

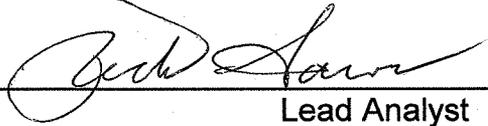
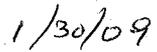
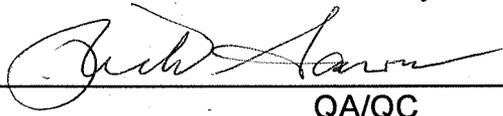
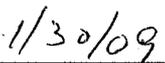
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Standard Operating Procedure XR-005.01

KEVEX SPECTROMETER DATA GENERATION, INTERPRETATION AND REPORTING CHESTER LABNET PROPRIETARY METHOD

Approvals:

 _____ Author	 _____ Date
 _____ Lead Analyst	 _____ Date
 _____ QA/QC	 _____ Date

Effective from: 1-30-09
Effective until: present

KEVEX SPECTROMETER DATA GENERATION, INTERPRETATION AND REPORTING CHESTER LABNET PROPRIETARY METHOD

1.0 Introduction

1.1 Test Method Reference ID: Chester LabNet Proprietary method

1.2 Applicability: This method is applicable to data generated by the Kevex Model Delta 770 energy dispersive XRF (EDXRF).

1.3 Detection Limit: N/A

1.4 Method Performance: N/A

2.0 Summary

2.1 Scope and Application: This method is applicable to data generated by the Kevex Model Delta 770 energy dispersive XRF (EDXRF). Chester LabNet currently operates two of these instruments, informally named "770" and "772". The process by which data is processed from each of these machines is essentially identical. This SOP *should never* be performed by anyone lacking extensive XRF data processing and interpretation skills.

2.2 Summary of Method: Once analysis is complete, data is transferred to a data processing computer, where it is processed from raw counts to final concentrations. During this process, the data is checked for spectral interferences and corrected for interelement interferences as well as size attenuation and other affects. The final processed data is then transferred to the LIMS.

2.3 Interferences: N/A.

2.4 Sample collection/preservation/shipment/storage: N/A

3.0 Safety

3.1 This method poses no risks beyond those normally associated with computer usage.

4.0 Pollution Prevention and Waste Management

4.1 No chemicals are utilized in this method.

5.0 Apparati, Equipment and Supplies

5.1 Data processing computer loaded with Windows compatible operating system, Microsoft excel and Chester LabNet's proprietary data processing spreadsheets.

5.2 Flash drive(s)

6.0 Reagents and Standards

6.1 N/A

7.0 Preparation, Calibration and Standardization

7.1 Samples should be analyzed as per SOP XR-002.

8.0 Procedure

8.1 Transfer the spectral files:

8.1.1 From the 770 and 772 data collection computer, copy all spectral files associated with the analytical run onto the proper subdirectory on the data processing computer using the Ethernet. Spectral files take the form of *.sp* files.

8.2 Process the QS data.

8.2.1 Open the QS processing workbook in Excel to process the QS data.

8.2.2 Enter the QS (Quality Standard) ID to be processed in the cell labeled "QGSNIST".

- 8.2.3 click 'Start'.
- 8.2.4 After processing is complete, verify that the QS data has passed QC by checking the data in the QS tab of the worksheet. Print out the QS data sheet and keep it with the XRF request form for that particular analysis.
- 8.2.5 Enter the date of analysis and the normalized gross counts per second for each element in each excitation condition, XRF run number, Analysis protocol, and number of samples analyzed into the proper '770QS' or '772QS' archive file in Excel.

8.3 Process Sample Data.

- 8.3.1 Open the appropriate LabNet XRF Data Processing workbook in Excel and select the 'IDs' worksheet. Also open a blank report workbook and rename it as ANNN-XXX where:

- A = the client letter prefix
- NNN = the client number, and
- XXX = the run number

Save this file as .XLS

- 8.3.2 In the LabNet XRF Data Processing workbook, return to the 'IDs' worksheet.
- 8.3.3 In the 'IDs' worksheet, enter the following demographics for each sample, as expressed on the XRF runsheet: File name, LIMS ID, Particle Size, deposit mass, deposit area.
- 8.3.4 After all demographics have been entered, highlight and copy them to the 'SAMPLE LOG' worksheet in the workbook created in section 8.3.1..
- 8.3.5 Return to the 'IDs' worksheet in the Processing workbook and left click on the *Start* button..

- 8.3.6 When the calculations have been completed, the program will move to the 'LIMS(2)' window. At this point the peaks have been integrated and corrected for spectral overlap interference as described in section 10.1.
- 8.3.7 The particle size corrections have been made for Al, Na, Mg and Si as described in section 10.3.
- 8.3.8 The net uncertainty for each final concentration has been determined as described in section 10.4.
- 8.3.9 Create a report file:
- 8.3.9.1 Select the proper LIMS format worksheet within the processing workbook (XRF, RTI, Precise, etc). Highlight the data, along with the header, and copy to the "LIMS" worksheet in the report workbook created in 8.3.1. This worksheet will automatically calculate the best candidates for the replicate sample analysis. The number of analytes which are both greater than 3x their uncertainty and greater than the mean value for each analyte in the group of samples analyzed will be displayed in a column at the far right-hand side of the file. Once the replicate sample has been chosen, perform the analysis using the next lesser analysis protocol.
 - 8.3.9.2 Amend the "SAMPLE LOG" worksheet in the report workbook with the replicate ID (normally the original sample ID with an "R" prefix) and the proper demographics. If the replicate is run on a different instrument, use the prefix "X" and the original sample ID. Once the replicate analysis has been performed, the processing can commence by copying the updated demographics to the ID worksheet in a newly opened processing workbook, and pressing "START" as in 8.3.5.
 - 8.3.9.3 When the processing is completed, go to the "result (2)" worksheet. This file contains the raw data as well as corrected concentrations for each excitation condition for each sample. Execute the following commands: "edit" "move or copy sheet..." "create a copy" "to book (new book)" "ok".

This creates a copy of the raw data in the proper format for printing on the line printer. Save this file under the same filename given the report workbook as a space delimited file (ANNN-XXX.prn).

8.3.9.4 Move the prn file to the report workbook using the following commands: "edit" "move or copy sheet..." "to book (ANNN-XXX.xls)". In the report workbook, scroll down the replicate sample analysis printout to the "Corrected Conc." Section. Highlight the area starting one row above the "Lab ID" header, down through the uncertainty for the last analyte in the "Corrected Conc." Column. Copy the highlighted portion to the "Replicate" worksheet in the report workbook and use "paste values" command in cell "A1".

8.3.9.5 Return to the worksheet with the raw data and scroll up to the "Corrected Conc." Section of the original analysis, then highlight and copy the data to the "Original" worksheet as described in 8.3.9.4.

8.3.9.6 Proceed to the "report" worksheet within the report workbook. The replicated report will appear, ready to print. Create a printout of the replicate report on the Laser Jet printer.

8.3.9.7 The report file can now be saved and closed. The raw data is then printed out on the lineprinter from the "Command Prompt" program using the command "p ANNN-XXX.prn" from the subdirectory in which the .prn file was saved.

8.3.9.8 All printouts are kept with the XRF run sheet prior to inspection, QA, and LIMS entry.

8.4 At this point, the processed data is checked for anomalies and corrections made in the 'LIMS' worksheet of the run file. Some anomalies include:

8.4.1 Over-subtraction of very intense peaks. Peaks that exceed 10000x the background counts can become over-corrected for background counts as the background subtraction channels begin to 'ride' up the sides of the analyte peak.

8.4.2 'False positives' for analytes in the 'noisier' background regions of the spectra; most notably Rh through La in the high energy (55 kV) excitation condition, and Y through Mo in the 35 kV direct excitation condition.

8.4.3 *Only a qualified XRF spectroscopist should critique the XRF spectra. Data corrections are made in red ink on the XRF printout. The data is then amended with the corrections.*

8.5 Once the data file has been amended and saved, transfer the data to the LIMS.

8.5.1 When all data changes and corrections have been made and saved in the replicate workbook, save a copy of the LIMS data for importing into the LIMS.

8.5.1.1 Go to the LIMS worksheet in the run file workbook.

8.5.1.2 Select all Sample IDs, concentrations and uncertainties and copy to a new workbook. Do not select the header row (Row 1).

8.5.1.3 Save this new workbook as *****.csv** (comma delimited) file onto the worklist directory, where ******* is the worklist name, which indicates the species to be transferred to the LIMS.

8.5.2 Access the LIMS by clicking on the LIMS icon. The mouse is inoperable in the LIMS program.

8.5.3 From the LIMS main menu choose option 3 (Worklist Management), then choose 1 (Create/Fill/Distribute). Note: striking the 'Enter' key must follow all commands.

8.5.4 The program will then ask for the analyst's number. Each analyst has a unique number that identifies the person entering data into the LIMS. Enter your analyst number.

8.5.5 Next type 'i' (for Instrument), then 'i' (for Import), then 'n' (for New).

- 8.5.6 The program will then ask for the 'worklist format name:', type appropriate worklist name (see step 7.8.1.3), usually 'xrf', and press 'Enter'.
- 8.5.7 The program will then ask for 'status report to:', type 's' (for **S**creen) and press 'Enter'.
- 8.5.8 The program then asks 'continue or quit:', type 'c' and press 'Enter'.
- 8.5.9 The program will then display a screen asking the analyst to enter the analyst's number, date of analysis, time of analysis, and instrument (770, 771, 772). After entering the instrument ID, check the entries for errors, then press 'Enter'.
- 8.5.10 The program then displays the first sample ID as well as the analytes, concentrations, and uncertainties.
- 8.5.11 Proofread the data:
- 8.5.11.1 Check to be sure that all of the changes made in section 8.4 coincide with the data on the screen.
 - 8.5.11.2 It is possible to scroll from sample to sample by using the 'Page Up' and 'Page Down' keys.
 - 8.5.11.3 If any corrections were missed, they may be entered at this time in the LIMS program.
- 8.5.12 Once all of the corrections have been confirmed, press the 'Home' key, type 's' to save, and 'y' for yes.
- 8.5.13 The worklist may now be distributed from the 'Worklist Management' screen: type 'd' (for **D**istribute), enter the worklist number (usually the default value on screen), enter the destination (usually the default value on screen), and then type 'c' (for **C**omplete).

8.5.14 Once the worklist has been distributed, the analyst may then exit the LIMS program.

8.6 Archive raw data:

8.6.1 Hardcopy data is archived by client name, project number, and analysis date. In each file the following documents are kept: run sheets, QS reports, replicate reports and the XRF data printouts. These files are held for three years prior to disposal, unless otherwise requested.

8.6.2 Electronic data is archived on the C drive of the data processing computer and on a flash drive. Each instrument has an associated subdirectory for archived data. The data files are moved into a subdirectory and named after the report number. The files are copied onto a CD on a routine basis for archiving.

9.0 QA/QC

9.1.1 N/A

10.0 Calculations

10.1 Peaks are integrated and corrected for spectral overlap interference in the following sequence:

$G_{i,j}$ = the sum of all counts in the FWHM window for element i in excitation condition j (gross counts)

$$B_{i,j} = n_{i,j} (mx + b) = \text{the background counts}$$

where: $n_{i,j}$ = the number of channels in the FWHM window for element i in excitation condition j .

x = the channel number of the centroid of the FWHM window for element i in excitation condition j .

$$m = \text{the slope of the background} = (\Sigma_h - \Sigma_l) / (C_h - C_l)$$

where: Σ_h = the sum of the counts in the HEB window for element i in excitation condition j (see figure 1).

Σ_l = the sum of the counts in the LEB window for element i in excitation condition j .

C_h = the centroid for the HEB window for element i in excitation condition j .

C_l = the centroid for the LEB window for element i in excitation condition j .

b = the y-intercept of the background = $\Sigma_n - (m C_n)$

$$N_{i,j} = G_{i,j} - B_{i,j}$$

where: $N_{i,j}$ = net counts in the FWHM window for element i in excitation condition j .

$$N_{c,i,j} = N_{i,j} - \Sigma(L_{n,i,j} N_j)$$

where: $N_{c,i,j}$ = the interference corrected net counts for element i in excitation condition j .

$L_{n,i,j}$ = the normalized interference correction factor for element i from element j .

N_j = the net counts for interfering element j .

$$L_{n,i,j} = L_{i,j} [(t_i C_i) / (t_j C_j)]$$

where: $L_{i,j}$ = the interference correction factor for element i from element j .
 t_i = the counting lifetime for the excitation condition in which element i was analyzed.

C_i = the current (mA) used for the excitation condition in which element i was analyzed.

t_j = the counting lifetime for the excitation condition in which the interfering element j was analyzed.

C_j = the current (mA) used for the excitation condition in which the interfering element j was analyzed.

$$C = (N_{c,i,j} F_n C_i) / t$$

where: C = the empirical concentration ($\mu\text{g}/\text{cm}^2$)

F_n = the normalized calibration factor [$(\mu\text{g}/\text{cm}^2) / (\text{cts}/\text{sec})$]

t = the counting lifetime (sec)

10.2 The absorption corrected concentration is calculated using the mass absorption coefficients:

$$C_a = C / A$$

where: C_a = the absorption corrected concentration ($\mu\text{g}/\text{cm}^2$)

C = the empirical concentration ($\mu\text{g}/\text{cm}^2$)

A = the absorption correction factor

The absorption correction algorithm is iterative and begins its corrections with C_a . All detected analytes are divided by the area density of the deposit ($\mu\text{g}/\text{cm}^2$) to determine their mass fractions. The carbon mass fraction (mf_c) is then estimated:

$$mf_c = (1 - (\Sigma mf_i + \Sigma mf_{i0})) / 1.3$$

where: mf_i = the mass fraction of element i

mf_{i0} = the mass fraction of oxygen related to element i

The oxygen mass fraction (mf_o) is then estimated:

$$mf_o = 1 - (\Sigma mf_i + mf_c)$$

The absorption correction algorithm then takes the corrected Ca concentration into account as it sequentially moves to correct K, then Cl...to Na

10.3 The particle size corrections for Na, Mg, Al, Si are determined as follows:

$$C_{a,s} = C_a / A_p$$

where: $C_{a,s}$ = the size and absorption corrected concentration ($\mu\text{g}/\text{cm}^2$)
 A_p = size correction factor

10.4 The net uncertainty for each final concentration is determined as follows:

$$\delta_{\text{conc}} = (\delta_{\text{net}} F_n) / t$$

where: δ_{conc} = the net concentration uncertainty ($\mu\text{g}/\text{cm}^2$)
 F_n = the normalized calibration factor (Section 6.4.4)
 t = counting lifetime

$$\delta_{\text{net}} = (\delta_c^2 + \delta_l^2 + \delta_s^2 + \delta_a^2)^{1/2}$$

where: δ_{net} = the net uncertainty (counts)

$$\delta_c = (G+B)^{1/2}$$

where: δ_c = is the counting uncertainty expressed as a function of the uncorrected net counts

G = the gross counts in the FWHM window

B = the background counts in the FWHM window

$$\delta_l = \sum (\delta_{c,j} L_{n,j})$$

where: δ_l = is the spectral overlap uncertainty (counts)

$\delta_{c,j}$ = the counting uncertainty for each interfering element j.

$L_{n,j}$ = the normalized spectral overlap correction factor for each interfering element j (step 6.4.7)

$$\delta_s = 0.05 N_c$$

where: δ_s = the calibration uncertainty which is assumed to be 5% as per manufacturer's specification.

N_c = net counts corrected for spectral overlap

$$\delta_a = (\delta_c^2 + \delta_l^2 + \delta_s^2)^{1/2} / (A^2 A_p^2)$$

where: δ_a = the absorption correction uncertainty (counts)

A = the absorption correction factor (steps 6.5.1 through 6.5.4)

A_p = the size correction factor

11.0 References

- 11.1 Kevex Operator's Manual
- 11.2 Practical X-Ray Spectrometry, R. Jenkins and J.L. De Vries, second edition, Philips Technical Library, Springer-Verlag New York Inc.
- 11.3 X-Ray Fluorescence Analysis of Environmental Samples, Jaklevic, et al, Ed. by T.G. Dzubay, Ann Arbor Sci.
- 11.4 Self Absorption Corrections for X-Ray Fluorescence Analysis of Aerosols, T.G. Dzubay and R.O. Nelson, in Advances in X-Ray Analysis, Vol 18, 619-631.
- 11.5 Quantitative Analysis of Aluminum and Silicon in Air Particulate Deposits on Teflon Membrane Filters by X-Ray Fluorescence Analysis, J.A. Cooper, L.M. Valdovinos, J.R. Sherman, W.L. Pollard, R.H. Sarver, and J.K. Weider, report by NEA, Inc., Beaverton, OR, July 15, 1987.
- 11.6 Round Robin Evaluation: Elemental Analysis of Bulk Samples and PM₁₀ Loaded Teflon Filters, presented at the 82nd Annual Meeting of AWMA, Anaheim, CA, June 24-30, 1989.

12.0 Definitions

- 12.1 Analyst: the designated individual who performs the "hands-on" method and who is the one responsible for applying required laboratory practices and other pertinent quality controls to meet the required level of quality.
- 12.2 Analysts' Notes: Non-essential aspects of a method, which may help the analyst during some phase of the method. Notes may include, but not be limited to, historical aspects of the method, "tricks" of the method, unexpected issues to be aware of, or other facts or opinions related to the method, but not directly part of the procedure.
- 12.3 Batch: environmental samples that are prepared and/or analyzed together with the same process and personnel, using the same lot(s) of reagents.
 - 12.3.1 Analytical Batch: a group of prepared samples (extracts/digests etc) that are analyzed together as a group, although they may have been prepared separately.
 - 12.3.2 Preparation Batch: a group of one to 20 samples of the same matrix which are prepared together as a group, and which share common QC samples.

12.4 Calculations (Data Reduction): the mathematical process of transforming raw data into a more useable form.

12.5 Laboratory Information Management System (LIMS): a comprehensive computerized database system that a laboratory uses for sample tracking and data management, from sample receipt to reporting and archiving.

12.6 Matrix/Matrices: the component or substrate that contains the analyte of interest. In this case, the matrix should consist of a bicarbonate impregnated cellulose filter.

12.7 QA/QC: Quality Assurance/Quality Control. A series of samples or metrics designed to show precision, accuracy and bias of the procedure are within acceptable limits.

12.8 QC Statistic: any of a number of statistical permutations performed on raw data to generate a metric capable of being subjected to control limits and corrective actions.

12.9 Reagent: a single chemical or combination of chemicals or a chemical solution used in the preparation or analysis of samples.

13.0 Analysts' Notes

13.1 N/A

SP0	LEB				Analyte				HEB				Avg Counts				Calibration	
	L	H	C	#	L	H	C	#	L	H	C	#	LEB	HEB	m	b	Factors	
Na	91	93	92	3	95	110	102.5	16	114	116	115	3	69.3	61.0	-0.3623	102.6667	0.04273	0.03205
Mg	114	116	115	3	118	133	125.5	16	133	134	133.5	2	61.0	67.0	0.3243	23.7027	0.01930	0.01447
Al	137	139	138	3	142	157	149.5	16	158	160	159	3	47.7	60.0	0.5873	-33.3810	0.00932	0.00699
Si	158	160	159	3	167	182	174.5	16	188	191	189.5	4	60.0	79.5	0.6393	-41.6557	0.00516	0.00387
P	191	192	191.5	2	193	209	201.0	17	210	211	210.5	2	78.0	98.5	1.0789	-128.6184	0.00336	0.00252
S	199	201	200	3	223	239	231.0	17	249	251	250	3	75.7	179.3	2.0733	-339.0000	0.00245	0.00184
SP1																		
Al	113	117	115	5	142	157	149.5	16	298	302	300	5	88.8	63.6	-0.1362	104.4649	0.19094	0.57283
Si	113	117	115	5	167	182	174.5	16	298	302	300	5	88.8	63.6	-0.1362	104.4649	0.10518	0.31555
P	113	117	115	5	193	209	201.0	17	298	302	300	5	88.8	63.6	-0.1362	104.4649	0.06828	0.20484
S	113	117	115	5	223	239	231.0	17	298	302	300	5	88.8	63.6	-0.1362	104.4649	0.04921	0.14764
Cl	113	117	115	5	254	270	262.0	17	298	302	300	5	88.8	63.6	-0.1362	104.4649	0.03526	0.10577
K	298	302	300	5	324	341	332.5	18	414	416	415	3	63.6	208.3	1.2586	-313.9652	0.01943	0.05829
Ca	298	302	300	5	361	378	369.5	18	414	416	415	3	63.6	208.3	1.2586	-313.9652	0.01460	0.04381
Ti MS	113	117	115	5	443	460	451.5	18	524	528	526	5	88.8	11.4	-0.1883	110.4569		
SP2																		
K	298	302	300	5	324	341	332.5	18	421	425	423	5	78.2	55.4	-0.1854	133.8098	0.01706	0.05117
Ca	298	302	300	5	361	378	369.5	18	421	425	423	5	83.2	55.4	-0.2260	151.0049	0.01300	0.03900
Sc	298	302	300	5	401	418	409.5	18	421	425	423	5	83.2	55.4	-0.2260	151.0049	0.01026	0.03077
Ti	421	425	423	5	443	460	451.5	18	517	521	519	5	55.4	85.4	0.3125	-76.7875	0.00809	0.02427
V	421	425	423	5	487	505	496.0	19	517	521	519	5	55.4	85.4	0.3125	-76.7875	0.00633	0.01900
Cr	512	521	516.5	10	533	551	542.0	19	564	573	568.5	10	79.4	123.7	0.8519	-360.6183	0.00491	0.01474
Fe MS	316	320	318	5	631	650	640.5	20	737	741	739	5	77.8	24.6	-0.1264	117.9843		
SP3																		
Cr	420	424	422	5	533	551	542.0	19	564	568	566	5	41.4	21.4	-0.1389	100.0111	0.01279	0.03838
Mn	564	568	566	5	581	599	590.0	19	726	730	728	5	21.4	27.6	0.0383	-0.2617	0.01033	0.03100
Fe	564	568	566	5	631	650	640.5	20	726	730	728	5	21.4	27.6	0.0383	-0.2617	0.00826	0.02478
Co	564	568	566	5	684	703	693.5	20	726	730	728	5	21.4	27.6	0.0383	-0.2617	0.00660	0.01981
Ni	667	671	669	5	738	758	748.0	21	767	771	769	5	20.8	27.0	0.0620	-20.6780	0.00563	0.01690
Cu	767	771	769	5	795	815	805.0	21	833	837	835	5	27.0	44.0	0.2576	-171.0758	0.00483	0.01450
Zn	833	837	835	5	854	875	864.5	22	883	887	885	5	44.0	102.8	1.1760	-937.9600	0.00404	0.01211
Sm	516	520	518	5	554	572	563.0	19	726	730	728	5	34.2	27.6	-0.0314	50.4800	0.02698	0.08095
Eu	516	520	518	5	575	593	584.0	19	726	730	728	5	34.2	27.6	-0.0314	50.4800	0.03800	0.11401
Tb	516	520	518	5	688	708	698.0	21	726	730	728	5	34.2	27.6	-0.0314	50.4800	0.02563	0.07690
Ge MS	725	734	518	10	978	999	988.5	22	1136	1140	1138	5	25.7	10.6	-0.0244	38.3158		
SP4																		
Zn	767	771	769	5	854	875	864.5	22	891	895	893	5	24.2	25.4	0.0097	16.7581	0.01733	0.05200
Ga	891	895	893	5	915	936	925.5	22	1017	1021	1019	5	25.4	25.6	0.0016	23.9825	0.01483	0.04450
Ge	891	895	893	5	978	999	988.5	22	1017	1021	1019	5	25.4	25.6	0.0016	23.9825	0.01298	0.03895
As	1017	1021	1019	5	1044	1065	1054.5	22	1153	1157	1155	5	25.6	21.8	-0.0279	54.0721	0.01166	0.03497
Se	1017	1021	1019	5	1111	1133	1122.0	23	1153	1157	1155	5	25.6	21.8	-0.0279	54.0721	0.01086	0.03257
Br	1153	1157	1155	5	1181	1204	1192.5	24	1227	1231	1229	5	21.8	19.2	-0.0351	62.3811	0.00991	0.02973
Rb	1299	1303	1301	5	1327	1352	1339.5	26	1376	1379	1377.5	4	26.0	37.8	0.1536	-173.8268	0.00850	0.02550
Sr	1376	1379	1377.5	4	1404	1430	1417.0	27	1454	1458	1456	5	37.8	67.8	0.3828	-489.5605	0.00784	0.02351
Y	1454	1458	1456	5	1481	1508	1494.5	28	1533	1537	1535	5	67.8	105.0	0.4709	-617.8101	0.00733	0.02200
Zr	1533	1537	1535	5	1562	1590	1576.0	29	1615	1619	1617	5	105.0	158.2	0.6488	-890.8780	0.00678	0.02034
Hg	891	895	893	5	989	1010	999.5	22	1017	1021	1019	5	25.4	25.6	0.0016	23.9825	0.02201	0.06604
Pb	1222	1231	1226.5	10	1252	1273	1262.5	22	1296	1305	1300.5	10	20.9	29.4	0.1149	-119.9818	0.02563	0.07688
SP5																		
Pd	2061	2080	2070.5	20	2095	2130	2112.5	36	2145	2164	2154.5	20	13.4	14.5	0.0137	-14.9961	0.01458	0.04373
Ag	2158	2177	2167.5	20	2192	2229	2210.5	38	2244	2263	2253.5	20	13.6	13.7	0.0012	11.0797	0.01402	0.04205
Cd	2258	2277	2267.5	20	2292	2331	2311.5	40	2346	2365	2355.5	20	13.8	13.7	-0.0011	16.3767	0.01375	0.04125
In	2360	2379	2369.5	20	2394	2435	2414.5	42	2450	2469	2459.5	20	14.0	15.5	0.0161	-24.1753	0.01375	0.04125
Sn	2463	2482	2472.5	20	2497	2540	2518.5	44	2555	2574	2564.5	20	15.9	18.5	0.0288	-55.3688	0.01415	0.04246
Sb	2569	2588	2578.5	20	2603	2649	2626.0	47	2664	2683	2673.5	20	17.5	23.1	0.0589	-134.5458	0.01503	0.04508
Cs	3021	3040	3030.5	20	3055	3112	3083.5	58	3127	3146	3136.5	20	39.2	49.1	0.0934	-243.8373	0.02475	0.07424
Ba	3143	3162	3152.5	20	3177	3236	3206.5	60	3251	3270	3260.5	20	47.5	55.0	0.0699	-172.9331	0.03037	0.09110
La	3265	3284	3274.5	20	3299	3361	3330.0	63	3376	3395	3385.5	20	58.3	58.7	0.0041	44.9750	0.03836	0.11508

Figure 1. Calibration data used in data processing.

Figure 2. Overlap correction factors used in data processing.

Analyte to be corrected	sp	Interferent	sp	Factor	Amount Subtracted	Corrected Net Counts	Corrected Uncertainty
K	1	Cd	5	0	0.00	0	60
Sn	5	Ag	5	0	0.00	110	40
K	1	Sn	4	0	0.00	0	60
Ca	1	Sn	4	0	0.00	0	71
Sb	5	Cd	5	0.13207	1.98	12	44
K	1	Sb	5	0	0.00	0	60
Ca	1	SB	5	0	0.00	0	71
Ca	1	K	1	0.07171	0.00	0	71
Ca	2	K	2	0.07171	5.37	45	50
Sc	2	Ca	2	0.092	4.12	0	45
Ba	5	I	5	0	0.00	10	78
Ti	2	BA	5	0.3332	0.00	345	52
Ti	2	Fe MS	2	0.0012	381.35	0	64
V	2	BA	5	0.1321	0.00	0	49
V	2	TI	2	0.13371	0.00	0	49
Cr	2	V	2	0.13568	0.00	0	62
Mn	3	CR	3	0.1257	18.74	65	31
Fe	3	MN	3	0.08087	5.27	415	37
Cu	3	Ge MS	3	0.0017	209.02	32	47
Pb	4	SE	4	0.07656	0.00	0	33
S	1	PB	4	0.11478	0.00	0	49
Cl	1	PB	4	0.02922	0.00	689	55
Cl	1	S	1	0.0175	0.00	689	55
Cl	1	Ti MS	1	0.0021	645.80	43	85
S	1	CL	1	0	0.00	0	49
Co	3	FE	3	0.06992	29.00	0	30
Sm	3	Cr	3	0.0762	11.36	0	32
Sm	3	Mn	3	0.0172	1.12	0	32
Eu	3	Cr	3	0.0611	9.11	0	32
Eu	3	Mn	3	0.8262	53.88	0	41
Tb	3	Fe	3	0.1	41.47	0	31
Tb	3	Co	3	0.9369	0.00	0	42
Co	4	FE	4	0.06007	10.75	0	32
Ga	4	PB	4	0.06488	0.00	28	34
As	4	PB	4	1.200648	0.00	0	31
Ge	4	ZN	3	0	0.00	0	32
Ge	4	Hg	4	0	0.00	0	32
Br	4	AS	4	0.04556	0.00	43	32
Rb	4	BR	4	0.13207	5.73	24	41
Y	4	PB	4	0.06959	0.00	0	67
Y	4	RB	4	0	0.00	0	67
Hf	4	Pb	4	0.0174	0.00	0	33
Hf	4	Cu	4	0.0883	13.99	0	33
Ga	4	Ta	4	0.65672	41.21	0	41

Figure 3. Replicate report.

REPLICATE REPORT

Original ID: 02-T5786

Replicate ID: RT5786

Deposit Mass: 214 µg

Deposit Area: 11.3 cm²

Particle Size: F

Element	Original ug/cm2		Replicate ug/cm2		Difference ug/cm2		RPD						
Na	0.0921	+-	0.0452	0.0381	+-	0.0476	0.0540	+-	0.0656				
Mg	0.0000	+-	0.0158	0.0325	+-	0.0176	-0.0325	+-	0.0236				
Al	0.0271	+-	0.0077	0.0173	+-	0.0083	0.0098	+-	0.0114	+	44.0	+-	51.2
Si	0.0965	+-	0.0116	0.0957	+-	0.0118	0.0007	+-	0.0165	+	0.8	+-	17.2
P	0.0000	+-	0.0026	0.0000	+-	0.0030	0.0000	+-	0.0040				
S	0.5519	+-	0.0623	0.5804	+-	0.0658	-0.0285	+-	0.0906	+	-5.0	+-	16.0
Cl	0.0104	+-	0.0038	0.0124	+-	0.0046	-0.0019	+-	0.0059				
K	0.0527	+-	0.0062	0.0589	+-	0.0071	-0.0061	+-	0.0094	+	-11.0	+-	16.8
Ca	0.0437	+-	0.0052	0.0446	+-	0.0055	-0.0009	+-	0.0076	+	-2.1	+-	17.2
Sc	0.0000	+-	0.0010	0.0006	+-	0.0013	-0.0006	+-	0.0017				
Ti	0.0089	+-	0.0011	0.0109	+-	0.0015	-0.0020	+-	0.0019	0	-20.6	+-	18.8
V	0.0011	+-	0.0006	0.0002	+-	0.0009	0.0009	+-	0.0011				
Cr	0.0006	+-	0.0006	0.0013	+-	0.0008	-0.0007	+-	0.0010				
Mn	0.0004	+-	0.0009	0.0040	+-	0.0012	-0.0036	+-	0.0015				
Fe	0.1003	+-	0.0053	0.1014	+-	0.0056	-0.0011	+-	0.0076	+	-1.1	+-	7.6
Co	0.0000	+-	0.0008	0.0000	+-	0.0010	0.0000	+-	0.0013				
Ni	0.0000	+-	0.0005	0.0001	+-	0.0007	-0.0001	+-	0.0008				
Cu	0.0899	+-	0.0046	0.0902	+-	0.0048	-0.0003	+-	0.0067	+	-0.3	+-	7.4
Zn	0.0023	+-	0.0007	0.0033	+-	0.0010	-0.0010	+-	0.0012	+	-37.3	+-	43.9
Ga	0.0000	+-	0.0015	0.0000	+-	0.0022	0.0000	+-	0.0026				
As	0.0028	+-	0.0010	0.0001	+-	0.0013	0.0027	+-	0.0017				
Se	0.0013	+-	0.0008	0.0005	+-	0.0012	0.0007	+-	0.0015				
Br	0.0044	+-	0.0009	0.0034	+-	0.0012	0.0010	+-	0.0015	+	25.1	+-	38.4
Rb	0.0000	+-	0.0009	0.0000	+-	0.0012	0.0000	+-	0.0015				
Sr	0.0000	+-	0.0010	0.0001	+-	0.0014	-0.0001	+-	0.0018				
Y	0.0015	+-	0.0012	0.0000	+-	0.0017	0.0015	+-	0.0021				
Zr	0.0029	+-	0.0015	0.0000	+-	0.0020	0.0029	+-	0.0025				
Nb	0.0005	+-	0.0017	0.0000	+-	0.0023	0.0005	+-	0.0029				
Mo	0.0028	+-	0.0019	0.0000	+-	0.0027	0.0028	+-	0.0033				
Ag	0.0000	+-	0.0037	0.0042	+-	0.0055	-0.0042	+-	0.0066				
Cd	0.0017	+-	0.0039	0.0000	+-	0.0054	0.0017	+-	0.0066				
In	0.0000	+-	0.0041	0.0000	+-	0.0055	0.0000	+-	0.0068				
Sn	0.0192	+-	0.0070	0.0148	+-	0.0068	0.0044	+-	0.0097				
Sb	0.0021	+-	0.0055	0.0058	+-	0.0074	-0.0037	+-	0.0092				
Cs	0.0091	+-	0.0144	0.0174	+-	0.0199	-0.0083	+-	0.0245				
Ba	0.0189	+-	0.0196	0.0466	+-	0.0275	-0.0277	+-	0.0338				
La	0.0000	+-	0.0265	0.0000	+-	0.0368	0.0000	+-	0.0453				
Ce	0.0071	+-	0.0373	0.1106	+-	0.0529	-0.1035	+-	0.0647				
Hg	0.0000	+-	0.0017	0.0000	+-	0.0023	0.0000	+-	0.0029				
Pb	0.0005	+-	0.0022	0.0006	+-	0.0030	-0.0001	+-	0.0038				

RPD: Relative Percent Difference $(X1-X2)/[(X1+X2)/2]*100$. RPD is calculated when original value is greater than three times its uncertainty.

C:\XR\F\QS024.sp0 sp0

Livetime	Target	Filter	kV	mA	
50	Direct	Cel	7.5	0.1	5

	Gross Counts	Normalized (gross/sec)	Avg cts/sec	Recovery	
Si	9004	1801	1706	1.056	PASS

C:\XR\F\QS024.sp1 sp1

Livetime	Target	Filter	kV	mA	
50	Direct	Cu	20	0.2	2

	Gross Counts	Normalized (gross/sec)	Avg cts/sec	Recovery	
Si	416	41.6			
Ti	8621	862.1	871.9261	0.989	PASS
Fe	17790	1779.0	1822.317	0.976	PASS

C:\XR\F\QS024.sp2 sp2

Livetime	Target	Filter	kV	mA	
50	Ge	0	30	1	2

	Gross Counts	Normalized (gross/sec)	Avg cts/sec	Recovery	
Ti	10138	202.76	205.4454	0.987	PASS
Fe	24524	490.48	493.9854	0.993	PASS

C:\XR\F\QS024.sp3 sp3

Livetime	Target	Filter	kV	mA	
50	8	Rh	35	1	1

	Gross Counts	Normalized (gross/sec)	Avg cts/sec	Recovery	
Ti	3566	71.32	68.11	1.047	PASS
Fe	8901	178.0	176.8	1.007	PASS
Se	10624	212.5	206.8	1.027	PASS
Pb	13075	261.5	260.8	1.003	PASS

C:\XR\F\QS024.sp4 sp4

Livetime	Target	Filter	kV	mA	
50	Direct	W	55	0.6	0

	Gross Counts	Normalized (gross/sec)	Avg cts/sec	Recovery	
Cd	5561	185.4	187.7	0.987	PASS

Figure 4. QS data report.