

CHESTER LabNet

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Chester LabNet

**Standard Operating Procedure
XR-005.01**

^{XRF}
KEVEX ~~770~~ SPECTROMETER DATA GENERATION, INTERPRETATION AND REPORTING
CHESTER LABNET PROPRIETARY METHOD

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SOP: XR-005.01

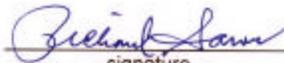
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REVIEW HISTORY

Review date:	Changes made:	Changes made by:
4/24/02	No changes. Date of origination. Original text found in SOP XR-002, written by Rick Sarver in 1998.	Sheri Heldstab

ANNUAL REVIEW

The undersigned attests that this standard operating procedure has undergone annual review for adherence to current practices and the latest QA/QC protocols:


signature

Richard Sarver
printed name/title

7.9.03
date

minor changes to text 7.9.03 SH

**KEVEX-770 SPECTROMETER DATA GENERATION, INTERPRETATION AND REPORTING
CHESTER LABNET PROPRIETARY METHOD**

1.0 Scope and Application

1.1 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.

1.2 This SOP *should never* be performed by anyone lacking extensive XRF data processing and interpretation skills.

2.0 Summary

2.1 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.

3.0 Sampling and Storage

3.1 N/A

4.0 Apparatus

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

4.2 3.5" floppy disks

5.0 Reagents

5.1 N/A

6.0 Calibration/Preparation

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

7.0 Procedure

7.1 Transfer the spectral files:

7.1.1 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 either the Ethernet. Spectral files take the form of *.sp* files.

7.2 Process the QS data.

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

7.2.2 Select the 'raw-in' worksheet

7.2.3 On the toolbar, click on 'edit' and then 'replace'.

7.2.4 Enter the ID to be replaced in the 'find what' box.

7.2.5 Enter the ID to be processed in the 'replace with' box, and then click on the 'replace all' button.

7.2.6 On the toolbar, click 'Run' then 'Start' then double click on 'V4RawData' to initiate data processing.

- 7.2.7 After processing is complete, the program will advance to the 'result' window and display the QS data sheet. Print out the QS data sheet and keep it with the XRF request form for that particular analysis.
- 7.2.8 Enter the date of analysis and the normalized gross counts per second for each element in each excitation condition into the proper 'KevexQS' archive file in Excel.

7.3 Process Sample Data.

- 7.3.1 Open the LabNet XRF Data Processing workbook (XRFV4.xls) in Excel and select the 'raw-in' worksheet. Also open a blank replicate report workbook and select the "original" worksheet.
- 7.3.2 In the LabNet XRF Data Processing workbook (XRFV4.xls), select the 'raw-in' worksheet
- 7.3.3 On the toolbar, click on 'edit' and then 'replace'.
- 7.3.4 Enter the ID to be replaced in the 'find what' box.
- 7.3.5 Enter the ID to be processed in the 'replace with' box, and then click on the 'replace all' button.
- 7.3.6 On the toolbar, click 'Run' then 'Start' then double click on 'V4RawData' to initiate data processing.
- 7.3.7 When the calculations have been completed, the program will move to the 'result' window. At this point the peaks have been integrated and corrected for spectral overlap interference as described in section 9.1.
- 7.3.8 Next, enter sample specific information in the 'result' window:
 - 7.3.8.1 Enter the LIMS ID into cell 'A2'

7.3.8.2 Enter the particle size (N = none, F = fine or PM_{2.5}, C = coarse, P = PM₁₀, T = total) into cell 'B2'

7.3.8.3 Enter the deposit mass (µg) into cell 'D2'

7.3.8.4 Enter the deposit area (cm²) into cell 'F2'.

At this point the program uses the deposit density to correct elements Na through Ca for mass absorption attenuation as described in section 9.2. The absorption corrected concentration is then calculated as described in section 9.3.

7.3.9 The particle size corrections are then made for Al, Na, Mg and Si as described in section 9.4.

7.3.10 The net uncertainty for each final concentration is determined as described in section 9.5.

7.3.11 Create a replicate report:

7.3.11.1 When the sample being used for the replicate is being processed, click on the name box and select "B".

7.3.11.2 Copy the highlighted area and paste values into the "original" worksheet in the blank replicate workbook opened in section 7.3.1.

7.3.11.3 Save the replicate file as A###-xxx.xls where 'A###' is the client number and 'xxx' is the run number. Verify that the "run file" workbook has been saved into the proper subdirectory on the data processing computer.

7.3.11.4 Perform steps 7.3.8.1 through 7.3.8.3 again for the replicate analysis data, with the exception of pasting the values from the replicate into the worksheet called "replicate" rather than the worksheet called "original" in the "run file" workbook.

7.3.11.5 Within the run file workbook, print out the worksheet called "report".

7.4 Compile sample data for all samples in the run:

7.4.1 To compile data manually:

7.4.1.1 While still in the 'result' window, click on the Name Box.

7.4.1.2 Either type in "a" or pull down the Name Box menu and choose "a". By clicking on 'a' the entire result sheet will be highlighted.

7.4.1.3 'copy' this area to the worksheet named 'result (2)'. To ensure proper formatting, use 'paste values' and 'paste formats'.

7.4.1.4 The first entry should be copied into cell 'A1' in window 'result (2)'. The following entries are made starting at the 'A' cell just below the highlighted area of the preceding sample file.

7.4.2 To compile data automatically, use the macro shortcut key combination "ctrl x". Note that this macro shortcut compiles both the sample data and LIMS data simultaneously, thus by using "ctrl x" at this stage, the analyst does not need to perform step 7.6.

7.4.3 Repeat steps 7.3.2 through 7.4.2 for all sample IDs on the XRF run sheet.

7.5 When all of the samples have been processed in this manner, save the 'result (2)' worksheet onto the disk containing the spectral files, and print the compiled results.

7.5.1 In 'result (2)' choose 'edit' then 'move or copy sheet'.

7.5.2 This will display the 'Move or Copy' window. Click on the 'Create a Copy' box in the lower left corner of the dialogue box.

7.5.3 Next click on the box labeled 'To Book' and choose (new book). Then click 'OK' and the 'result (2)' file will be copied into a new Excel workbook.

7.5.4 Save the new workbook onto the same disk that the original *.sp* files are stored. Save it as a space delimited (.prn) file, using the file nomenclature 'A###-xxx.prn' where 'A###' is the client number and 'xxx' is the run number. After saving the .prn file, use "move or copy sheet" to move this sheet to the "run file" workbook, then save the run file.

7.5.5 Using the DOS prompt within Windows, print the .prn file using the command:
COPY A###-xxx.prn LPT1

7.6 Compile LIMS data for all samples in the run:

7.6.1 As the samples are being processed, the data processing program also creates data suitable for transfer to the Laboratory Information Management System (LIMS) located in the 'LIMS' worksheet.

7.6.2 To compile LIMS data manually:

*7.6.2.1 When manually compiling data, it is imperative to never use "paste" to move data. Due to the high number of formulas and references in this workbook, "paste special" and "values" **OR** "paste values" should always be used.*

7.6.2.2 For each sample, click on the 'LIMS' worksheet at the bottom of the processing program screen.

7.6.2.3 The LIMS ID and each associated analyte followed by its uncertainty will be displayed horizontally across the 'LIMS' worksheet in atomic order and will be highlighted.

7.6.2.4 Copy the highlighted area from the 'LIMS' worksheet and "paste values" into cell 'A2' (for the first sample) of the 'LIMS (2)' worksheet. Row one is reserved for column descriptions.

7.6.2.5 Repeat this process for each sample, pasting the values into the next available row.

7.6.3 The use of macro shortcut key combination “ctrl x” automatically performs the LIMS data compilation. Note that the use of the “ctrl x” macro in step 7.4.2 of this method will automatically perform the LIMS data compilation as well. *If “ctrl x” was used at that point, do not use it again at this stage.*

7.6.4 When all of the samples have been processed in this manner, save the ‘LIMS (2)’ worksheet into the run file workbook.

7.6.4.1 In the ‘LIMS (2)’ worksheet of the processing workbook, highlight and copy the headers and all data except for the replicate data and paste to the LIMS worksheet in the run file workbook.

7.6.4.2 Corrections to data generated in step 7.7 will be made and saved in this worksheet.

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

7.7.1 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.

7.7.2 ‘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.

7.7.3 *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.*

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

7.8.1 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.

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

- 7.8.1.2 Select all Sample IDs, concentrations and uncertainties and copy to a new workbook. Do not select the header row (Row 1).
- 7.8.1.3 Save this new workbook as *****.csv** (comma delimited) file onto the 1Kermit directory, where ******* is the worklist name, which indicates the species to be transferred to the LIMS.
- 7.8.2 Access the LIMS by clicking on the LIMS icon. The mouse is inoperable in the LIMS program.
- 7.8.3 From the LIMS main menu choose option 2 (Worklist Management). Note: striking the 'Enter' key must follow all commands.
- 7.8.4 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.
- 7.8.5 Next type 'i' (for Instrument), then 'i' (for Import), then 'n' (for **N**ew).
- 7.8.6 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'.
- 7.8.7 The program will then ask for 'status report to:', type 's' (for **S**creen) and press 'Enter'.
- 7.8.8 The program then asks 'continue or quit:', type 'c' and press 'Enter'.
- 7.8.9 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'.
- 7.8.10 The program then displays the first sample ID as well as the analytes, concentrations, and uncertainties.

7.8.11 Proofread the data:

7.8.11.1 Check to be sure that all of the changes made in section 7.7 coincide with the data on the screen.

7.8.11.2 It is possible to scroll from sample to sample by using the 'Page Up' and 'Page Down' keys.

7.8.11.3 If any corrections were missed, they may be entered at this time in the LIMS program.

7.8.12 Once all of the corrections have been confirmed, press the 'Home' key, type 's' to save, and 'y' for yes.

7.8.13 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).

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

7.9 Archive raw data:

7.9.1 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.

7.9.2 Electronic data is archived on the C drive of the data processing computer. 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.

8.0 QA/QC

8.1 N/A

9.0 Calculations

9.1 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 = $\Sigma_h - (m C_h)$

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

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 livetime 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 livetime 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 [$\mu\text{g}/\text{cm}^2$] / (cts/sec)]

t = the counting livetime (sec)

9.2 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:

$$mf_c = (1 - (\sum mf_i + \sum mf_{i_0})) / 1.3$$

where: mf_i = the mass fraction of element i

mf_{i_0} = the mass fraction of oxygen related to element i

The oxygen mass fraction (mf_o) is then estimated:

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

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

9.3 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

9.4 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 livetime

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

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

$$\delta_i = \sum (\delta_{e,j} L_{n,j})$$

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

$\delta_{e,j}$ = 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

$$\delta_a = [((\delta_c^2 + \delta_i^2 + \delta_s^2)^{1/2} / A)^2 + (0.1 N / A^2)^2]^{1/2} / A_p$$

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

10.0 References

- 10.1 Kevex Operator's Manual
- 10.2 Practical X-Ray Spectrometry, R. Jenkins and J.L. De Vries, second edition, Philips Technical Library, Springer-Verlag New York Inc.
- 10.3 X-Ray Fluorescence Analysis of Environmental Samples, Jaklevic, et al, Ed. by T.G. Dzubay, Ann Arbor Sci.

10.4 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.

10.5 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.

10.6 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.

11.0 Analyst Notes

11.1 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.

Analyte to be corrected	sp	Interferent	sp	Factor	Amount Subtracted	Corrected Net Counts	Corrected Uncertainty
K	1	Cd	5	0	0.00	0	0.00
Sn	5	Ag	5	0	0.00	110	0.00
K	1	Sn	4	0	0.00	0	0.00
Ca	1	Sn	4	0	0.00	0	0.00
Sb	5	Cd	5	0.13207	1.98	12	4.41
K	1	Sb	5	0	0.00	0	0.00
Ca	1	SB	5	0	0.00	0	0.00
Ca	1	K	1	0.07171	0.00	0	4.32
Ca	2	K	2	0.07171	5.37	45	3.05
Sc	2	Ca	2	0.092	4.12	0	4.59
Ba	5	I	5	0	0.00	10	0.00
Ti	2	BA	5	0.3332	0.00	345	0.00
Ti	2	Fe MS	2	0.0012	381.35	0	0.68
V	2	BA	5	0.1321	0.00	0	0.00
V	2	TI	2	0.13371	0.00	0	8.58
Cr	2	V	2	0.13568	0.00	0	6.69
Mn	3	CR	3	0.1257	18.74	65	4.15
Fe	3	MN	3	0.08087	5.27	415	2.50
Cu	3	Ge MS	3	0.0017	209.02	32	0.60
Pb	4	SE	4	0.07656	0.00	0	2.32
S	1	PB	4	0.11478	0.00	0	8.20
Cl	1	PB	4	0.02922	0.00	689	2.09
Cl	1	S	1	0.0175	0.00	689	0.86
Cl	1	Ti MS	1	0.0021	645.80	43	1.17
S	1	CL	1	0	0.00	0	0.00
Co	3	FE	3	0.06992	29.00	0	2.61
Sm	3	Cr	3	0.0762	11.36	0	2.51
Sm	3	Mn	3	0.0172	1.12	0	0.53
Eu	3	Cr	3	0.0611	9.11	0	2.02
Eu	3	Mn	3	0.8262	53.88	0	25.50
Tb	3	Fe	3	0.1	41.47	0	3.74
Tb	3	Co	3	0.9369	0.00	0	28.34
Co	4	FE	4	0.06007	10.75	0	2.18
Ga	4	PB	4	0.06488	0.00	28	2.16
As	4	PB	4	1.200648	0.00	0	0.00
Ge	4	ZN	3	0	0.00	0	0.00
Ge	4	Hg	4	0	0.00	0	0.00
Br	4	AS	4	0.04556	0.00	43	1.40
Rb	4	BR	4	0.13207	5.73	24	4.24
Y	4	PB	4	0.06959	0.00	0	1.78
Y	4	RB	4	0	0.00	0	0.00
Hf	4	Pb	4	0.0174	0.00	0	0.58
Hf	4	Cu	4	0.0883	13.99	0	3.05
Ga	4	Ta	4	0.65672	41.21	0	22.59

Figure 2. Overlap correction factors used in data processing.

REPLICATE REPORT

Original ID: 02-T5786

Replicate ID: RT5786

Deposit Mass: 214 µg

Deposit Area: 11.3 cm²

Particle Size: F

Element	Original		Replicate		Difference		RPD						
	ug/cm2		ug/cm2		ug/cm2								
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.

Figure 3. Replicate report.

C:\IXRF\QS1011.sp0		sp0			
770v13	Livetime	Target	Filter	kV	mA
	100	Direct	Cel	7.5	0.10
	Normalized				
	Gross Counts	Gross Counts per Second	Average Cts/Sec	Recovery	
Si	18836	188.36	191.16	0.985	PASS
C:\IXRF\QS1011.sp1		sp1			
	Livetime	Target	Filter	kV	mA
	100	Ti	0	25	3.00
	Normalized				
	Gross Counts	Gross Counts per Second	Average Cts/Sec	Recovery	
Si	6562	10.94	10.86	1.007	PASS
C:\IXRF\QS1011.sp2		sp2			
	Livetime	Target	Filter	kV	mA
	100	Fe	0	35	0.50
	Normalized				
	Gross Counts	Gross Counts per Second	Average Cts/Sec	Recovery	
Ti	12939	129.39	129.98	0.995	PASS
C:\IXRF\QS1011.sp3		sp3			
	Livetime	Target	Filter	kV	mA
	100	Ge	0	35	0.50
	Normalized				
	Gross Counts	Gross Counts per Second	Average Cts/Sec	Recovery	
Ti	5085	50.85	50.61	1.005	PASS
Fe	17844	178.44	177.51	1.005	PASS
C:\IXRF\QS1011.sp4		sp4			
	Livetime	Target	Filter	kV	mA
	100	Direct	Rh	35	0.75
	Normalized				
	Gross Counts	Gross Counts per Second	Average Cts/Sec	Recovery	
Ti	2081	6.94	7.04	0.985	PASS
Fe	7829	26.10	26.23	0.995	PASS
Se	14578	48.59	48.42	1.004	PASS
Pb	10564	35.21	35.23	1.000	PASS
C:\IXRF\QS1011.sp5		sp5			
	Livetime	Target	Filter	kV	mA
	100	Direct	W	55	0.60
	Normalized				
	Gross Counts	Gross Counts per Second	Average Cts/Sec	Recovery	
Cd	7988	33.28	32.29	1.031	PASS

Figure 4. QS data report.