	1.680	33.000	9.000	40.000	25.000	0.000		
W=2	19	754.000	802.000	4.830	283.000	44.000	87.000	17.000	2.000		
W=2	20	689.000	768.000	4.920	332.000	72.000	166.000	21.000	2.000		
W=2	21	395.000	798.000	4.280	176.000	69.000	88.000	20.000	2.000		
W=14	22	0.000	517.000	2.900	47.000	36.000	97.000	19.000	14.000		
W=0	23	108.000	599.000	3.730	84.000	26.000	57.000	17.000	0.000		
263127	24	0.000	346.000	2.270	46.000	16.000	59.000	21.000		64.513	–50.6
263129	25	186.000	694.000	4.520	127.000	99.000	105.000	23.000		64.525	–50.7
263152	26	10.000	352.000	2.540	64.000	14.000	52.000	12.000		64.295	–51.4
263154	27	293.000	548.000	3.670	159.000	27.000	74.000	13.000		64.295	–51.4
263156	28	639.000	797.000	5.000	288.000	51.000	123.000	16.000		64.294	–51.4
263162	29	420.000	650.000	3.780	196.000	41.000	63.000	13.000		64.293	–51.4
263166	30	377.000	587.000	3.580	163.000	39.000	57.000	15.000		64.290	–51.4
263168	31	194.000	912.000	4.930	134.000	76.000	87.000	19.000		64.290	–51.4
263170	32	141.000	869.000	5.230	122.000	74.000	101.000	21.000		64.289	–51.4
263174	33	73.000	832.000	4.760	108.000	135.000	55.000	16.000		64.281	–51.4
263180	34	0.000	562.000	4.290	71.000	127.000	103.000	14.000		64.271	–51.4
263192	35	0.000	403.000	2.360	48.000	28.000	42.000	16.000		64.299	–51.1
263200	36	51.000	609.000	3.180	120.000	71.000	83.000	14.000		64.311	–51.2
263230	37	0.000	405.000	2.590	47.000	14.000	49.000	15.000		64.492	–50.8
263236	38	32.000	379.000	2.230	37.000	16.000	35.000	18.000		64.496	–49.8
263240	39	0.000	273.000	1.660	11.000	2.000	43.000	19.000		64.540	–50.7
263248	40	0.000	381.000	2.370	24.000	9.000	47.000	15.000		64.570	–50.6
263274	41	14.000	403.000	2.460	47.000	11.000	52.000	15.000		64.572	–50.4
263276	42	0.000	361.000	2.740	50.000	17.000	56.000	12.000		64.572	–50.4
263278	43	0.000	508.000	3.520	60.000	33.000	49.000	19.000		64.770	–50.7
263282	44	68.000	565.000	3.630	87.000	47.000	62.000	22.000		64.763	–50.6
263284	45	0.000	418.000	2.920	80.000	22.000	49.000	15.000		64.749	–50.6
263290	46	0.000	373.000	3.200	57.000	29.000	38.000	12.000		64.728	–50.7
263292	47	208.000	528.000	3.240	218.000	17.000	56.000	16.000		64.330	–51.3
263320	48	78.000	521.000	3.340	113.000	57.000	79.000	16.000		64.360	–51.1
263322	49	99.000	642.000	4.080	65.000	52.000	77.000	23.000		64.368	–51.1
263324	50	5.000	429.000	3.200	35.000	28.000	54.000	10.000		64.368	–51.1
263326	51	0.000	584.000	4.120	31.000	46.000	76.000	16.000		64.367	–51.1
263330	52	3.000	685.000	3.760	60.000	66.000	94.000	16.000		64.365	–51.1
263332	53	0.000	568.000	3.880	40.000	39.000	57.000	17.000		64.366	–51.1
263334	54	0.000	361.000	2.650	28.000	20.000	50.000	11.000		64.371	–51.1

		Rb	Sr	Y	Zr	Nb	U	K	Ca	Ti	V
		1	2	3	4	5	6	7	8	9	10
263338	55	155.000	150.000	26.000	194.000	9.000	40.900	1.900	2.220	0.468	82.000
263348	56	87.000	293.000	16.000	213.000	6.000	35.200	1.610	2.570	0.331	22.000
263350	57	53.000	177.000	43.000	272.000	9.000	52.800	1.210	2.270	0.322	21.000
263358	58	152.000	222.000	22.000	360.000	15.000	40.800	1.540	2.330	0.313	0.000
263376	59	130.000	198.000	20.000	349.000	7.000	5.850	1.870	2.740	0.244	0.000
263378	60	160.000	149.000	21.000	332.000	15.000	43.600	1.890	2.080	0.279	0.000
263384	61	99.000	155.000	32.000	331.000	7.000	2.770	1.520	4.000	0.426	91.000
306345	62	52.000	255.000	13.000	245.000	7.000	7.900	1.130	3.330	0.383	43.000
306347	63	38.000	224.000	13.000	317.000	9.000	4.300	1.060	2.880	0.418	54.000
306348	64	50.000	239.000	9.000	246.000	7.000	7.900	0.970	2.850	0.360	0.000
306349	65	76.000	250.000	19.000	296.000	4.000	3.300	1.490	3.220	0.429	9.000
306351	66	125.000	265.000	19.000	344.000	9.000	3.600	1.980	2.640	0.296	2.000
306353	67	81.000	237.000	19.000	310.000	10.000	7.700	1.550	2.750	0.299	16.000
306355	68	55.000	226.000	23.000	209.000	4.000	24.600	1.110	2.320	0.295	0.000
306356	69	66.000	220.000	29.000	220.000	1.000	34.600	1.500	2.270	0.334	0.000
306360	70	50.000	182.000	39.000	219.000	1.000	67.600	0.750	2.180	0.256	0.000
306362	71	81.000	265.000	16.000	241.000	2.000	3.100	1.950	2.740	0.299	0.000
306363	72	64.000	243.000	17.000	309.000	5.000	14.500	1.390	2.420	0.211	0.000
306366	73	39.000	221.000	15.000	257.000	4.000	6.600	1.160	2.540	0.218	0.000
306367	74	67.000	226.000	42.000	342.000	8.000	8.400	1.560	2.780	0.327	0.000

		Cr	Mn	Fe	Ni	Cu	Zr	Ga	heelite gr	ATITUD	ONGIT
		11	12	13	14	15	16	17	18	19	20
263338	55	252.000	777.000	5.040	166.000	122.000	138.000	16.000		64.434	–51.08
263348	56	12.000	512.000	3.410	60.000	81.000	82.000	15.000		64.497	–50.48
263350	57	0.000	603.000	2.920	33.000	43.000	58.000	9.000		64.489	–50.06
263358	58	0.000	570.000	3.160	71.000	53.000	75.000	14.000		64.254	–51.22
263376	59	85.000	418.000	2.540	83.000	6.000	43.000	15.000		64.121	–51.24
263378	60	0.000	405.000	2.460	54.000	12.000	56.000	17.000		64.131	–51.08
263384	61	433.000	817.000	5.120	160.000	90.000	86.000	22.000		64.180	–51.49
306345	62	32.000	629.000	3.550	76.000	170.000	67.000	14.000		64.276	–51.43
306347	63	30.000	405.000	2.920	86.000	35.000	41.000	9.000		64.364	–51.36
306348	64	44.000	444.000	3.170	86.000	32.000	45.000	13.000		64.362	–51.36
306349	65	55.000	583.000	3.520	79.000	32.000	57.000	12.000		64.362	–51.32
306351	66	0.000	399.000	2.570	55.000	22.000	41.000	12.000		64.605	–49.87
306353	67	0.000	392.000	2.590	41.000	21.000	40.000	11.000		64.618	–49.87
306355	68	0.000	317.000	2.650	21.000	9.000	39.000	10.000		64.618	–49.83
306356	69	0.000	574.000	3.120	26.000	20.000	48.000	11.000		64.618	–49.83
306360	70	0.000	910.000	2.720	29.000	28.000	64.000	5.000		64.645	–50.47
306362	71	0.000	459.000	2.480	35.000	17.000	45.000	13.000		64.656	–50.50
306363	72	2.000	380.000	2.640	23.000	19.000	56.000	11.000		64.659	–50.55
306366	73	0.000	629.000	2.240	30.000	10.000	49.000	7.000		64.636	–50.49
306367	74	66.000	470.000	3.050	77.000	33.000	79.000	14.000		64.638	–50.48