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Tests on the suitability of the S360 SEM for microanalysis of heavy mineral grain mounts.

Laboratory Operations Programme

Internal Report IR/06/020

BRITISH GEOLOGICAL SURVEY

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Foreword

This report is the published product of a study by the British Geological Survey (BGS). It provides a brief account of an assessment of the suitability of our Cambridge-Leica S360 Scanning Electron Microscope for the analysis of grain mounts of heavy minerals. This type of analysis has up to now been conducted using an aging, Cambridge Instruments Microscan5 electron microprobe, which is coming to the end of its useful working life.

Acknowledgements

John Mckervey carried out the Cameca SX50 microprobe analyses on the G-probe samples quoted in section 3.4. The heavy mineral grain mounts samples for analysis in this comparison were provided by Andy Morton of HMRA. This work was carried out under the laboratory maintenance and development of capability (MaDCap) programme funded through the laboratory operations manager (Shaun Reeder).

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1 Introduction

BGS has traditionally undertaken microchemical analysis of heavy mineral grain mounts using a Cambridge Instruments Microscan 5 Electron Probe Micro-Analyser (EPMA), with a Link Systems AN10,000 Energy Dispersive X-ray Analyser (EDXA) – hereafter referred to as the "*Microscan*". This instrument is over 30 years old and has proved itself to be a dependable workhorse over this period, generating large amounts of quantitative data for BGS and external clients. It is recognised that the equipment is old, and for many of the types of analysis it can perform, it has now been superseded by other equipment within BGS i.e. the more modern Cameca SX-50 EPMA and our two Scanning Electron Microscopes (SEM).

The microscan, due to a combination of its good optical microscope system and its high "take-off" angle for X-ray analysis, has proved itself to be ideally suited to the analysis of grain mounts, which has, to date, proved difficult to perform by any other method. Consequently, this instrument has been kept running for the past several years almost solely for the purposes of performing these analyses.

Given the age of the Microscan, in the event of serious breakdown, repairs are likely to be at best difficult and time consuming, with ever increasing uncertainty as to the availability of suitable spare parts. Therefore, a contingency is required to maintain our capability in the analysis of grain mount material (to our knowledge, the University of Aberdeen and ourselves are currently the only institutions capable of offering this analysis).

In 2003 we acquired a Cambridge-Leica S360 SEM – hereafter referred to as the "*S360*" – from BAS. This instrument is well-equipped to undertake X-ray microanalysis with a modern, high specification EDXA system (Oxford Instruments GEM detector with INCA processing hardware and software), and there has been much debate as to whether this equipment could be used to undertake analyses equivalent to those performed on the Microscan.

This short study was undertaken to determine the feasibility of analysing grain mounts on the S360, and to provide a set of data allowing direct comparison with data previously generated using the Microscan. The work was carried out in two distinct periods. The first batch of analyses on garnet grains were conducted in the period Nov-Dec 2005. Subsequently, a series of tourmaline analyses were carried out in Nov 2006. In the period between these two sets of analyses, considerable additional operator experience of the S360 instrument had been gained, and this improved the overall speed of the analyses.

2 Materials and Methods

Two grain mount samples comprising "columns" of separated garnet and tourmaline grains were analysed using the Microscan and the S360, and the data were compared on a grain-by-grain basis. Each instrument was run using broadly comparable analysis conditions (see Table 1).

The garnet analyses were conducted in Nov-Dec 2005, the tourmaline analyses were conducted in Nov 2006. In the interval between these analyses, considerable additional experience of the more detailed intricacies of the S360 has been gained, enabling a considerably improved work throughput.

Table 1 Operating conditions employed on the Microscan and S360 instruments for analysis.

	Microscan	S360	Units
Accelerating Voltage	20	20	kV
Probe Current	0.5	0.5	nA
EDXA hardware	Link Si[Li] detector and AN10000 pulse processor	Oxford Instruments GEM detector and INCA pulse processor	
Live Time The target analysis duration (excluding dead time).	30	30	Seconds
Approximate Dead Time Dead time is the time during which the detector cannot detect incoming X-rays because is it still processing X-rays received already. Usually expressed as a percent of the total analysis duration. Live time + Dead time = Analysis Duration.	30-35	10-15	%
X-ray processing time The time spent by the X-ray signal processor determining the energy of each incident X-ray. There is a trade-off between dead time, count rate and spectral resolution. 1 = low dead time, higher counts, lower spectral resolution 6 = high dead time, lower counts, higher spectral resolution	n/a	5	-
Elements Analysed	Mg, Al, Si, Ca, Ti, Cr, Mn, Fe		
Oxygen Content	By Stoichiometry		
Working Distance The distance between the final condenser lens and the specimen	unknown	25	mm
X-ray "take-off" angle The angle between the trajectory of an X-ray that will enter the X-ray detector and the surface of the sample.	75	45	°

2.1 BEAM-SAMPLE-DETECTOR GEOMETRY

Raw X-ray count data are converted into quantitative results by comparing the X-ray intensities derived from the unknown material with X-ray intensities derived from standards of known composition, and it is broadly true that the more abundant an element is within the analysed material the greater intensity of X-rays will be generated. However, in reality a number of factors additional to concentration, such as absorption and fluorescence, affect X-ray intensity. These matrix-dependent factors are corrected through the application of "matrix corrections".

The majority of the effects corrected for by matrix corrections (but most significantly X-ray absorption effects) are proportional to the "path length" that X-rays must travel from the excitation volume to exit the sample (Figure 1). This path length is normally constrained by the analyst having knowledge of the working distance, spectrometer take-off angle (Table 1) and the sample orientation. This is conventionally achieved by using perfectly polished samples placed orthogonal to the beam. Furthermore, by setting the working distance correctly, the analyst ensures the correct positioning of the sample relative to the detector and hence that the take-off angle is correct.

However, in the analysis of rough grains, the orientation of the sample surface relative to the beam and detector are poorly constrained, as is illustrated schematically in Figure 1. It is apparent that when a sample surface is inclined away from the detector, the path-length from excitation volume to the sample surface is proportionally longer, and also that the excitation volume is on average further from the sample surface than is the case for an orthogonal sample. The net result of this is that the analysis software under-compensates for X-ray absorption, and an anomalously low analytical total results. The opposite effect occurs when the sample surface is oriented towards the detector, and anomalously high analytical totals result.

Furthermore, on rough surfaces, raised areas between the analysis point and the detector may cause additional "shadowing" of the generated X-rays, resulting in a reduction in X-ray count rate and hence analytical totals.

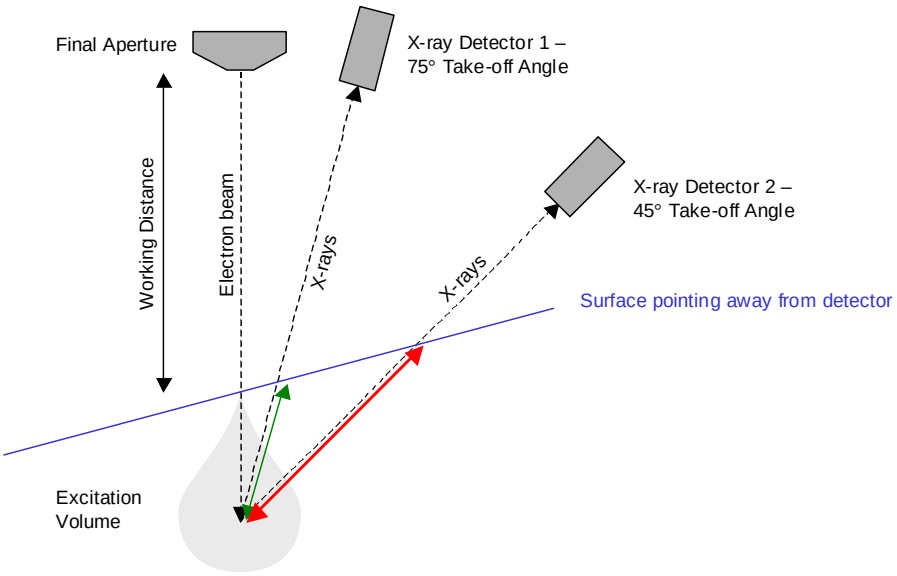
Therefore, when analysing grain mounts, the analyst has to make a judgement as to the optimum position for analysis on a given grain, usually attempting to locate a "flat-spot" on the grain, which is not shadowed by adjacent high points.

The magnitude of the potential error is ultimately controlled by two factors:

1) the take-off angle of the instrument. In the case of the instruments being compared here, the high take-off angle of the Microscan, (75°) means that variations in sample surface orientation result in relatively small variations in path-length, and hence the system is relatively insensitive to X-ray attenuation/enhancement due to variations in sample geometry. In the case of the S360, the lower take-off angle renders the system more susceptible to the effects of poor matrix correction. As will be discussed below, these effects are reflected in the results from the two instruments.

2) the energy of the X-ray. Low energy X-rays from light elements are much more likely to be absorbed within the sample than higher energy X-rays from heavy elements. Consequently, light element analyses are more likely to be adversely affected by poorly constrained sample surface geometries than analyses of heavier elements.

(A)



(B)

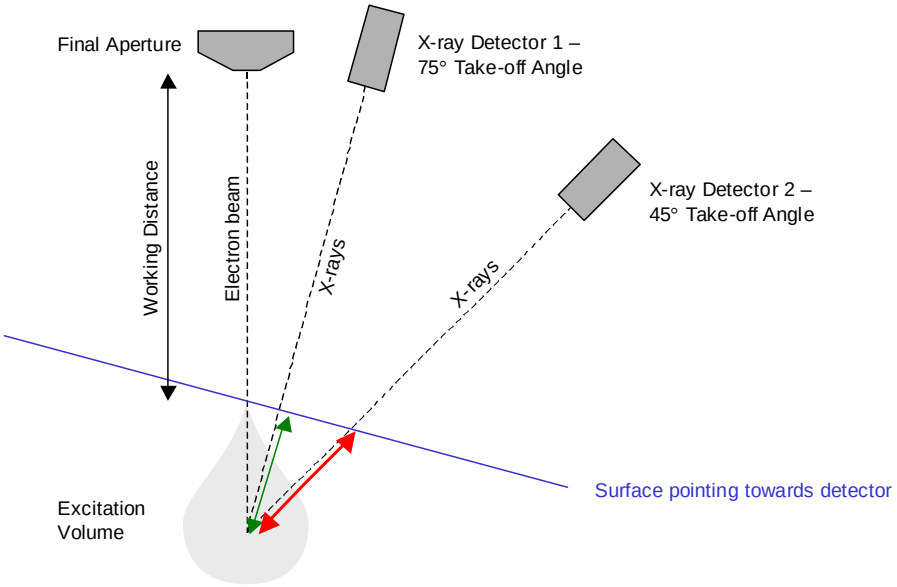


Figure 1 Illustration of the significance of beam-sample-detector geometry with respect to X-ray absorption within the sample.

In (A) the sample surface is tilted away from the detector, and in (B) the sample surface is tilted towards the detector. It is apparent from comparison of these images that the lower take-off angle of the S360 produces far larger variations in path-length (red arrows) than the higher take-off angle of the Microscan (green arrows).

2.2 ANALYSIS PROTOCOLS

2.2.1 Microscan Analysis

The garnet and tourmaline grains were analysed using the established protocols for this type of analysis, which have been in use for a number of years. Selection of the analysis points most likely to yield good results (i.e. with totals close to 100%) was guided by the optical microscope system which readily identifies likely suitable locations as "bright spots", and the probe current meter which can be used to further constrain analysis points that are likely to yield appropriate analytical totals.

The correct working distance was obtained as soon as the bright spot on the specimen came into focus. The protocol is to accept garnet analyses if they have analytical totals in the range c.90-101 wt%, and to accept tourmalines with analytical totals of > c.80-90 wt% (note: the presence of c.10 wt% BO_3 and structural water that can not be measured quantitatively using this instrument, mean that a "perfect" tourmaline analysis should yield an analytical total in the general range 85-88 wt%).

2.2.2 S360 Analysis

The same garnet and tourmaline grains were then analysed using the S360.

For the **garnet** analyses two different runs were undertaken:

1) A slow run ("S360-Slow"). During this run, great care was taken in the selection of analysis points. However, no mechanism equivalent to the optical microscope system of the microscan exists in the S360, and consequently a considerable amount of effort was expended in order to constrain which specific surface features on an individual garnet grain contributed to generating a "good" or a "bad" analysis. The beam was repositioned on a given grain until an analysis yielded a total in the range 90-102%. This acceptance range is broadly comparable with that applied during analysis with the Geoscan. Analysis according to this protocol proved time consuming (considerably longer than that required for analysis on the Microscan), and frustrating for the analyst, with the analysis point having to be shifted repeatedly until an acceptable analysis was obtained. Attempts to use probe current readings, and X-ray count rates as indicators of likely analysis quality had only limited success.
2) A fast run ("S360-Fast"). During this run, relatively short amounts of time were expended in attempts to identify suitable analysis positions, and analyses were accepted with totals in the range 90-110%.

For the **tourmaline** analysis, a single run on the S360 was carried out using the same acceptance threshold as that which is applied to the Microscan data (i.e. anything between approximately 80-90%). As noted in the introduction, in the period between carrying out the garnet analyses and the tourmaline analyses, considerable additional experience of the S360 instrument had been gained. This made it possible to locate suitable analysis points, using a combination of the SEM image and the probe current meter/and or analytical count rate, more quickly than had been possible during the garnet analyses.

2.2.3 Data manipulation and interpretation

Following analysis, the data were extracted from the analysis systems, and loaded into MS Excel for processing and comparison. All analyses were recalculated into formula units on the basis of 24 oxygen atoms (assuming all Fe was present as FeO) as is the convention for garnet and tourmaline analyses. The data from all five runs are presented in Appendix 1, and compared in the subsequent sections.

3 Results

3.1 ANALYSIS TIMES

The Microscan protocols were used as a benchmark against which to compare the analysis time using the S360. Approximate total analysis times are indicated in Table 2.

Actual analysis times for individual points are marginally quicker on the S360 relative to the Microscan, due to its more modern hardware being capable of processing X-rays more rapidly. However, the rate limiting step for the analyses is actually in the identification of the next grain for analysis and in finding a suitable location on that grain to analyse.

For the garnet analysis runs it proved quite difficult to identify successive analysis points, and for the S360-Slow run, this proved to be highly time consuming. If the analyst is prepared to accept a broader range of totals, as was the case for the S360-Fast run, then it is possible to undertake analysis on the S360 at approximately the same rate as is possible on the Microscan.

For tourmaline analyses, analysis times using the S360 were broadly comparable with the analysis times on the Microscan. This reflects the fact that in the period between carrying out the garnet and the tourmaline analyses considerable experience of the S360 instrument had been gained by the analyst, enabling the more rapid identification of suitable analysis points.

The S360 does, however, have the advantage of a much more rapid data extraction method, with data simply being cut and pasted from the X-ray analysis software into Excel. In the case of the Microscan, data extraction is a laborious process involving creation and transfer of text files from the X-ray analyser, via floppy disk, followed by pasting of the text into Excel, and parsing into columns. Furthermore, the small hard drive space available on the Microscan X-ray analysis system prevents systematic archiving of the full results of analyses and full analysis results are periodically deleted in order to make space for new analyses. The S360 system automatically saves the full results of each analysis into an "INCA" project file. The quantity of storage space available on the BGS Storage Area Network system is such that space limitations for storage of full analysis results is not likely to ever become a problem.

Table 2 Comparison of analysis and data extraction times for the various analytical runs

Run	Analysis Date	Total Analysis Time	Data extraction time	Total Time
GARNET (Sample GM101_C1)				
Microscan	Nov 2005	c. 90 minutes	20 minutes	c. 1:50
S360-Fast	Dec 2005	c. 2 hours	2 minutes	c. 2:02
S360-Slow	Dec 2005	c. 5 hours	2 minutes	c. 5:00
TOURMALINE (Sample GM119_C1)				
Microscan	Nov 2006	c. 90 Minutes	20 minutes	c. 1:50
S360	Nov 2006	c. 2 hours	2 minutes	c. 2:02

3.2 GARNET ANALYSES

3.2.1 Analytical Totals

The range of analytical totals obtained during a given run obviously reflects the rigour with which analyses were accepted or rejected.

Using the **Microscan,** the majority of analyses return totals in the range 95-100% (Figure 2A), with a definite skew towards analytical totals of around 100%. Totals in excess of 100% are relatively rarely encountered.

The **S360-Slow** data (Figure 2B) display a tighter distribution relative to the Microscan data, due to the narrower band for acceptance of analyses, but analyses are more evenly distributed around 100%, and totals in excess of 100% are relatively common.

Finally, the **S360-Fast** data (Figure 2C) reflect the broad acceptance band for analyses, displaying a broad range of analytical totals, which are commonly well in excess of 100%.

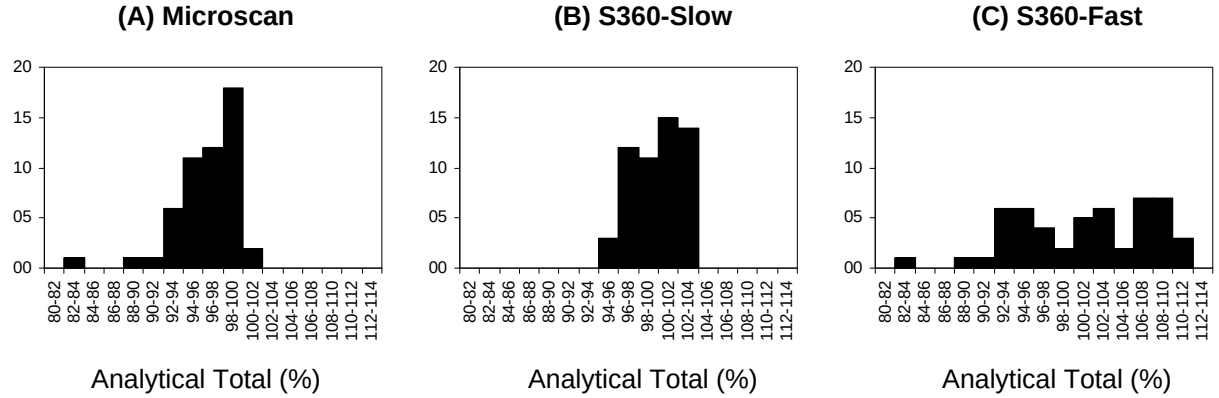


Figure 2 Frequency distributions for analytical totals obtained from the garnet analyses.

3.2.2 Compositional data

Given the variability in analytical totals described above, the data from all three analytical runs are remarkably consistent. Figure 3 uses cross plots to compare raw element percent data derived using the Microscan and the S360, for the major elements analysed during this test. The solid line on all plots represents unity, which is where all the analyses should, theoretically, plot. A degree of departure from unity would be expected due to inhomogeneities within individual garnet grains – and this probably accounts for the majority of the analysis points that deviate significantly from unity. This effect is further compounded by the fact that individual analyses of different grains have different analytical totals (largely caused by the poorly constrained take-off angle discussed in Section 2), which will artificially reduce or elevate the measured concentrations of individual elements.

Al and Si concentrations are more widely scattered when determined using S360 (in both the Slow and the Fast runs) relative to the data derived using the Microscan (Figure 3A and B). Furthermore, the scatter is more pronounced in the S360-Fast data than the S360-Slow data.

Irrespective of instrument, there are good correlations between Si and Al concentration and analytical total (Figure 4). Given the relatively poor constraints on take-off angle in both the Microscan and the S360, it would be anticipated that measured concentrations of all elements would show some variation with the quality of the analysis - i.e. for analyses with relatively high analytical totals (generated by analysis of grain surfaces that are tilted towards the X-ray

detector), all elements should have artificially elevated concentrations. For most of the elements analysed in garnet, this variability is masked somewhat by the natural variations in concentrations. However, for Si and Al, which only display limited variations in abundance in garnets, the relationship between analytical total and individual element concentration is apparent. The effect may be compounded by the relatively light nature of these elements and the relatively low energies of the measured X-rays, which renders them more susceptible to absorption effects than X-rays from the heavier elements that may not be correctly corrected for by the matrix correction software when surface geometry is not correctly constrained.

The relationships between analytical total and Si and Al concentrations is seen in both the data derived from the Microscan and that from the S360 (both runs), and the magnitude of the effect is largely controlled by the analytical total – consequently the Microscan and the S360-Slow run data show less variability in measured Si and Al concentrations that the S360-fast run.

In spite of the low atomic number of Mg, **Mg concentrations** show excellent agreement between the two instruments. The fact that Mg is present at relatively low concentrations (typically < 5 element wt%), and that it is involved in solid-solution series with the other garnet end-member components (Ca, Fe, Mn), probably masks any relationship between measured concentrations and analytical totals that might be anticipated to occur.

The X-ray lines used to determine **Fe, Mn, and Ca concentrations** are of relatively high energy and consequently X-ray absorption is less significant relative to the lower energy X-rays used to quantify the lighter elements. Consequently, errors in the calculation of X-ray absorption effects become of lesser significance with increasing atomic number.

Fe, Mn and Ca all display very good agreement between the data derived in the different analytical runs (Figure 3C-F).

3.2.3 Normalised Data

When analyses are normalised into formula units, based on a total of 24 oxygen atoms, as is normally the case when garnet analyses are presented, Al and Si concentrations determined on both instruments display a very close level of agreement with a strong clustering of analyses around the expected values of 4 and 6 formula units respectively (Figure 5). This indicates that, whilst the poor constraint on beam-sample-detector geometry adversely affects quantification for light elements, relative proportions of elements appear to be reliable.

Garnet are commonly represented using triangular diagrams, which plot the relative proportions of Mg (pyrope end member), Fe+Mn (Almandine and Spessartine) and Ca (Grossular). A key factor in assessing the suitability of the S360 for analysis of garnets is in the quality of the data when plotted in this manner. Figure 6 is a series of triangular diagrams for each analytical run, showing the overall distribution of data. It is clear that analysis in all of the runs generates a remarkable level of consistency when the data are plotted in this manner, with the same general groupings of garnet compositional types observed in all three datasets.

When the data is explored in more detail, it is apparent that individual garnet grains typically plot in the same position on the diagram irrespective of the instrument used to generate the data (see plots in Appendix 2).

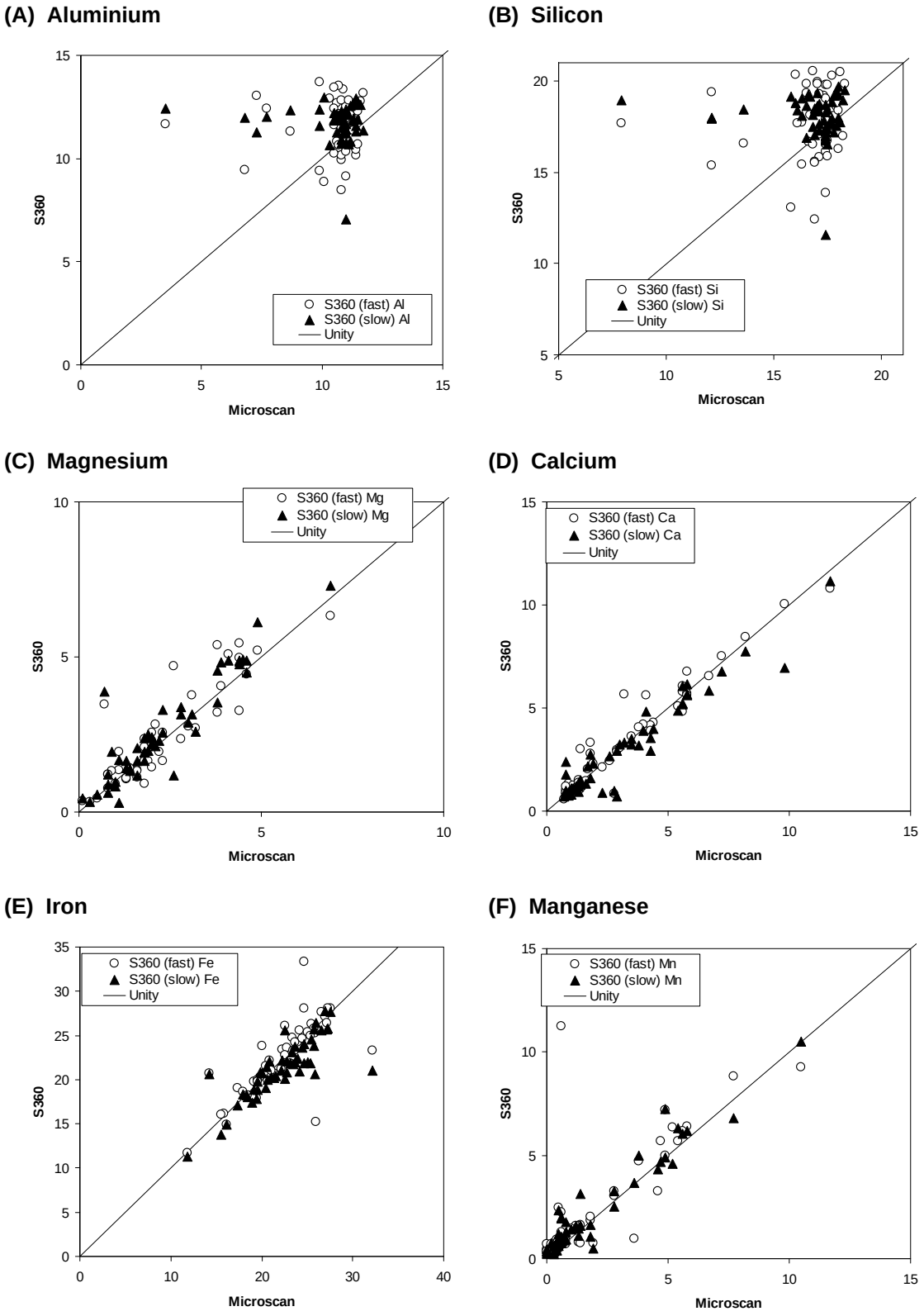


Figure 3 Comparison of garnet elemental data derived using the Microscan and the S360.

All plots have element % determined using the Microscan on the X axis, and element % determined using the S360 plotted on the Y axis. Closed symbols compare date from the Microscan run with date from the S60-slow run, open symbols compare date from the Microscan run with date from the S360-fast run.

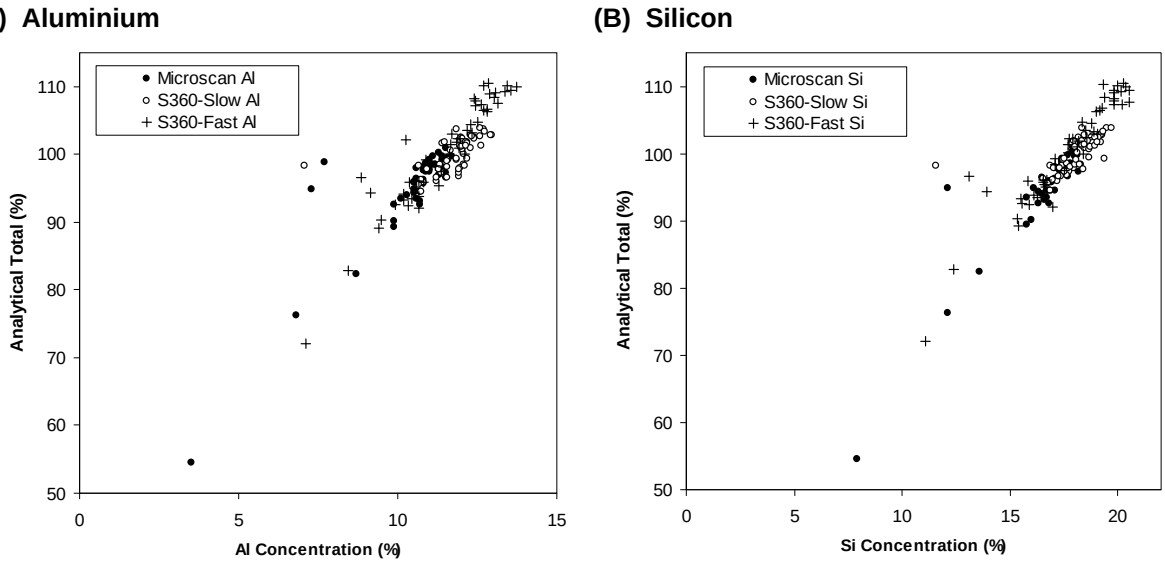


Figure 4 Relationship between light-element concentrations and analytical total in garnets. For all the analytical runs, a strong relationship between Al and Si concentrations and analytical total is observed.

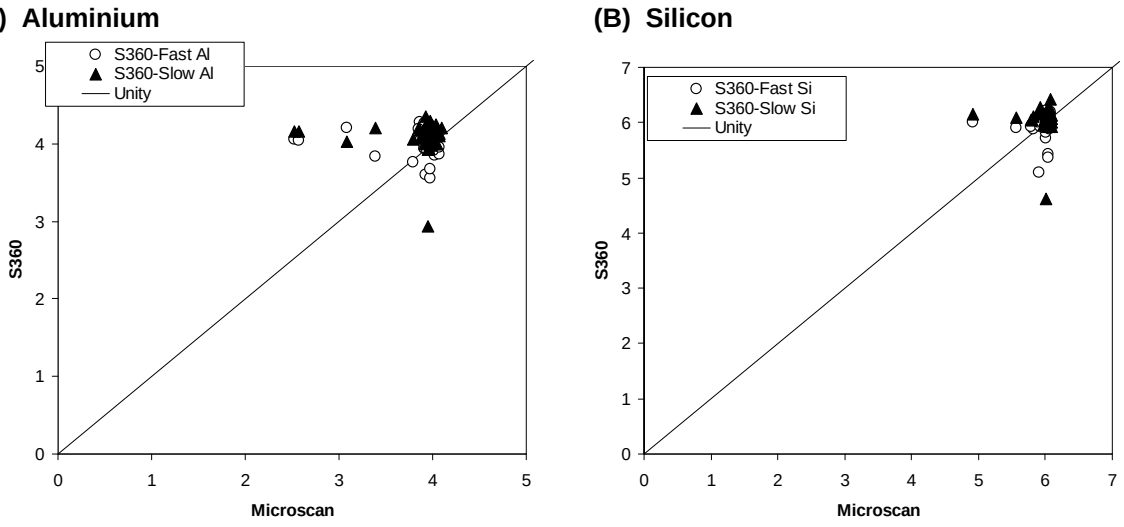
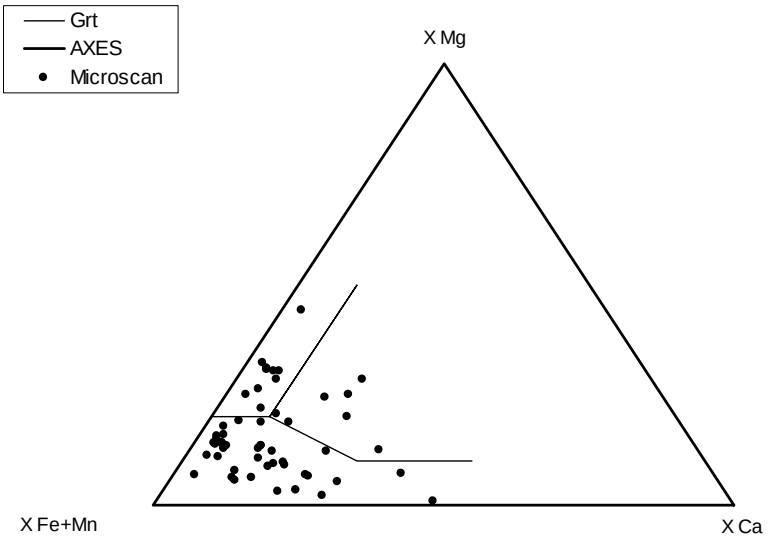
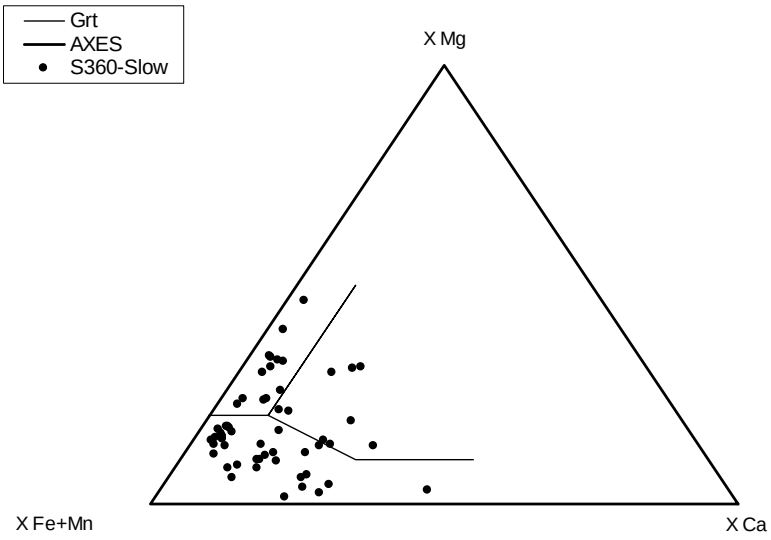


Figure 5 Cross plots comparing data normalised into formula units for garnet analyses. Data from both instruments show a high degree of clustering around 4 formula units Al, and 6 formula units Si, which are the expected values for garnets.

(A) Microscan



(B) S360 Slow



(C) S360 fast

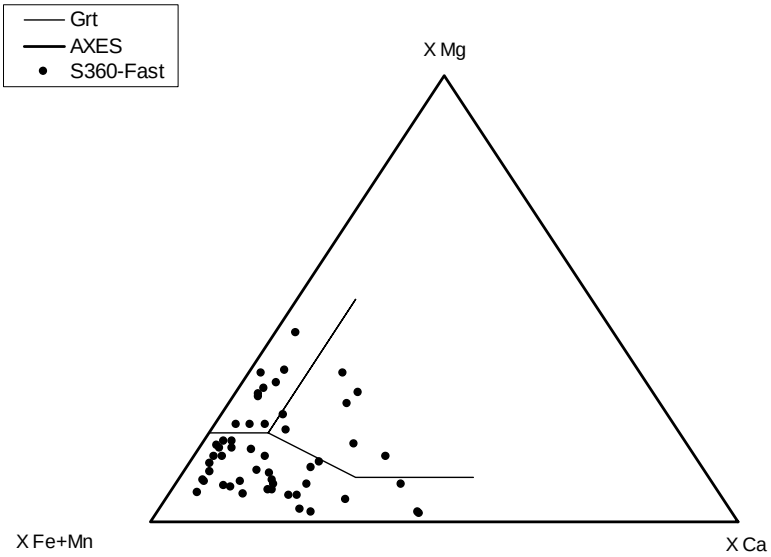


Figure 6 Triangular diagrams of the type used for discriminating different garnet populations with different chemistries. Excellent agreement is observed between the different analytical runs.

3.3 TOURMALINE ANALYSES

3.3.1 Analytical Totals

Analyses generated using the **Microscan** return analytical totals in the range 78-85% (Figure 7A). As seen for the garnet analyses, this distribution is skewed towards the higher totals in this range. However, none of the analyses yield totals within the ideal range for tourmaline (i.e. 85-88%).

The **S360** data (Figure 7B) show a broader spread of analytical totals, with a more even "normal"-style distribution of values than is seen in the Microscan data. Importantly however, it proved possible to obtain a greater proportion of analyses within the "ideal" range for tourmaline (85-88%) using this instrument relative to the Microscan.

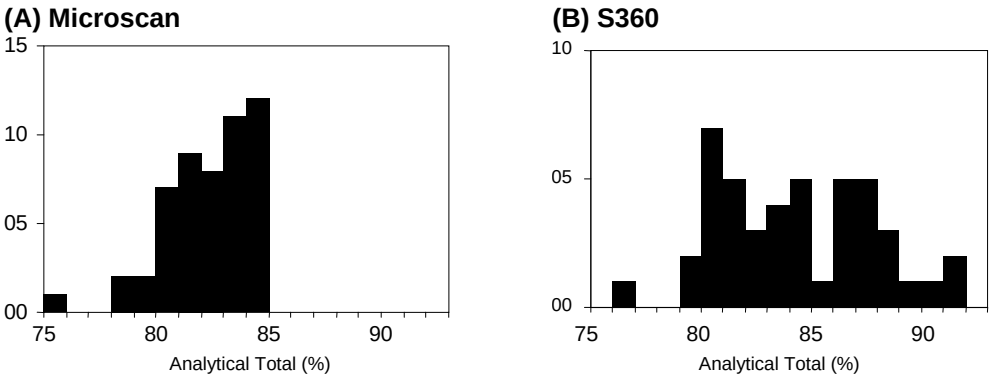


Figure 7 Frequency distributions for analytical totals obtained from the tourmaline analyses.

3.3.2 Compositional data

Figure 8 and Figure 9 use cross plots to compare concentration data (as raw element weight %) derived using the Microscan and the S360 for most of the elements analysed during this test. As seen for the garnet data, for the major elements very good agreement between the data derived using the Microscan and that derived using the S360 is observed. As expected, the degree of scatter increases in the plots for the less abundant elements as detection limits are approached and analytical uncertainty increases.

The relationship between Si, Al concentrations and analytical total seen in the garnet analyses is also evident within the tourmaline data, and can be explained in the same manner.

3.3.3 Normalised Data

When the data are normalised into formula units (on the basis of 24 oxygen atoms) as is conventional for tourmaline analyses where boron data is not reported, Al and Si concentrations determined on both instruments display a very close level of agreement with a strong clustering of analyses around the expected values of 5.5-6.5 and 6 formula units for Al and Si respectively (Figure 10). Cation totals are also broadly comparable between the two instruments (Table 7 and Table 8).

As for garnets, tourmaline analyses are commonly presented graphically through the use of triangular diagrams, which plot the relative proportions of Al (Elbaite end member $[Na(Li,Al)_3Al_6B_3Si_6O_{27}(OH,F)_4]$), Fe (Schorl $[Na(Fe,Mn)_3Al_6B_3Si_6O_{27}(OH,F)_4]$) and Mg (Dravite $[NaMg_3Al_6B_3Si_6O_{27}(OH,F)_4]$). A key factor in assessing the suitability of the S360 for

analysis of tourmalines is in the quality of the data when plotted in this manner. Figure 11 is a pair of triangular diagrams for showing the overall distribution of data derived using the Microscan and the S360. It is clear that analysis in all of the runs generates a remarkable level of consistency when the data are plotted in this manner, with the same general groupings of tourmaline compositional types observed in both datasets.

When the data is explored in more detail, it is apparent that individual grains typically plot in the same position on the diagram irrespective of the instrument used to generate the data (see plots in Appendix 3).

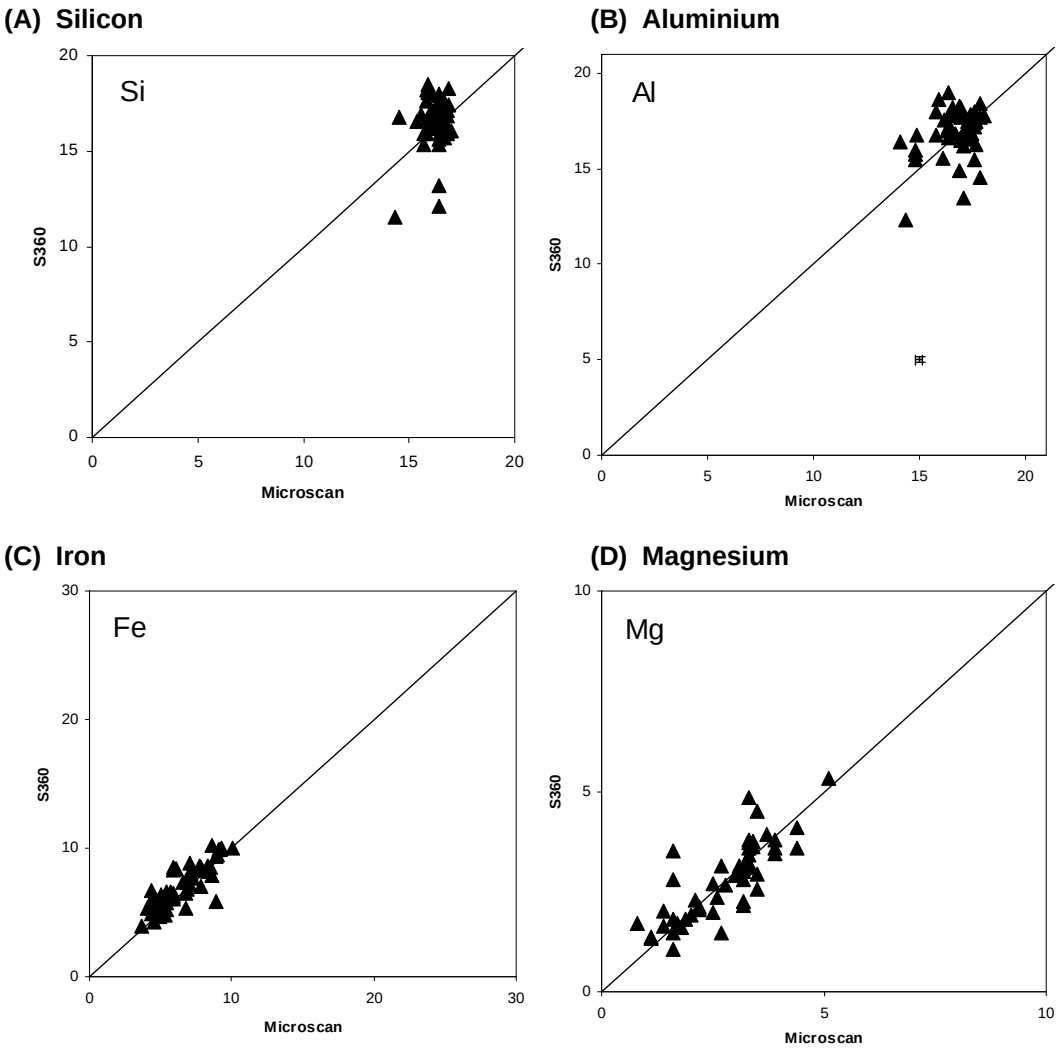


Figure 8 Comparison of tourmaline major element data derived using the Microscan and the S360.

All plots have element % determined using the Microscan on the X axis, and element % determined using the S360 plotted on the Y axis. The solid line on all plots represents unity, which is where all the analyses should, theoretically, plot. Statistical counting errors are smaller than the symbols used to plot the analyses.

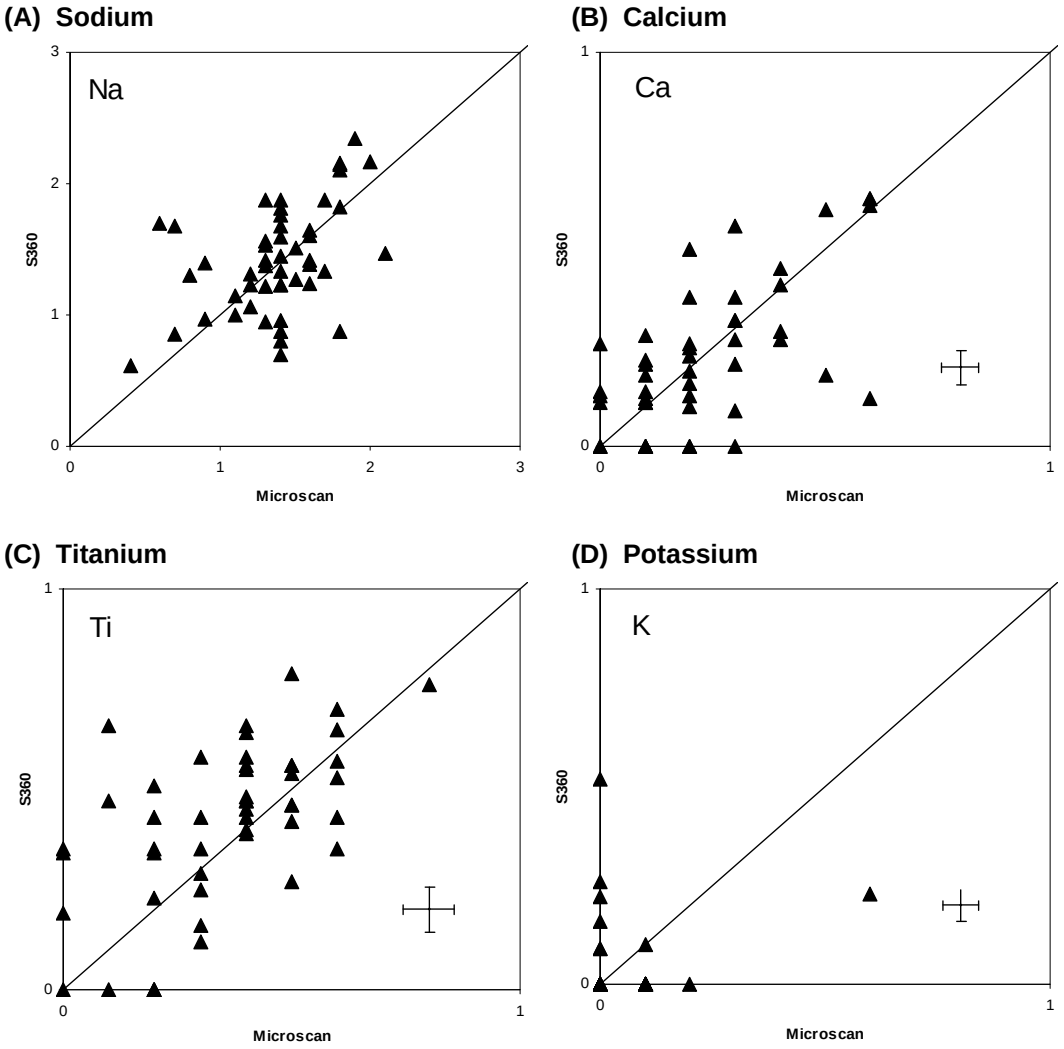


Figure 9 Comparison of tourmaline minor element data derived using the Microscan and the S360.

All plots have element % determined using the Microscan on the X axis, and element % determined using the S360 plotted on the Y axis. The solid line on all plots represents unity, which is where all the analyses should plot. Representative error bars are shown for Ca, Ti and K.

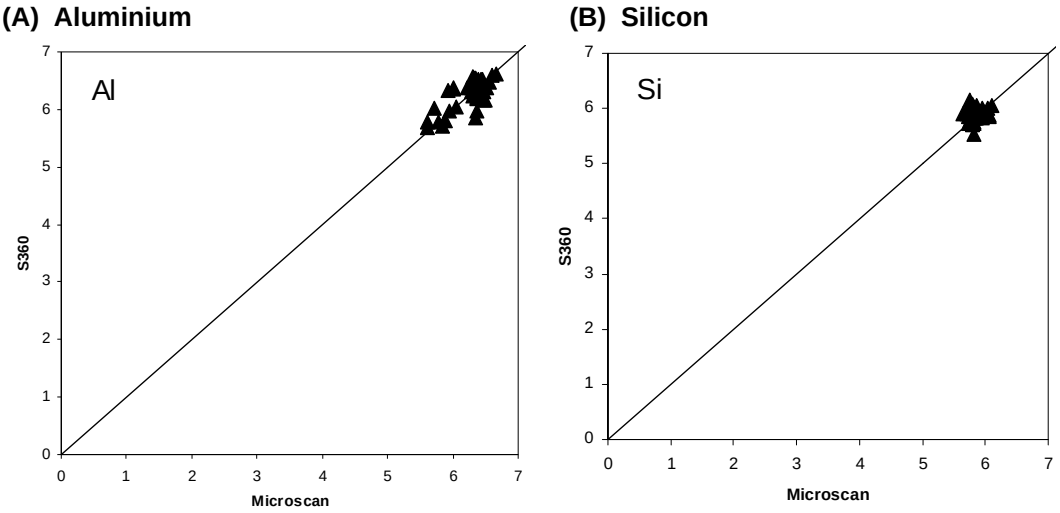
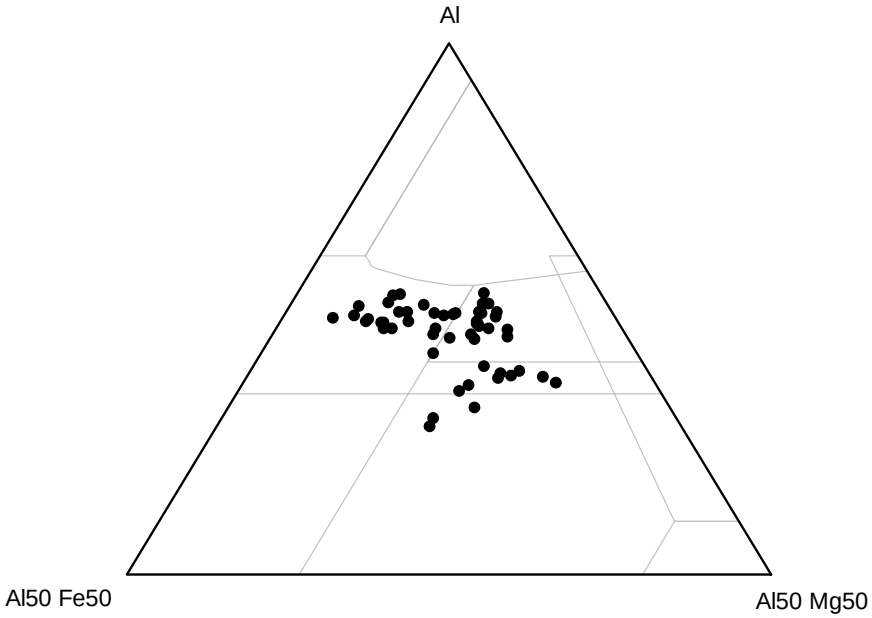


Figure 10 Cross plots comparing data normalised into formula units for tourmaline analyses. Data from both instruments show a high degree of clustering around 5.5-6.5 formula units Al, and 6 formula units Si, which are the expected values for tourmaline.

(A) Microscan



(B) S360

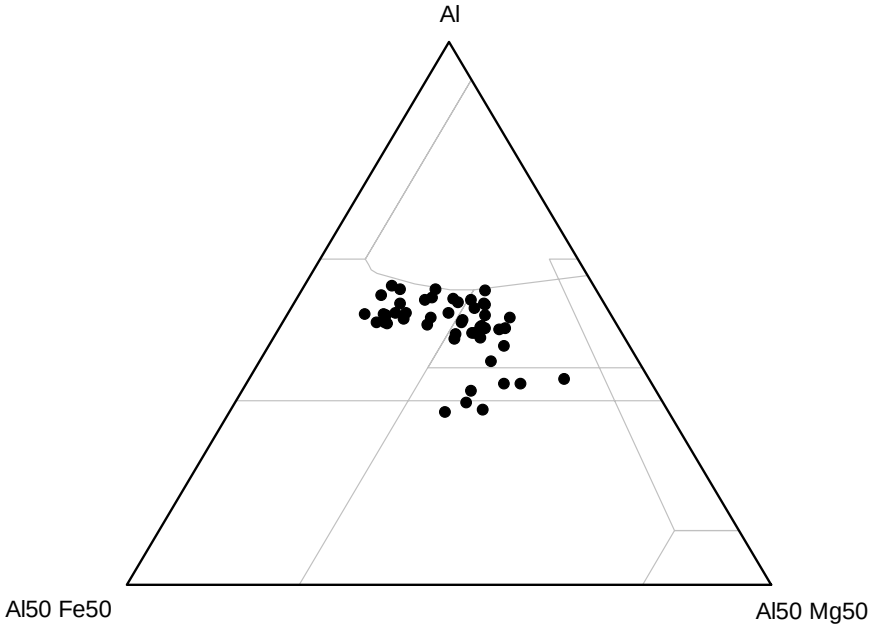


Figure 11 Triangular diagrams of the type used for discriminating different tourmaline populations with different chemistries. Excellent agreement is observed between the different analytical runs.

3.4 G-PROBE ANALYSIS

"G-Probe" is an approximately bi-annual proficiency test for microprobe laboratories organised by the International Association of Geoanalysts (IAG), which is designed to measure and report the average composition of an unknown sample using *routine* microprobe tests. BGS participated in round 2 of this test (G-Probe-2; Potts *et al.* 2006) and submitted data generated by our Cameca SX-50 microprobe only. Our performance in G-probe-2 was very good and all the elements analysed (with the exception of P and Ba; these are elements we don't normally analyse and consequently we don't have well-defined calibrations for them) were well within the "satisfactory" range. Indeed a comparison of the scores for the individual laboratories places our data within the top 10 of the approximately 60 labs that participated in G-Probe-2 (Figure 12).

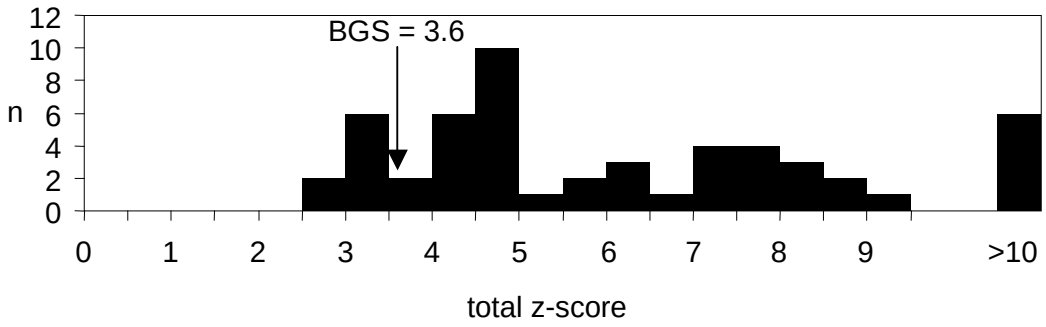


Figure 12 Comparison of BGS data relative to data from other labs participating in the G-Probe-2 proficiency test.

This plot was constructed by summing together the absolute "z-scores" for each element determined by a given laboratory, and then plotting these as a histogram. The z-score reflects the accuracy of the analyses relative to the known actual concentration for a given determinant, with a score of zero indicating a perfect match between the analysed and the known concentration. Therefore, a perfect analysis which exactly matched the composition of the unknown sample for all elements, would have a total Z-score of zero, and progressively less accurate analyses have progressively higher total z-scores. This compilation excludes P determinations for all laboratories, as we do not currently have a "good" calibration for P on the SX50.

We have just completed the latest round of this test (G-Probe-3) using the SX50. We also took the opportunity to analyse the unknown sample using the S360, to enable a direct comparison of results from this instrument with results from the SX-50, which will ultimately be compared with a number of other international microbeam analysis laboratories.

The sample comprised 2 pieces of fused glass, of unknown composition. These were prepared as polished blocks. The use of a polished block enabled us to remove the uncertainty introduced into the S360 analyses by the rough surfaces of the previously-analysed heavy mineral grain mounts. Table 3 and Figure 13 give summary results from both the SX50 and the S360 analyses and it is apparent that the results derived using the S360 are within error of those derived from the SX50 over the concentration range c. 0.2-55 oxide wt%. This gives us a significant degree of confidence in the validity of our existing calibrations on the S360.

Note the higher precision, expressed in terms of standard deviations, of the SX50 relative to the S360 reflects the fact that the SX50 analyses were conducted using, the inherently more precise, wavelength-dispersive rather than energy-dispersive spectrometry. Unfortunately, no comparable data are available from the Microscan microprobe as the instrument was unusable at the time of analysis due to problems with the gun and/or gun power supply.

Table 3 Summary SX50 and S360 analyses of the G-Probe-3 glass sample.

	SX50 DATA				S360 DATA			
Glass piece #	1		2		1		2	
n	5		5		15		15	
	Mean	St. Dev.	Mean	St. Dev.	Mean	St. Dev.	Mean	St. Dev.
SiO2	53.788	0.193	54.006	0.121	53.57	0.52	53.44	0.44
TiO2	1.065	0.061	1.111	0.022	1.17	0.12	1.24	0.16
Al2O3	18.527	0.061	17.944	0.139	18.95	0.33	18.5	0.36
Fe2O3T	9.460	0.209	9.465	0.113	9.38	0.37	9.57	0.32
MnO	0.225	0.035	0.218	0.045	0.23	0.10	0.25	0.12
MgO	4.217	0.019	4.272	0.040	4.14	0.14	4.14	0.18
CaO	7.057	0.062	7.067	0.083	7.18	0.22	7.31	0.21
Na2O	2.817	0.053	3.043	0.039	3.06	0.21	3.22	0.23
K2O	1.745	0.025	1.794	0.046	1.77	0.15	1.75	0.07
P2O5	0.307	0.022	0.339	0.017	n/a	n/a	n/a	n/a
TOTAL	99.208	-	99.259	-	99.450	-	99.420	-

(A) Glass 1 **(B) Glass 2**

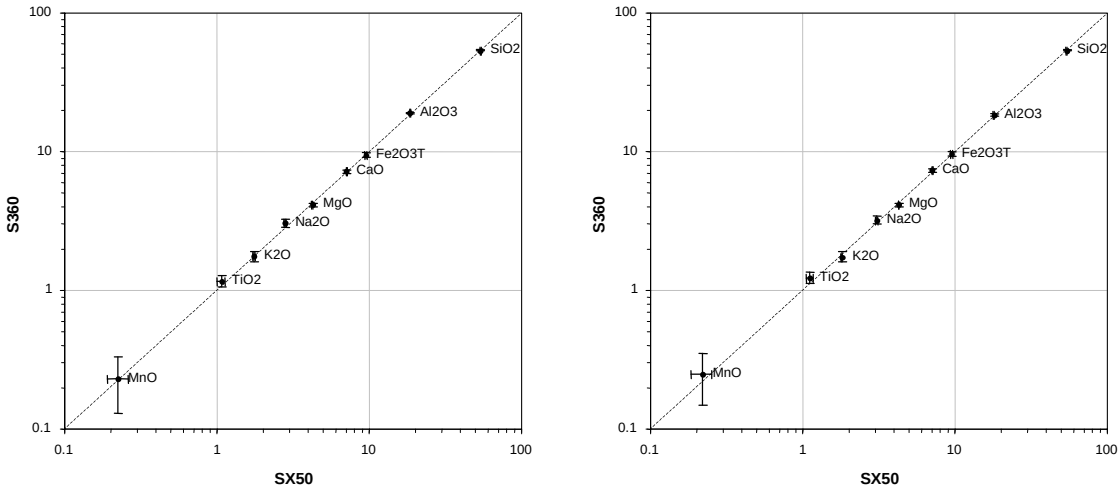


Figure 13 Comparison of S360 data and SX50 data for G-Probe-3 analyses. Note, that the analyses plot within error of unity.

4 Conclusions

The results of this study are very promising and it is our recommendation that the S360 can and should be used to undertake analyses of rough surfaces of heavy mineral grain mounts currently undertaken on the Microscan.

- The S360 is capable of producing data of equivalent quality to that generated using the old Microscan 5 electron microprobe. We have a high level of confidence in the quality of the calibrations on the S360 as evidenced by the excellent agreement observed between data generated from polished blocks using the S360 with data from the Cameca SX50 electron microprobe on the same blocks.
- The S360 has more modern analysis software making extraction of analysis data from the system at the end of a run much simpler (simple copy and paste into MS Excel) than is possible using the Microscan.
- During the first batch of analyses on garnets it proved difficult and significantly more time-consuming to locate suitable analysis points using the S360 than had been previously possible on the Microscan. However, during the subsequent round of tourmaline analyses, after additional operator experience of the instrument had been gained, this problem became notably less pronounced and similar analysis times/sample throughputs can now be achieved using the S360 as were possible on the Microscan.
- The results from the Microscan and the S360 differ slightly in that, using the Microscan it is relatively unusual to derive an analytical total in excess of the theoretical maximum for a mineral (i.e. 100% for garnet and 88% for tourmaline), and histograms of analytical totals are typically positively skewed towards the “correct” maximum value. In contrast, on the S360, histograms of analytical totals tend to be centred around the “correct” value, in approximately normal distributions, with the degree of scatter around the mean largely controlled by the amount of experience the operator has in identifying (and/or the amount of effort/time that can be spent locating) suitable analysis points that present perpendicular, flat surfaces to the X-ray detector.
- Normalised data generated using the S360 are indistinguishable from those derived using the Microscan. This applies to analyses gathered paying very careful attention to analytical total, and also to analyses where analytical totals are less carefully considered.
- The largest source of error in the determination of absolute abundances in the analyses is the poorly constrained sample geometry. This influences the results from both the Microscan and the S360, although it appears to be marginally more significant in the S360 relative to the Microscan due to its lower take-off angle. However, as noted above it is possible to minimise the effects of this through careful selection of analysis points.
- In order to remove this uncertainty the use of polished surfaces is recommended. In this case, it would be possible to automate the analysis to a higher degree using the new X-ray analysis hardware/software that will soon be commissioned at BGS and hence to increase analytical throughput and data quality further.

5 References

P.J.Potts, Thompson, M. and Wilson, S. 2002 G-Probe-1 - An international proficiency test for microprobe laboratories-Report on round 1: February 2002 (TB-1 basaltic glass). Geostandards Newsletter Vol. 26, p. 197-235.

Potts P.J., Thompson M., Wilson S.A. and Webb P.C. 2006 G-Probe-2 An international proficiency test for microbeam laboratories Report on Round 2 / May 2005 (NKT-1G basaltic glass). Geostandards and Geoanalytical Research Vol.30.

Appendix 1 Data Listings

For all the data listings in this appendix the analytical totals are colour-coded according to the nearness of the total to the ideal value.

For garnet:

blue	98-100%	
green	95-98%	100-103%,
yellow	90-95%	103-105%,
orange	<90%	>105%

For Tourmaline:

blue	85-88%	
green	82-85%	88-91%,
yellow	79-82%	91-94%,
orange	<79%	>94%

Table 4 EDXA data for garnet derived from Microscan run.

		Microscan Data																		
Garnet Grain ID	Spectrum Label	Element %										Formula Units (24 Oxygens)								
		Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	O	Total	Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Total Cations
GNT1	GT1	18.3	-	11.3	17.3	0.4	4.4	5.6	-	41.1	98.3	6.09	-	3.91	2.89	0.07	1.69	1.31	-	15.96
GNT2	GT2	16.5	-	10.3	20.9	5.8	0.8	2.6	-	37.1	94.0	6.08	-	3.95	3.87	1.09	0.34	0.67	-	16.01
GNT3	GT3	17.1	-	10.9	21.4	3.8	0.5	5.6	-	38.9	98.1	6.01	-	3.99	3.78	0.68	0.20	1.38	-	16.05
GNT4	GT4	17.4	-	11.0	15.8	2.8	1.1	9.8	-	39.6	97.5	6.01	-	3.95	2.74	0.49	0.44	2.37	-	16.01
GNT5	GT5	17.8	0.1	11.2	18.3	0.8	1.9	8.2	-	40.2	98.5	6.05	0.02	3.96	3.13	0.14	0.75	1.95	-	16.01
GNT6	GT6	17.5	-	10.8	19.8	4.9	1.8	3.5	-	39.3	97.7	6.09	-	3.91	3.46	0.87	0.72	0.85	-	15.91
GNT7	GT7	17.3	-	11.0	27.0	0.5	2.0	0.9	-	39.0	97.5	6.06	-	4.01	4.76	0.09	0.81	0.22	-	15.96
GNT7	GT8	16.7	-	10.6	22.8	1.7	2.7	1.2	-	37.7	93.4	6.06	-	4.00	4.16	0.32	1.13	0.30	-	15.97
GNT8	GT9	18.1	-	11.7	19.4	1.3	3.8	4.4	-	41.1	99.7	6.02	-	4.05	3.25	0.22	1.46	1.03	-	16.03
GNT9	GT10	17.4	-	10.8	27.6	0.5	1.6	1.4	-	39.0	98.2	6.10	-	3.94	4.87	0.09	0.65	0.34	-	15.99
GNT10	GT11	17.5	-	10.9	27.2	0.4	2.1	1.2	-	39.4	98.6	6.07	-	3.94	4.75	0.07	0.84	0.29	-	15.96
GNT11	GT12	12.1	-	6.8	25.8	1.4	0.9	0.8	-	28.5	76.3	5.80	-	3.40	6.22	0.34	0.50	0.27	-	16.54
GNT12	GT13	15.8	-	10.1	24.7	3.6	1.6	0.9	0.2	36.6	93.5	5.90	-	3.93	4.64	0.69	0.69	0.24	0.04	16.12
GNT13	GT14	17.1	-	10.7	22.3	-	4.6	1.0	-	38.8	94.5	6.03	-	3.92	3.95	-	1.87	0.25	-	16.02
GNT14	GT15	16.9	-	10.8	26.0	0.6	1.8	1.4	-	38.2	95.7	6.05	-	4.02	4.68	0.11	0.74	0.35	-	15.96
GNT15	GT16	17.4	-	11.4	23.2	2.8	1.9	2.9	-	39.8	99.2	5.98	-	4.08	4.01	0.49	0.75	0.70	-	16.01
GNT16	GT17	17.1	-	10.6	16.1	10.5	1.6	3.2	-	38.9	97.9	6.01	-	3.88	2.85	1.89	0.65	0.79	-	16.06
GNT17	GT18	16.8	-	10.7	20.6	0.6	4.4	1.3	-	38.2	92.7	6.01	-	3.99	3.71	0.11	1.82	0.33	-	15.96
GNT18	GT19	16.9	-	10.8	23.4	0.7	1.3	4.3	-	38.3	95.7	6.03	-	4.01	4.20	0.13	0.54	1.08	-	15.99
GNT19	GT20	16.5	-	10.6	24.2	0.3	4.1	1.3	0.7	38.7	96.4	5.83	-	3.90	4.30	0.05	1.67	0.32	0.13	16.21
GNT20	GT21	12.1	-	7.3	32.2	0.8	1.1	4.1	3.6	33.7	94.8	4.91	-	3.08	6.57	0.17	0.52	1.17	0.79	17.20
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT21	GT22	17.6	-	11.3	21.1	0.8	4.6	1.6	-	40.0	97.0	6.02	-	4.02	3.63	0.14	1.82	0.38	-	16.00
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT22	GT23	17.4	-	11.0	24.0	1.8	1.4	4.0	-	39.5	99.1	6.02	-	3.96	4.18	0.32	0.56	0.97	-	16.01
-	GT24	15.8	-	9.9	17.9	5.2	0.4	4.3	0.2	35.6	89.3	6.07	-	3.96	3.46	1.02	0.18	1.16	0.04	15.88
GNT23	GT25	18.0	-	11.4	24.5	0.5	3.8	0.9	-	40.6	99.6	6.06	-	4.00	4.15	0.09	1.48	0.21	-	15.98
GNT24	GT26	16.6	-	10.7	25.5	0.3	1.9	0.8	-	37.4	93.2	6.07	-	4.07	4.69	0.06	0.80	0.20	-	15.89
GNT25	GT27	17.4	-	11.1	17.9	4.6	0.8	7.2	-	39.6	98.6	6.01	-	3.99	3.11	0.81	0.32	1.74	-	15.98
GNT26	GT28	26.2	-	7.7	14.2	4.9	0.8	1.7	-	43.4	98.8	8.25	-	2.52	2.25	0.79	0.29	0.38	-	14.48
GNT27	GT29	17.4	-	10.9	27.3	-	2.2	0.8	-	39.0	97.4	6.10	-	3.98	4.81	-	0.89	0.20	-	15.98
GNT28	GT30	18.0	-	11.6	22.8	-	4.4	1.8	-	41.0	99.6	6.00	-	4.03	3.82	-	1.70	0.42	-	15.97
GNT29	GT31	17.7	-	11.0	22.8	0.4	2.8	3.5	-	39.8	97.8	6.08	-	3.93	3.94	0.07	1.11	0.84	-	15.98
GNT30	GT32	16.3	-	9.9	11.8	5.6	0.1	11.7	-	37.1	92.6	6.01	-	3.80	2.19	1.06	0.04	3.02	-	16.11
GNT30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT31	GT33	17.1	-	10.8	20.5	1.3	1.8	5.8	-	38.9	96.3	6.01	-	3.95	3.62	0.23	0.73	1.43	-	15.98
GNT32	GT34	17.8	0.2	11.4	22.6	-	4.9	0.7	-	40.6	98.2	5.99	0.04	4.00	3.83	-	1.91	0.17	-	15.93
GNT33	GT35	17.7	-	11.5	21.6	0.3	4.5	1.0	-	40.0	96.6	6.05	-	4.09	3.71	0.05	1.78	0.24	-	15.92
GNT34	GT36	16.9	-	10.8	25.8	0.5	2.3	1.0	-	38.4	95.8	6.02	-	4.00	4.62	0.09	0.95	0.25	-	15.93
GNT35	GT37	17.9	-	11.3	22.6	1.9	3.2	2.8	-	40.6	100.3	6.03	-	3.96	3.83	0.33	1.25	0.66	-	16.05
GNT36	GT38	16.7	-	10.7	19.1	0.4	3.0	5.8	0.3	38.6	94.6	5.92	-	3.94	3.40	0.07	1.23	1.44	0.06	16.06
GNT37	GT39	17.4	0.1	11.0	20.7	5.2	1.3	3.8	-	39.5	98.9	6.02	0.02	3.96	3.60	0.92	0.52	0.92	-	15.97
GNT38	GT40	16.0	-	9.9	22.2	0.6	3.1	1.8	-	36.4	90.1	6.01	-	3.87	4.19	0.12	1.35	0.47	-	16.01
GNT38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT39	GT41	18.0	-	11.2	18.9	0.4	3.9	5.4	-	40.7	98.5	6.05	-	3.92	3.19	0.07	1.51	1.27	-	16.01
GNT40	GT42	17.0	-	10.5	26.6	0.2	2.0	1.1	0.2	38.2	95.8	6.08	-	3.91	4.79	0.04	0.83	0.28	0.04	15.96
GNT41	GT43	16.8	-	10.7	23.7	0.8	1.4	4.3	-	38.3	96.0	6.00	-	3.98	4.25	0.15	0.58	1.08	-	16.03
GNT42	GT44	18.2	-	11.5	18.4	0.3	6.9	0.9	-	41.2	97.3	6.04	-	3.97	3.07	0.05	2.65	0.21	-	15.99
GNT43	GT45	17.4	-	10.9	23.5	0.6	1.0	5.6	-	39.3	98.2	6.05	-	3.95	4.11	0.11	0.40	1.37	-	15.99
GNT44	GT46	7.9	-	3.5	20.0	1.2	0.7	1.9	-	19.4	54.6	5.57	-	2.57	7.09	0.43	0.57	0.94	-	17.16
GNT45	GT47	17.7	0.1	11.1	19.5	4.7	1.0	5.8	-	40.0	99.8	6.05	0.02	3.95	3.35	0.82	0.39	1.39	-	15.98
GNT46	GT48	13.6	-	8.7	19.5	5.4	1.8	1.3	-	32.1	82.3	5.79	-	3.86	4.18	1.18	0.89	0.39	-	16.28
GNT47	GT49	17.0	-	10.5	15.5	7.7	0.3	6.7	-	38.2	95.9	6.08	-	3.91	2.79	1.41	0.12	1.68	-	16.00
GNT48	GT50	16.3	-	10.5	25.1	1.4	2.6	0.8	-	37.6	94.3	5.93	-	3.97	4.59	0.26	1.09	0.20	-	16.05
GNT49	GT51	17.5	-	11.0	23.7	1.0	2.8	2.3	-	39.5	97.8	6.06	-	3.96	4.13	0.18	1.12	0.56	-	16.00
GNT50	GT52	16.1	-	10.5	25.9	1.8	2.3	0.8	-	37.4	94.8	5.89	-	4.00	4.76	0.34	0.97	0.20	-	16.16
GNT51	GT53	17.4	-	11.0	24.7	0.6	2.0	2.9	-	39.4	98.1	6.04	-	3.97	4.31	0.11	0.80	0.71	-	15.94
GNT52	GT54	17.9	-	11.5	25.4	0.5	2.0	3.0	-	40.6	100.9	6.03	-	4.03	4.30	0.09	0.78	0.71	-	15.93

Table 5 EDXA data for garnet derived from S360 FAST run.

		S360 "FAST" data																		
Garnet Grain ID	Spectrum Label	Element %										Formula Units (24 Oxygens)								
		Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	O	Total	Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Total Cations
GNT1	Spectrum 1	19.8	0.1	12.5	19.1	0.5	5.0	5.8	0.2	45.0	107.9	6.03	0.01	3.94	2.91	0.08	1.74	1.24	0.04	15.98
GNT2	Spectrum 2	19.8	-	12.9	22.2	6.4	1.2	2.4	0.1	44.0	109.0	6.16	-	4.17	3.46	1.01	0.43	0.53	0.01	15.76
GNT3	Spectrum 3	17.1	0.2	10.9	20.8	4.7	0.5	6.0	-	39.2	99.3	5.95	0.03	3.95	3.64	0.84	0.18	1.47	-	16.07
GNT4	Spectrum 4	19.8	0.1	12.6	16.2	3.1	1.4	10.1	-	44.3	107.3	6.12	0.01	4.06	2.51	0.48	0.48	2.18	-	15.85
GNT5	Spectrum 5	18.9	-	12.3	18.1	0.7	2.3	8.5	-	42.6	103.2	6.06	-	4.12	2.92	0.12	0.86	1.90	-	15.97
GNT6	Spectrum 6	16.7	-	10.6	20.3	5.0	1.6	3.6	-	38.2	96.0	5.98	-	3.94	3.65	0.91	0.68	0.91	-	16.07
GNT7	Spectrum 7	19.2	-	12.7	27.1	0.9	2.6	0.8	-	43.2	106.4	6.07	-	4.19	4.32	0.15	0.93	0.19	-	15.84
GNT7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT8	Spectrum 8	20.5	-	13.2	17.9	0.8	5.4	4.3	-	45.6	107.6	6.15	-	4.10	2.70	0.12	1.86	0.90	-	15.83
GNT9	Spectrum 9	16.5	-	10.4	28.1	0.8	1.4	1.1	0.1	37.6	95.8	6.01	-	3.93	5.13	0.14	0.57	0.27	0.01	16.05
GNT10	Spectrum 10	19.8	0.1	13.4	26.4	0.9	2.8	1.2	0.0	44.7	109.3	6.06	0.02	4.26	4.06	0.14	1.00	0.26	0.00	15.79
GNT11	Spectrum 11	15.4	0.0	9.5	26.1	1.7	1.3	1.0	0.1	35.2	90.3	5.96	0.00	3.83	5.10	0.33	0.59	0.27	0.02	16.11
GNT12	Spectrum 13	13.1	-	8.9	33.3	1.0	1.1	1.3	2.8	35.1	96.6	5.09	-	3.59	6.52	0.19	0.50	0.37	0.59	16.86
GNT13	Spectrum 12	18.5	0.9	12.2	23.5	0.3	4.4	1.0	0.1	42.7	103.5	5.93	0.17	4.06	3.78	0.05	1.64	0.22	0.02	15.86
GNT14	Spectrum 14	12.4	0.1	8.5	15.3	11.3	0.9	3.0	0.1	31.3	82.8	5.43	0.03	3.85	3.36	2.52	0.46	0.92	0.03	16.60
GNT15	Spectrum 15	16.7	-	10.2	21.9	3.3	1.7	3.0	-	37.6	94.1	6.09	-	3.86	4.01	0.60	0.70	0.76	-	16.01
GNT16	Spectrum 16	15.8	0.2	10.8	14.9	9.3	1.3	5.7	0.1	37.9	96.0	5.71	0.04	4.06	2.71	1.71	0.55	1.44	0.01	16.21
GNT17	Spectrum 17	20.5	0.1	13.5	21.3	0.8	5.5	1.5	0.1	46.1	109.4	6.09	0.02	4.18	3.18	0.12	1.87	0.31	0.02	15.79
GNT18	Spectrum 18	15.6	-	9.9	24.8	0.7	1.1	4.1	0.1	36.3	92.5	5.87	-	3.90	4.70	0.14	0.47	1.09	0.02	16.19
GNT19	Spectrum 19	19.4	0.1	12.7	25.5	0.2	5.1	1.2	0.9	45.1	110.2	5.87	0.02	4.01	3.90	0.03	1.78	0.26	0.14	16.03
GNT20	Spectrum 20	19.4	0.1	13.0	23.3	1.1	1.9	5.6	-	44.1	108.4	6.00	0.01	4.20	3.62	0.17	0.69	1.22	-	15.92
-	Spectrum 21	11.1	0.1	7.1	21.1	0.9	2.9	1.3	-	27.7	72.0	5.48	0.01	3.66	5.23	0.22	1.64	0.46	-	16.70
GNT21	Spectrum 22	17.5	0.2	11.4	21.0	0.9	4.8	1.4	0.1	40.2	97.4	5.96	0.03	4.03	3.60	0.15	1.87	0.34	0.01	15.99
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT22	Spectrum 23	18.4	0.1	12.5	24.3	1.8	1.3	4.2	-	42.1	104.7	5.96	0.01	4.23	3.96	0.31	0.49	0.96	-	15.92
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT23	Spectrum 24	16.3	-	10.4	24.6	0.6	3.2	0.9	-	37.5	93.4	5.94	-	3.97	4.52	0.10	1.35	0.24	-	16.11
GNT24	Spectrum 25	16.7	0.1	10.5	26.3	0.6	2.1	0.8	0.0	37.9	95.1	6.02	0.02	3.95	4.77	0.12	0.89	0.21	0.00	15.99
GNT25	Spectrum 26	19.0	-	11.7	18.6	3.3	0.8	7.5	0.1	41.9	103.0	6.20	-	3.98	3.06	0.54	0.29	1.72	0.02	15.81
GNT26	Spectrum 27	20.2	-	12.4	20.7	7.2	1.2	2.0	-	43.6	107.2	6.33	-	4.06	3.26	1.15	0.44	0.45	-	15.69
GNT27	Spectrum 28	17.1	-	11.2	28.0	0.5	1.9	0.9	-	39.1	98.3	5.99	-	4.07	4.93	0.08	0.78	0.22	-	16.08
GNT28	Spectrum 29	19.0	0.1	12.8	23.6	0.7	3.3	3.3	-	43.5	106.3	5.97	0.02	4.19	3.73	0.12	1.18	0.73	-	15.93
GNT29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT30	Spectrum 30	15.4	-	9.4	11.7	6.2	0.3	10.8	0.1	35.5	89.2	5.94	-	3.77	2.27	1.22	0.15	2.91	0.01	16.27
GNT30	Spectrum 31	20.1	0.1	13.1	13.2	5.9	0.3	11.6	-	44.9	109.2	6.12	0.02	4.14	2.03	0.91	0.11	2.47	-	15.80
GNT31	Spectrum 32	19.3	0.1	12.8	21.5	1.6	2.1	5.7	-	43.7	106.7	6.03	0.01	4.18	3.39	0.25	0.76	1.25	-	15.87
GNT32	Spectrum 33	18.1	0.0	11.9	22.8	0.4	5.2	0.6	0.3	41.7	100.9	5.94	0.00	4.07	3.76	0.06	1.97	0.13	0.06	15.99
GNT33	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT34	Spectrum 34	15.5	0.0	10.2	25.7	2.5	1.7	1.1	0.2	36.4	93.2	5.83	0.01	3.97	4.86	0.47	0.72	0.28	0.03	16.16
GNT35	Spectrum 35	18.6	0.0	11.9	26.1	0.8	2.7	0.8	-	41.5	102.3	6.12	0.01	4.08	4.31	0.13	1.03	0.19	-	15.86
GNT36	Spectrum 36	18.2	0.0	11.8	19.8	0.7	2.8	6.8	-	41.7	101.8	5.96	0.01	4.04	3.27	0.12	1.05	1.56	-	16.01
GNT37	Spectrum 38	17.9	0.0	12.0	19.9	6.4	1.1	4.1	-	41.0	102.3	5.97	0.01	4.15	3.34	1.09	0.42	0.96	-	15.94
GNT38	Spectrum 37	20.4	0.1	13.7	21.2	2.2	3.8	2.8	0.0	45.8	109.9	6.08	0.02	4.27	3.18	0.34	1.30	0.58	0.00	15.77
GNT38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT39	Spectrum 39	18.4	0.0	12.1	18.1	0.6	4.1	5.1	-	41.8	100.0	6.02	0.00	4.13	2.98	0.09	1.54	1.17	-	15.93
GNT40	Spectrum 40	20.0	0.0	13.4	27.7	0.7	2.3	1.2	-	44.8	110.1	6.09	0.00	4.27	4.24	0.11	0.81	0.26	-	15.78
GNT41	Spectrum 41	16.6	-	10.7	24.3	1.2	1.4	3.9	0.1	38.1	96.0	5.94	-	3.98	4.38	0.21	0.58	0.98	0.01	16.09
GNT42	Spectrum 42	17.0	-	10.7	18.2	0.3	6.3	0.9	0.1	38.7	92.0	6.01	-	3.93	3.23	0.05	2.58	0.21	0.02	16.03
GNT43	Spectrum 43	16.1	0.1	10.7	23.3	0.7	0.9	4.8	-	37.3	93.8	5.92	0.02	4.07	4.30	0.12	0.37	1.24	-	16.04
GNT44	Spectrum 44	17.7	-	11.7	23.8	1.6	3.5	2.3	-	41.0	101.4	5.90	-	4.05	4.00	0.27	1.34	0.53	-	16.09
GNT45	Spectrum 45	20.3	0.2	12.8	20.0	5.7	0.9	5.6	0.1	44.9	110.4	6.18	0.03	4.07	3.06	0.88	0.32	1.20	0.01	15.76
GNT46	Spectrum 46	16.6	-	11.3	19.8	5.7	2.4	1.4	-	38.4	95.4	5.92	-	4.19	3.54	1.04	0.97	0.34	-	16.00
GNT47	Spectrum 47	19.8	0.1	12.4	16.1	8.8	0.3	6.6	0.2	43.8	108.2	6.18	0.03	4.03	2.52	1.41	0.12	1.43	0.04	15.76
GNT48	Spectrum 48	17.8	0.5	10.3	25.4	0.7	4.7	1.2	0.7	41.0	102.2	5.92	0.10	3.56	4.25	0.12	1.81	0.28	0.12	16.16
GNT49	Spectrum 49	15.9	0.1	10.3	23.3	1.5	2.4	2.1	0.0	36.8	92.3	5.89	0.02	3.99	4.34	0.28	1.01	0.56	0.00	16.10
GNT50	Spectrum 50	17.7	-	11.6	25.3	2.0	2.6	0.7	0.1	40.3	100.1	6.01	-	4.12	4.32	0.35	1.00	0.16	0.02	15.97
GNT51	Spectrum 51	13.9	0.1	9.2	28.1	1.3	1.5	2.9	2.0	35.5	94.3	5.36	0.03	3.67	5.44	0.25	0.65	0.78	0.41	16.57
GNT52	Spectrum 52	18.8	0.1	12.3	25.0	0.5	2.2	3.1	0.0	42.4	104.4	6.06	0.02	4.13	4.05	0.08	0.82	0.69	0.01	15.86

Table 6 EDXA data for garnet derived from S360 SLOW run.

		S360 "SLOW" data																		
Garnet Grain ID	Spectrum Label	Element %										Formula Units (24 Oxygens)								
		Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	O	Total	Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Total Cations
GNT1	Spectrum 1	19.5	0.2	12.7	17.0	0.4	4.9	5.2	-	43.9	103.8	6.07	0.03	4.12	2.67	0.07	1.76	1.14	-	15.85
GNT2	Spectrum 2	16.9	0.1	10.7	22.0	6.2	0.9	2.7	0.2	38.6	98.3	5.98	0.02	3.93	3.92	1.12	0.36	0.66	0.04	16.03
GNT3	Spectrum 3	18.4	0.1	11.8	20.2	5.0	0.6	6.1	0.1	41.6	103.8	6.04	0.02	4.05	3.34	0.84	0.21	1.39	0.01	15.91
GNT4	Spectrum 4	11.6	0.0	7.1	30.7	2.5	0.3	7.0	4.9	34.2	98.2	4.63	0.00	2.94	6.17	0.51	0.13	1.95	1.05	17.38
GNT5	Spectrum 5	17.2	-	10.8	18.2	0.9	2.0	7.8	0.1	39.1	96.0	6.02	-	3.94	3.20	0.17	0.80	1.90	0.02	16.05
GNT6	Spectrum 6	16.6	-	10.7	20.8	4.9	1.7	3.5	0.0	38.2	96.3	5.92	-	4.00	3.75	0.89	0.68	0.87	0.01	16.12
GNT7	Spectrum 7	17.9	-	11.4	27.8	1.0	2.2	0.8	0.1	40.5	101.6	6.03	-	4.01	4.71	0.17	0.85	0.20	0.02	15.97
GNT7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT8	Spectrum 8	17.7	0.1	11.4	17.8	1.1	4.6	4.0	0.2	40.5	97.3	5.99	0.01	4.00	3.03	0.19	1.78	0.94	0.03	15.97
GNT9	Spectrum 9	18.3	0.0	11.5	27.7	0.6	1.7	1.3	-	40.8	101.8	6.14	0.01	4.01	4.67	0.11	0.64	0.30	-	15.86
GNT10	Spectrum 10	17.4	-	11.6	25.7	0.8	2.1	1.2	-	39.5	98.1	6.02	-	4.16	4.47	0.14	0.84	0.29	-	15.93
GNT11	Spectrum 11	18.0	-	12.0	25.7	1.6	2.0	1.0	0.0	40.7	100.9	6.05	-	4.20	4.35	0.27	0.76	0.23	0.00	15.85
GNT12	Spectrum 12	19.2	0.1	13.0	21.8	3.7	2.1	0.8	-	42.3	102.8	6.19	0.01	4.35	3.54	0.60	0.77	0.18	-	15.65
GNT13	Spectrum 13	17.6	-	12.1	22.1	0.4	4.5	1.0	0.1	40.7	98.5	5.93	-	4.23	3.74	0.07	1.74	0.24	0.01	15.97
GNT14	Spectrum 14	17.0	0.0	10.9	26.4	1.1	1.9	1.5	0.1	38.9	97.8	5.99	0.00	4.00	4.66	0.19	0.79	0.37	0.01	16.01
GNT15	Spectrum 15	17.5	0.1	11.6	21.8	3.3	2.0	2.9	0.1	40.0	99.1	5.97	0.01	4.13	3.75	0.57	0.78	0.70	0.03	15.94
GNT16	Spectrum 16	17.3	0.1	11.3	14.9	10.5	1.2	3.3	-	39.3	97.9	6.02	0.03	4.09	2.61	1.87	0.47	0.82	-	15.91
GNT17	Spectrum 17	18.2	0.1	12.1	21.4	0.8	4.8	1.2	0.1	41.5	100.1	5.98	0.01	4.14	3.54	0.14	1.81	0.28	0.02	15.93
GNT18	Spectrum 19	18.5	-	12.1	23.1	0.9	1.7	3.5	-	41.1	100.7	6.14	-	4.17	3.86	0.15	0.64	0.83	-	15.80
GNT19	Spectrum 20	18.7	-	12.2	20.9	0.2	4.9	0.9	-	41.7	99.4	6.12	-	4.15	3.44	0.04	1.85	0.21	-	15.82
GNT20	Spectrum 21	17.9	-	11.3	21.0	1.3	1.7	4.8	-	39.9	97.8	6.15	-	4.03	3.62	0.22	0.66	1.16	-	15.85
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT21	Spectrum 22	17.8	0.1	12.0	20.3	0.9	4.9	1.3	-	40.8	97.9	5.97	0.02	4.18	3.43	0.16	1.89	0.32	-	15.95
-	Spectrum 23	19.3	-	12.3	20.8	0.6	2.2	5.4	-	42.5	102.8	6.21	-	4.11	3.36	0.10	0.80	1.22	-	15.81
GNT22	Spectrum 24	18.7	-	11.7	22.4	1.7	1.4	3.9	-	41.0	100.6	6.23	-	4.04	3.75	0.28	0.53	0.91	-	15.75
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT23	Spectrum 25	18.0	0.1	11.3	23.6	0.7	3.5	0.9	0.0	40.3	98.4	6.11	0.01	4.00	4.03	0.12	1.38	0.22	0.01	15.88
GNT24	Spectrum 26	19.2	-	12.1	24.5	0.6	2.5	1.0	-	41.8	101.6	6.29	-	4.11	4.03	0.10	0.94	0.22	-	15.69
GNT25	Spectrum 27	16.8	0.0	10.7	18.3	4.3	0.6	6.8	-	38.2	95.5	6.00	0.01	3.98	3.30	0.79	0.26	1.70	-	16.04
GNT26	Spectrum 28	18.2	0.1	12.0	20.6	7.2	1.2	2.2	-	41.1	102.4	6.05	0.01	4.16	3.45	1.23	0.47	0.51	-	15.88
GNT27	Spectrum 29	17.0	-	11.2	25.8	0.4	2.3	0.9	-	38.6	96.1	6.01	-	4.13	4.59	0.07	0.94	0.23	-	15.98
GNT28	Spectrum 30	19.3	0.0	12.6	20.8	0.3	4.9	1.6	0.1	43.1	102.7	6.11	0.01	4.16	3.32	0.06	1.78	0.35	0.01	15.80
GNT29	Spectrum 31	18.9	-	12.4	22.1	0.6	3.2	3.2	-	42.3	102.5	6.09	-	4.17	3.58	0.09	1.18	0.73	-	15.85
GNT30	Spectrum 32	18.1	-	11.6	11.3	6.0	0.5	11.2	0.0	40.6	99.1	6.09	-	4.06	1.91	1.04	0.18	2.63	0.00	15.91
GNT30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GNT31	Spectrum 33	18.7	0.1	12.3	19.1	1.5	1.9	5.6	-	41.7	100.9	6.13	0.02	4.20	3.15	0.24	0.73	1.29	-	15.76
GNT32	Spectrum 34	19.2	-	12.9	20.1	0.3	6.1	0.7	-	43.5	102.8	6.04	-	4.23	3.18	0.04	2.23	0.15	-	15.87
GNT33	Spectrum 35	17.6	0.1	11.9	20.4	0.6	4.9	0.8	-	40.3	96.7	5.98	0.02	4.20	3.48	0.11	1.93	0.19	-	15.91
GNT34	Spectrum 36	18.3	0.1	12.1	23.8	2.3	2.6	1.1	0.1	41.4	101.8	6.05	0.01	4.18	3.96	0.39	0.97	0.26	0.02	15.84
GNT35	Spectrum 37	17.6	0.1	11.9	25.6	0.5	2.6	1.0	-	40.1	99.2	5.98	0.02	4.20	4.38	0.08	1.02	0.23	-	15.91
GNT36	Spectrum 38	19.1	0.1	12.0	18.9	0.8	2.9	6.2	-	42.5	102.4	6.15	0.02	4.02	3.05	0.12	1.07	1.39	-	15.84
GNT37	Spectrum 40	16.9	-	10.8	20.0	4.6	1.4	3.2	-	37.9	94.6	6.07	-	4.03	3.63	0.85	0.59	0.80	-	15.97
GNT38	Spectrum 39	18.8	0.2	12.4	21.0	2.0	3.2	2.8	0.0	42.3	102.5	6.07	0.03	4.17	3.41	0.32	1.18	0.62	0.00	15.81
GNT38	Spectrum 41	18.2	0.1	12.1	21.3	0.8	3.3	1.7	0.1	40.8	98.3	6.10	0.02	4.22	3.58	0.13	1.28	0.41	0.01	15.76
-	Spectrum 42	18.3	0.0	12.0	18.5	3.4	1.9	5.4	0.1	41.4	101.1	6.06	0.00	4.13	3.08	0.58	0.74	1.25	0.02	15.86
GNT39	Spectrum 43	19.7	0.1	12.6	17.4	0.4	4.8	4.9	-	43.9	103.8	6.14	0.02	4.08	2.73	0.06	1.73	1.06	-	15.81
GNT40	Spectrum 44	18.6	0.0	12.2	25.5	0.8	2.2	1.1	-	41.5	101.8	6.14	0.00	4.19	4.24	0.13	0.84	0.25	-	15.79
GNT41	Spectrum 45	17.5	0.1	11.9	22.0	1.8	1.3	2.9	0.1	39.6	97.3	6.05	0.03	4.30	3.82	0.31	0.53	0.70	0.02	15.77
GNT42	Spectrum 46	18.9	0.1	12.6	18.0	0.4	7.3	0.8	-	43.2	101.2	5.99	0.01	4.16	2.86	0.06	2.67	0.17	-	15.92
GNT43	Spectrum 47	17.4	0.0	11.5	21.7	0.7	0.8	5.2	0.1	39.2	96.6	6.07	0.01	4.19	3.82	0.13	0.33	1.27	0.02	15.82
GNT44	Spectrum 48	19.0	0.0	12.4	20.7	1.6	3.9	2.3	-	42.5	102.3	6.10	0.01	4.16	3.35	0.26	1.45	0.51	-	15.84
GNT45	Spectrum 49	18.0	0.1	12.1	18.9	4.7	1.0	5.7	0.4	41.1	101.8	5.97	0.02	4.20	3.15	0.80	0.37	1.32	0.06	15.88
GNT46	Spectrum 50	18.5	0.1	12.3	19.8	6.3	2.4	1.4	0.2	41.8	102.7	6.04	0.02	4.20	3.26	1.05	0.90	0.32	0.03	15.82
GNT47	Spectrum 51	19.4	0.1	11.9	13.8	6.8	0.3	5.9	0.0	41.2	99.3	6.43	0.02	4.10	2.31	1.15	0.12	1.36	0.00	15.50
GNT48	Spectrum 52	19.1	0.1	12.2	22.0	3.1	1.2	2.4	0.0	41.6	101.6	6.27	0.02	4.18	3.64	0.53	0.45	0.55	0.01	15.63
GNT49	Spectrum 53	18.4	-	12.2	23.7	1.4	3.4	0.9	0.0	41.5	101.3	6.07	-	4.17	3.92	0.24	1.29	0.20	0.00	15.89
GNT50	Spectrum 54	18.4	-	11.9	20.7	1.1	3.3	1.8	0.0	40.6	97.7	6.18	-	4.17	3.49	0.18	1.28	0.42	0.01	15.73
GNT51	Spectrum 55	17.3	-	11.2	24.0	2.0	2.4	0.7	0.1	39.0	96.6	6.05	-	4.10	4.23	0.36	0.98	0.18	0.02	15.93
GNT52	Spectrum 56	19.4	-	12.7	21.8	1.2	2.4	3.2	-	42.7	103.3	6.19	-	4.24	3.51	0.19	0.88	0.72	-	15.74

Table 7 EDXA data for tourmaline derived from Microscan run.

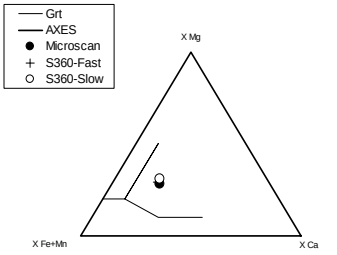
Tourmaline Grain ID	Spectrum Label	Microscan Data: Element %												Formula Units (24 Oxygens)										
		Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Na	K	O	Total	Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Na	K	Total Cations
TO_01	T2	16.4	0.5	17.7	6.8	*n.d.*	2.5	*n.d.*	*n.d.*	1.8	*n.d.*	38.9	84.4	5.76	0.10	6.48	1.20	*n.d.*	1.02	*n.d.*	*n.d.*	0.77	*n.d.*	15.33
TO_02	T3	16.5	0.4	17.6	5.0	*n.d.*	3.2	0.6	0.1	1.4	0.1	39.0	83.8	5.78	0.08	6.42	0.88	*n.d.*	1.30	0.15	0.02	0.60	0.03	15.26
TO_03	T4	16.2	0.2	16.6	6.1	*n.d.*	2.5	0.2	*n.d.*	1.1	0.1	37.3	80.4	5.94	0.04	6.33	1.12	*n.d.*	1.06	0.05	*n.d.*	0.49	0.03	15.07
TO_04	T5	14.5	0.4	14.1	8.9	*n.d.*	3.3	0.4	0.9	1.3	*n.d.*	35.1	78.8	5.65	0.09	5.72	1.74	*n.d.*	1.49	0.11	0.19	0.62	*n.d.*	15.60
TO_05	T6	15.8	0.2	17.0	5.9	*n.d.*	2.7	0.3	0.1	1.4	*n.d.*	37.4	80.7	5.78	0.04	6.47	1.08	*n.d.*	1.14	0.08	0.02	0.63	*n.d.*	15.23
TO_06	T7	15.8	0.2	14.9	6.6	*n.d.*	3.5	0.2	0.1	1.8	*n.d.*	36.3	79.2	5.95	0.04	5.84	1.25	*n.d.*	1.52	0.05	0.02	0.83	*n.d.*	15.51
TO_07	T8	16.4	0.4	17.2	5.9	*n.d.*	3.3	0.5	*n.d.*	1.4	*n.d.*	38.8	83.8	5.78	0.08	6.31	1.05	*n.d.*	1.34	0.12	*n.d.*	0.60	*n.d.*	15.29
TO_08	T9	16.9	0.4	18.1	4.4	0.2	3.1	0.2	*n.d.*	1.4	*n.d.*	39.6	84.3	5.83	0.08	6.50	0.76	0.04	1.24	0.05	*n.d.*	0.59	*n.d.*	15.10
TO_09	T11	15.9	0.2	16.4	4.2	*n.d.*	3.3	0.3	0.2	1.4	*n.d.*	36.8	78.6	5.91	0.04	6.34	0.78	*n.d.*	1.42	0.08	0.04	0.64	*n.d.*	15.25
TO_10	T10	16.8	*n.d.*	17.1	7.8	*n.d.*	2.1	*n.d.*	*n.d.*	1.2	*n.d.*	38.2	82.8	6.01	*n.d.*	6.37	1.40	*n.d.*	0.87	*n.d.*	*n.d.*	0.52	*n.d.*	15.18
TO_11	T12	15.9	0.3	16.7	7.1	*n.d.*	2.6	0.3	0.1	1.2	0.1	37.5	81.8	5.80	0.06	6.34	1.30	*n.d.*	1.10	0.08	0.02	0.53	0.03	15.25
TO_12	T13	16.3	0.4	14.8	8.9	*n.d.*	3.4	0.1	*n.d.*	1.9	*n.d.*	37.5	83.2	5.94	0.09	5.62	1.63	*n.d.*	1.43	0.03	*n.d.*	0.85	*n.d.*	15.58
TO_13	T14	16.2	0.5	14.8	7.1	*n.d.*	3.9	0.2	0.2	2.0	*n.d.*	37.5	82.4	5.91	0.11	5.62	1.30	*n.d.*	1.64	0.05	0.04	0.89	*n.d.*	15.56
TO_14	T15	16.4	0.3	17.1	5.0	*n.d.*	3.5	0.2	0.2	1.6	0.1	38.5	82.7	5.82	0.06	6.32	0.89	*n.d.*	1.44	0.05	0.04	0.69	0.03	15.34
TO_15	T16	16.8	0.4	16.3	5.3	*n.d.*	4.4	0.3	*n.d.*	2.1	*n.d.*	39.2	84.7	5.86	0.08	5.92	0.93	*n.d.*	1.77	0.07	*n.d.*	0.89	*n.d.*	15.53
TO_16	T17	16.0	0.6	17.1	5.3	*n.d.*	3.3	0.5	*n.d.*	1.4	0.1	38.2	82.5	5.73	0.13	6.37	0.95	*n.d.*	1.36	0.13	*n.d.*	0.61	0.03	15.31
TO_17	T18	17.0	0.1	17.0	7.8	*n.d.*	1.8	0.1	*n.d.*	0.8	0.6	38.3	83.5	6.07	0.02	6.32	1.40	*n.d.*	0.74	0.03	*n.d.*	0.35	0.15	15.08
TO_18	T19	16.4	0.6	17.6	5.0	*n.d.*	3.2	0.2	0.1	1.4	*n.d.*	38.8	83.3	5.78	0.12	6.46	0.89	*n.d.*	1.30	0.05	0.02	0.60	*n.d.*	15.22
TO_19	T20	15.7	0.4	16.9	9.0	*n.d.*	1.1	0.1	*n.d.*	1.4	*n.d.*	37.0	81.8	5.80	0.09	6.50	1.67	*n.d.*	0.47	0.03	*n.d.*	0.63	*n.d.*	15.19
TO_20	T21	16.0	0.4	17.6	6.9	*n.d.*	2.2	0.2	*n.d.*	1.6	*n.d.*	38.2	83.1	5.73	0.08	6.56	1.24	*n.d.*	0.91	0.05	*n.d.*	0.70	*n.d.*	15.27
TO_21	T22	16.8	0.6	17.9	4.7	*n.d.*	3.2	0.2	*n.d.*	1.3	*n.d.*	39.4	83.9	5.83	0.12	6.47	0.82	*n.d.*	1.28	0.05	*n.d.*	0.55	*n.d.*	15.12
TO_22	T23	14.3	0.5	14.4	5.9	*n.d.*	2.2	2.7	0.1	1.1	0.2	34.1	75.3	5.73	0.12	6.01	1.19	*n.d.*	1.02	0.76	0.02	0.54	0.06	15.45
TO_23	T24	16.8	*n.d.*	17.0	9.3	*n.d.*	1.4	*n.d.*	*n.d.*	0.4	*n.d.*	38.0	82.8	6.04	*n.d.*	6.37	1.68	*n.d.*	0.58	*n.d.*	*n.d.*	0.18	*n.d.*	14.85
TO_24	T25	16.1	0.2	17.9	7.9	*n.d.*	1.6	0.1	0.1	1.4	*n.d.*	38.2	83.3	5.76	0.04	6.67	1.42	*n.d.*	0.66	0.03	0.02	0.61	*n.d.*	15.21
TO_25	T26	16.9	0.4	17.6	5.4	*n.d.*	3.3	0.1	0.1	1.3	*n.d.*	39.4	84.5	5.86	0.08	6.36	0.94	*n.d.*	1.32	0.02	0.02	0.55	*n.d.*	15.16
TO_26	T27	15.8	0.5	17.0	4.5	*n.d.*	3.9	0.4	*n.d.*	1.6	0.1	37.9	81.5	5.70	0.11	6.38	0.82	*n.d.*	1.63	0.10	*n.d.*	0.71	0.03	15.46
TO_27	T28	16.3	0.4	17.4	4.4	*n.d.*	3.2	0.3	*n.d.*	1.3	0.1	38.3	81.7	5.82	0.08	6.47	0.79	*n.d.*	1.32	0.08	*n.d.*	0.57	0.03	15.15
TO_28	T29a	15.4	0.3	16.4	9.2	*n.d.*	1.1	*n.d.*	*n.d.*	1.3	*n.d.*	36.2	80.1	5.82	0.07	6.45	1.75	*n.d.*	0.48	*n.d.*	*n.d.*	0.60	*n.d.*	15.16
TO_29	T29b	15.6	0.2	16.5	10.1	*n.d.*	0.8	0.1	0.1	1.3	0.1	36.6	81.3	5.83	0.04	6.42	1.90	*n.d.*	0.35	0.03	0.02	0.59	0.03	15.20
TO_30	T30	16.7	0.5	17.4	4.4	*n.d.*	3.9	0.3	*n.d.*	1.7	*n.d.*	39.4	84.2	5.79	0.10	6.28	0.77	*n.d.*	1.56	0.07	*n.d.*	0.72	*n.d.*	15.31
TO_31	T32	16.6	0.5	17.2	6.8	*n.d.*	3.0	0.2	*n.d.*	1.2	*n.d.*	39.0	84.4	5.82	0.10	6.28	1.20	*n.d.*	1.22	0.05	*n.d.*	0.51	*n.d.*	15.18
TO_32	T33	16.6	0.1	16.8	7.1	*n.d.*	1.6	0.1	*n.d.*	0.7	*n.d.*	37.2	80.2	6.10	0.02	6.43	1.31	*n.d.*	0.68	0.03	*n.d.*	0.31	*n.d.*	14.88
TO_33	T34	16.3	0.6	17.4	5.9	*n.d.*	2.8	0.6	*n.d.*	1.3	*n.d.*	38.6	83.4	5.77	0.12	6.42	1.05	*n.d.*	1.15	0.15	*n.d.*	0.56	*n.d.*	15.22
TO_34	T35	17.4	0.3	16.2	4.1	*n.d.*	4.9	0.3	0.1	1.9	*n.d.*	39.6	84.7	6.01	0.06	5.82	0.71	*n.d.*	1.95	0.07	0.02	0.80	*n.d.*	15.45
TO_35	T36	16.7	0.8	17.4	5.4	*n.d.*	3.3	0.3	*n.d.*	1.4	*n.d.*	39.3	84.4	5.81	0.16	6.30	0.94	*n.d.*	1.33	0.07	*n.d.*	0.59	*n.d.*	15.21
TO_36	T37	16.4	0.4	15.8	3.7	*n.d.*	5.1	0.6	*n.d.*	1.7	0.1	38.2	82.0	5.87	0.08	5.89	0.67	*n.d.*	2.11	0.15	*n.d.*	0.74	0.03	15.53
TO_37	T38	15.9	0.3	14.8	7.1	*n.d.*	3.4	0.4	*n.d.*	1.8	0.1	36.5	80.2	5.96	0.07	5.77	1.34	*n.d.*	1.47	0.10	*n.d.*	0.82	0.03	15.56
TO_38	T39	15.8	*n.d.*	16.2	8.3	*n.d.*	1.6	0.1	*n.d.*	0.7	*n.d.*	36.2	79.0	5.97	*n.d.*	6.37	1.58	*n.d.*	0.70	0.03	*n.d.*	0.32	*n.d.*	14.96
TO_39	T40	16.8	0.1	17.5	7.7	*n.d.*	2.0	0.1	0.2	0.9	*n.d.*	38.8	84.1	5.92	0.02	6.42	1.36	*n.d.*	0.81	0.02	0.04	0.39	*n.d.*	14.99
TO_40	T41	16.4	0.2	17.9	8.3	*n.d.*	1.6	0.1	*n.d.*	1.4	*n.d.*	38.6	84.3	5.81	0.04	6.60	1.48	*n.d.*	0.65	0.02	*n.d.*	0.61	*n.d.*	15.21
TO_41	T42	16.8	0.3	16.1	4.8	*n.d.*	4.4	0.2	*n.d.*	1.8	*n.d.*	38.6	82.9	5.95	0.06	5.94	0.86	*n.d.*	1.80	0.05	*n.d.*	0.78	*n.d.*	15.43
TO_42	T43	16.4	*n.d.*	16.4	8.6	*n.d.*	1.7	*n.d.*	0.1	0.6	*n.d.*	37.0	80.7	6.06	*n.d.*	6.31	1.60	*n.d.*	0.73	*n.d.*	0.02	0.27	*n.d.*	14.98
TO_43	T44	16.4	0.2	16.9	9.1	*n.d.*	1.4	0.1	0.1	0.9	*n.d.*	37.7	82.8	5.95	0.04	6.38	1.66	*n.d.*	0.59	0.03	0.02	0.40	*n.d.*	15.06
TO_44	T45	16.1	0.5	16.6	5.7	*n.d.*	3.3	0.6	*n.d.*	1.4	*n.d.*	38.0	82.2	5.79	0.11	6.22	1.03	*n.d.*	1.37	0.15	*n.d.*	0.62	*n.d.*	15.28
TO_45	T47	15.9	0.6	15.8	7.3	*n.d.*	2.7	*n.d.*	*n.d.*	1.8	*n.d.*	37.1	81.4	5.86	0.13	6.06	1.35	*n.d.*	1.15	*n.d.*	*n.d.*	0.81	*n.d.*	15.36
TO_46	T48	16.5	0.6	17.3	4.9	*n.d.*	3.2	0.3	*n.d.*	1.5	*n.d.*	38.8	83.1	5.81	0.12	6.35	0.87	*n.d.*	1.30	0.07	*n.d.*	0.65	*n.d.*	15.17
TO_47	T49	16.8	0.4	17.7	4.4	*n.d.*	3.5	0.2	*n.d.*	1.6	*n.d.*	39.4	84.0	5.83	0.08	6.39	0.77	*n.d.*	1.40	0.05	*n.d.*	0.68	*n.d.*	15.20
TO_48	T50	16.1	0.5	15.9	5.9	*n.d.*	3.7	0.4	*n.d.*	1.6	*n.d.*	37.6	81.7	5.85	0.11	6.02	1.08	*n.d.*	1.55	0.10	*n.d.*	0.71	*n.d.*	15.43
TO_49	T51	16.4	0.3	15.6	5.4	*n.d.*	4.0	0.3	*n.d.*	1.7	*n.d.*	37.7	81.5	5.95	0.06	5.89	0.98	*n.d.*	1.68	0.08	*n.d.*	0.75	*n.d.*	15.39
TO_50	T52	15.7	0.3	16.4	8.5	*n.d.*	1.6	0.2	*n.d.*	1.4	0.1	36.7	80.8	5.85	0.07	6.36	1.59	*n.d.*	0.69	0.05	*n.d.*	0.64	0.03	15.27
TO_51	T53	16.4	0.4	15.8	5.7	*n.d.*	4.1	0.8	*n.d.*	1.5	0.1	38.3	83.2	5.85	0.08	5.87	1.02	*n.d.*	1.69	0.20	*n.d.*	0.65	0.03	15.40
TO_52	T54	16.3	0.3	17.0	8.6	*n.d.*	1.9	0.1	*n.d.*	1.5	*n.d.*	38.2	84.0	5.83	0.06	6.33	1.55	*n.d.*	0.79	0.03	*n.d.*	0.66	*n.d.*	15.24

Table 8 EDXA data for tourmaline derived from S360 run.

		S360_II Data																					
Tourmaline Grain ID	Spectrum Label	Element %												Formula Units (24 Oxygens)									
		Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Na	K	O	Total	Si	Ti	Al	Fe	Mn	Mg	Ca	Cr	Na	K	Total Cations
TO_01	Spectrum 1	16.9	0.6	16.3	5.4	*n.d.*	2.0	0.3	*n.d.*	0.9	1.1	37.6	81.0	6.16	0.12	6.17	0.99	*n.d.*	0.83	0.07	*n.d.*	0.39	0.27	15.01
TO_02	Spectrum 2	16.2	0.5	17.4	6.1	*n.d.*	2.2	0.1	*n.d.*	1.3	*n.d.*	38.0	81.8	5.83	0.10	6.53	1.11	*n.d.*	0.90	0.03	*n.d.*	0.59	*n.d.*	15.09
TO_03	Spectrum 4	17.0	0.2	17.9	5.5	*n.d.*	2.7	0.2	*n.d.*	1.2	*n.d.*	39.3	84.0	5.91	0.05	6.49	0.97	*n.d.*	1.09	0.05	*n.d.*	0.49	*n.d.*	15.03
TO_04	Spectrum 5	16.8	0.6	16.4	5.5	*n.d.*	3.8	0.5	*n.d.*	1.6	*n.d.*	38.9	83.9	5.89	0.12	6.01	0.97	*n.d.*	1.54	0.11	*n.d.*	0.67	*n.d.*	15.31
TO_05	Spectrum 6	15.9	*n.d.*	16.6	8.6	*n.d.*	1.5	0.1	*n.d.*	0.8	*n.d.*	36.7	80.2	5.94	*n.d.*	6.44	1.61	*n.d.*	0.64	0.02	*n.d.*	0.36	*n.d.*	15.01
TO_06	Spectrum 7	18.2	0.4	16.8	7.5	*n.d.*	4.5	0.3	*n.d.*	2.2	*n.d.*	41.9	91.6	5.94	0.07	5.71	1.23	*n.d.*	1.69	0.06	*n.d.*	0.86	*n.d.*	15.56
TO_07	Spectrum 8	15.6	0.6	16.6	5.4	*n.d.*	3.1	0.6	*n.d.*	1.2	*n.d.*	37.2	80.3	5.74	0.12	6.34	1.00	*n.d.*	1.32	0.15	*n.d.*	0.55	*n.d.*	15.23
TO_08	Spectrum 9	17.4	0.4	17.8	4.5	*n.d.*	3.1	*n.d.*	*n.d.*	1.2	*n.d.*	39.8	84.2	5.99	0.08	6.38	0.78	*n.d.*	1.24	*n.d.*	*n.d.*	0.52	*n.d.*	14.99
TO_09	Spectrum 10	18.1	0.5	17.2	5.3	*n.d.*	4.8	0.6	*n.d.*	1.8	*n.d.*	41.8	90.1	5.90	0.10	5.86	0.87	*n.d.*	1.83	0.13	*n.d.*	0.72	*n.d.*	15.42
TO_10	Spectrum 11	16.1	0.4	16.7	6.6	*n.d.*	2.3	0.1	*n.d.*	1.2	*n.d.*	37.3	80.6	5.89	0.08	6.38	1.21	*n.d.*	0.97	0.04	*n.d.*	0.55	*n.d.*	15.11
TO_11	Spectrum 12	16.7	0.3	16.9	6.9	*n.d.*	2.4	0.3	*n.d.*	1.1	*n.d.*	38.2	82.7	5.97	0.05	6.28	1.25	*n.d.*	0.97	0.08	*n.d.*	0.46	*n.d.*	15.06
TO_12	Spectrum 13	17.2	0.4	15.8	8.6	*n.d.*	3.6	0.1	*n.d.*	2.3	*n.d.*	39.6	87.6	5.93	0.08	5.67	1.49	*n.d.*	1.44	0.03	*n.d.*	0.99	*n.d.*	15.63
TO_13	Spectrum 14	17.0	0.8	16.0	7.0	*n.d.*	3.8	0.1	*n.d.*	2.2	*n.d.*	39.4	86.2	5.89	0.16	5.77	1.22	*n.d.*	1.52	0.02	*n.d.*	0.92	*n.d.*	15.51
TO_14	Spectrum 15	12.1	0.6	13.5	4.3	0.6	2.6	0.5	*n.d.*	1.4	*n.d.*	30.0	65.6	5.53	0.15	6.39	0.99	0.13	1.35	0.16	*n.d.*	0.79	*n.d.*	15.50
TO_15	Spectrum 16	16.3	0.5	17.0	4.5	*n.d.*	3.6	*n.d.*	*n.d.*	1.5	*n.d.*	38.2	81.5	5.84	0.10	6.33	0.80	*n.d.*	1.49	*n.d.*	*n.d.*	0.64	*n.d.*	15.20
TO_16	Spectrum 17	17.0	0.4	16.2	4.5	*n.d.*	3.7	0.2	*n.d.*	1.9	*n.d.*	38.6	82.6	6.03	0.09	5.97	0.81	*n.d.*	1.52	0.04	*n.d.*	0.81	*n.d.*	15.28
TO_17	Spectrum 19	16.1	0.7	16.5	8.2	*n.d.*	1.6	0.1	*n.d.*	1.3	0.2	37.4	82.1	5.87	0.14	6.28	1.51	*n.d.*	0.68	0.03	*n.d.*	0.58	0.06	15.16
TO_18	Spectrum 18	15.4	0.4	15.5	4.8	*n.d.*	2.2	1.8	*n.d.*	0.9	0.3	35.4	76.6	5.93	0.08	6.22	0.94	*n.d.*	1.00	0.48	*n.d.*	0.41	0.07	15.12
TO_19	Spectrum 20	15.3	0.6	14.9	7.3	*n.d.*	1.3	*n.d.*	*n.d.*	0.7	0.2	34.4	74.7	6.09	0.15	6.17	1.45	*n.d.*	0.62	*n.d.*	*n.d.*	0.34	0.06	14.88
TO_20	Spectrum 22	16.2	0.5	17.2	6.4	*n.d.*	2.1	0.2	*n.d.*	1.4	0.1	37.9	81.8	5.86	0.10	6.47	1.16	*n.d.*	0.86	0.04	*n.d.*	0.61	0.02	15.12
TO_21	Spectrum 21	16.8	0.7	17.7	5.0	*n.d.*	3.0	0.2	*n.d.*	1.4	*n.d.*	39.4	84.1	5.85	0.13	6.40	0.87	*n.d.*	1.21	0.06	*n.d.*	0.58	*n.d.*	15.10
TO_22	Spectrum 23	11.6	0.5	12.4	4.5	*n.d.*	2.1	0.1	*n.d.*	1.0	*n.d.*	27.6	59.7	5.73	0.13	6.38	1.13	*n.d.*	1.22	0.04	*n.d.*	0.61	*n.d.*	15.24
TO_23	Spectrum 26	17.1	*n.d.*	17.7	8.5	*n.d.*	1.7	*n.d.*	*n.d.*	0.6	*n.d.*	39.0	84.7	6.00	*n.d.*	6.46	1.50	*n.d.*	0.67	*n.d.*	*n.d.*	0.26	*n.d.*	14.89
TO_24	Spectrum 27	16.7	0.4	18.4	7.7	*n.d.*	1.5	0.1	*n.d.*	1.7	*n.d.*	39.6	86.1	5.78	0.09	6.63	1.33	*n.d.*	0.59	0.03	*n.d.*	0.71	*n.d.*	15.16
TO_25	Spectrum 24	18.3	0.4	18.0	4.6	0.1	3.2	0.3	*n.d.*	1.5	0.5	41.3	88.2	6.05	0.08	6.20	0.76	0.02	1.22	0.06	*n.d.*	0.62	0.12	15.15
TO_26	Spectrum 25	17.7	0.4	18.0	5.3	*n.d.*	3.4	0.4	*n.d.*	1.6	*n.d.*	41.0	87.9	5.90	0.08	6.26	0.89	*n.d.*	1.33	0.10	*n.d.*	0.65	*n.d.*	15.21
TO_27	Spectrum 28	16.2	0.7	16.6	4.5	*n.d.*	3.1	0.2	*n.d.*	1.4	*n.d.*	37.6	80.3	5.89	0.14	6.30	0.82	*n.d.*	1.29	0.05	*n.d.*	0.63	*n.d.*	15.13
TO_28	Spectrum 31	16.6	0.3	17.8	8.1	0.2	1.4	*n.d.*	*n.d.*	1.9	*n.d.*	38.8	85.0	5.83	0.06	6.52	1.44	0.04	0.55	*n.d.*	*n.d.*	0.80	*n.d.*	15.24
TO_29	Spectrum 32	17.0	*n.d.*	17.1	8.5	*n.d.*	1.7	*n.d.*	*n.d.*	1.0	*n.d.*	38.4	83.5	6.04	*n.d.*	6.32	1.52	*n.d.*	0.70	*n.d.*	*n.d.*	0.41	*n.d.*	14.99
TO_30	Spectrum 33	15.7	0.5	16.6	4.1	*n.d.*	3.6	0.3	*n.d.*	1.3	*n.d.*	37.1	79.2	5.78	0.10	6.37	0.76	*n.d.*	1.53	0.08	*n.d.*	0.60	*n.d.*	15.22
TO_31	Spectrum 35	16.7	0.5	17.2	5.6	*n.d.*	2.9	0.4	*n.d.*	1.3	*n.d.*	38.8	83.4	5.87	0.11	6.31	1.00	*n.d.*	1.18	0.09	*n.d.*	0.56	*n.d.*	15.13
TO_32	Spectrum 36	17.7	*n.d.*	17.9	8.2	*n.d.*	1.8	0.1	*n.d.*	0.9	*n.d.*	40.1	86.7	6.05	*n.d.*	6.37	1.41	*n.d.*	0.71	0.03	*n.d.*	0.35	*n.d.*	14.93
TO_33	Spectrum 37	16.7	0.5	17.7	6.1	*n.d.*	2.7	0.6	*n.d.*	1.2	0.2	39.3	84.9	5.81	0.11	6.40	1.07	*n.d.*	1.07	0.15	*n.d.*	0.52	0.04	15.16
TO_34	-																							
TO_35	Spectrum 39	17.5	0.8	17.9	5.4	*n.d.*	3.4	0.4	*n.d.*	1.5	*n.d.*	40.8	87.5	5.86	0.15	6.24	0.90	*n.d.*	1.33	0.09	*n.d.*	0.59	*n.d.*	15.16
TO_36	Spectrum 40	18.0	0.5	16.7	3.3	*n.d.*	5.3	0.6	*n.d.*	1.9	*n.d.*	41.1	87.4	5.99	0.09	5.80	0.55	*n.d.*	2.05	0.15	*n.d.*	0.76	*n.d.*	15.39
TO_37	Spectrum 41	16.3	0.4	15.5	7.3	0.2	3.8	0.3	*n.d.*	2.1	0.1	38.1	84.1	5.84	0.09	5.78	1.32	0.04	1.56	0.07	*n.d.*	0.92	0.03	15.64
TO_38	Spectrum 42	17.7	0.2	17.6	5.6	*n.d.*	3.5	0.2	*n.d.*	1.7	*n.d.*	40.5	87.0	5.96	0.04	6.18	0.95	*n.d.*	1.37	0.05	*n.d.*	0.69	*n.d.*	15.24
TO_39	Spectrum 43	16.1	0.5	16.9	7.6	*n.d.*	1.9	0.2	*n.d.*	1.0	*n.d.*	37.5	81.5	5.86	0.10	6.41	1.40	*n.d.*	0.80	0.05	*n.d.*	0.43	*n.d.*	15.04
TO_40	Spectrum 44	13.2	0.3	14.6	7.6	*n.d.*	1.1	*n.d.*	*n.d.*	1.0	*n.d.*	31.4	69.2	5.74	0.09	6.59	1.67	*n.d.*	0.53	*n.d.*	*n.d.*	0.51	*n.d.*	15.13
TO_41	Spectrum 46	15.9	0.4	15.5	5.4	*n.d.*	4.1	*n.d.*	*n.d.*	1.8	*n.d.*	37.0	80.1	5.87	0.08	5.97	1.00	*n.d.*	1.75	*n.d.*	*n.d.*	0.82	*n.d.*	15.47
TO_42	Spectrum 45	17.6	0.3	19.0	7.7	*n.d.*	1.7	0.1	*n.d.*	1.7	*n.d.*	41.2	89.4	5.85	0.07	6.56	1.29	*n.d.*	0.65	0.03	*n.d.*	0.69	*n.d.*	15.13
TO_43	Spectrum 47	17.9	*n.d.*	18.3	8.0	*n.d.*	2.0	*n.d.*	*n.d.*	1.4	0.1	40.8	88.5	6.00	*n.d.*	6.38	1.35	*n.d.*	0.78	*n.d.*	*n.d.*	0.57	0.02	15.10
TO_44	Spectrum 49	16.9	0.6	18.2	5.3	*n.d.*	3.6	0.6	*n.d.*	1.8	*n.d.*	40.6	87.5	5.70	0.11	6.38	0.90	*n.d.*	1.39	0.14	*n.d.*	0.72	*n.d.*	15.35
TO_45	Spectrum 51	18.5	0.7	18.0	6.8	*n.d.*	3.1	0.1	*n.d.*	2.2	*n.d.*	42.4	91.7	5.97	0.13	6.03	1.10	*n.d.*	1.17	0.03	*n.d.*	0.85	*n.d.*	15.29
TO_46	Spectrum 52	16.0	0.6	17.5	4.8	0.1	2.8	0.3	*n.d.*	1.3	*n.d.*	38.0	81.4	5.76	0.12	6.55	0.87	0.02	1.17	0.07	*n.d.*	0.56	*n.d.*	15.11
TO_47	Spectrum 53	16.2	0.6	17.5	4.0	0.2	2.9	0.3	*n.d.*	1.2	*n.d.*	38.1	80.9	5.82	0.12	6.53	0.73	0.03	1.22	0.06	*n.d.*	0.54	*n.d.*	15.05
TO_48	Spectrum 55	18.0	0.3	18.6	4.1	0.1	3.9	0.3	*n.d.*	1.7	*n.d.*	41.7	88.7	5.89	0.05	6.35	0.68	0.02	1.49	0.06	*n.d.*	0.66	*n.d.*	15.20
TO_49	-																							
TO_50	Spectrum 57	15.9	0.1	16.7	5.5	*n.d.*	2.8	0.1	*n.d.*	1.6	*n.d.*	37.1	79.8	5.86	0.03	6.40	1.03	*n.d.*	1.20	0.03	*n.d.*	0.72	*n.d.*	15.26
TO_51	-																							
TO_52	Spectrum 58	16.9	0.2	18.2	7.9	*n.d.*	1.8	0.2	*n.d.*	1.5	*n.d.*	39.7	86.3	5.83	0.03	6.54	1.36	*n.d.*	0.72	0.05	*n.d.*	0.64	*n.d.*	15.17

Appendix 2 Garnet Triangular Diagrams

Standard garnet classification triangular diagrams (below) compare, on a grain-by-grain basis data acquired from each analytical run. In almost all cases, the data from each run are almost indistinguishable when plotted in this manner. The numbers represent the garnet grain identifiers quoted in Appendix Tables 3, 4 and 5.



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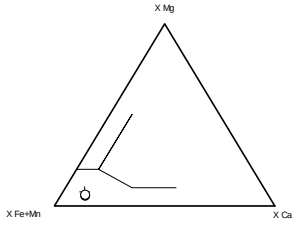

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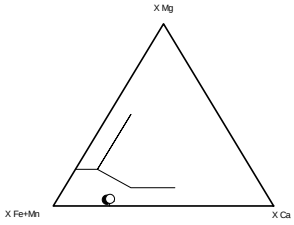

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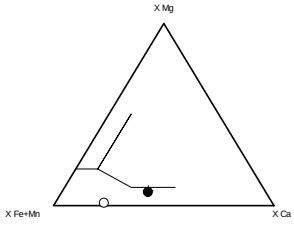

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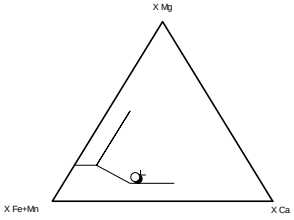

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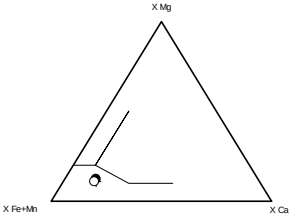

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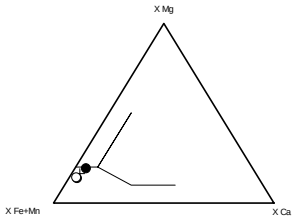

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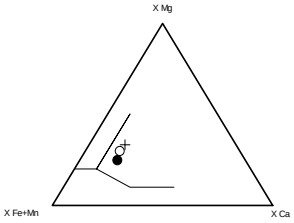

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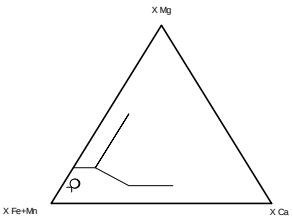

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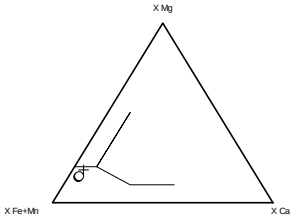

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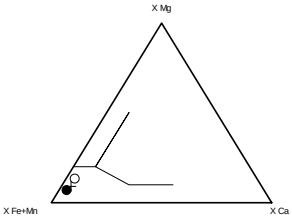

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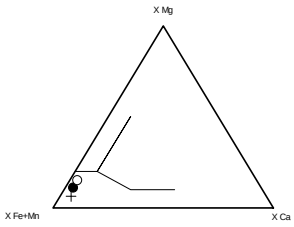

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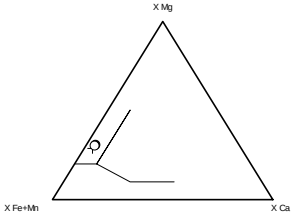

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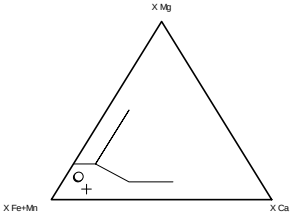

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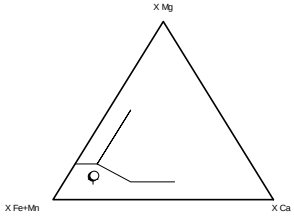

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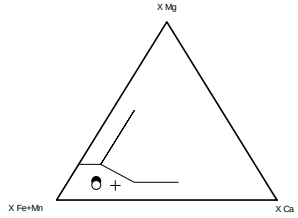

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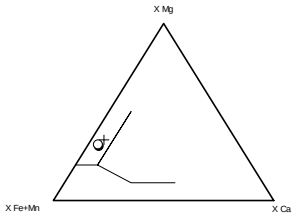

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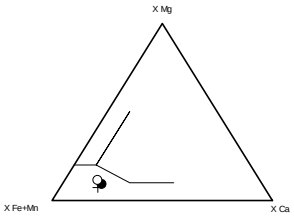

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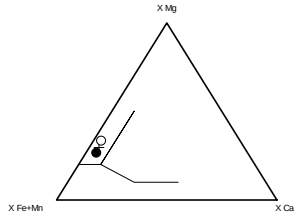

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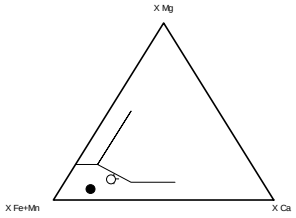

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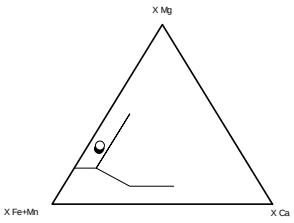

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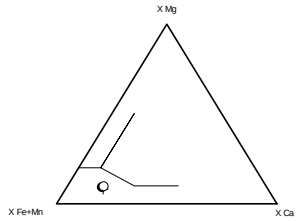

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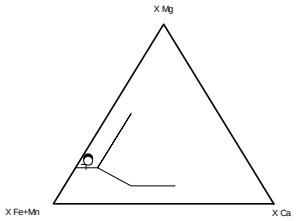

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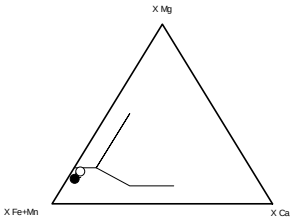

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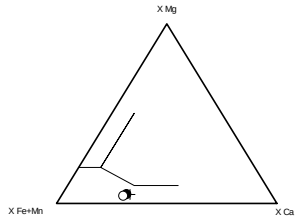

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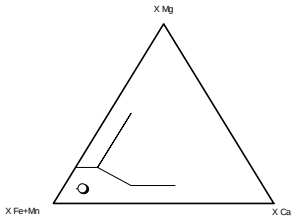

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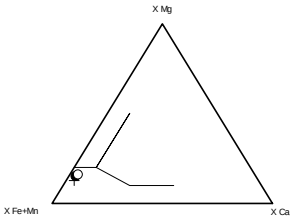

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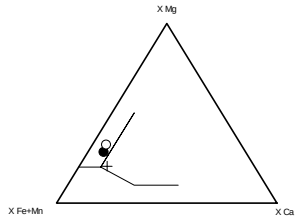

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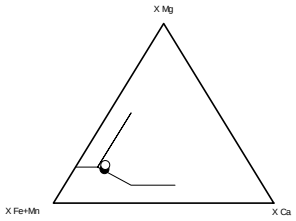

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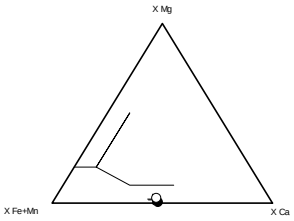

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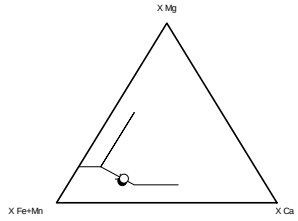

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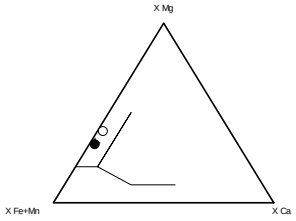

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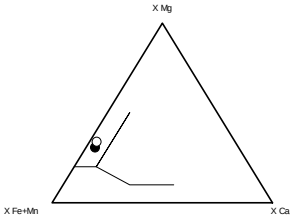

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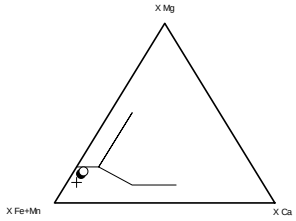

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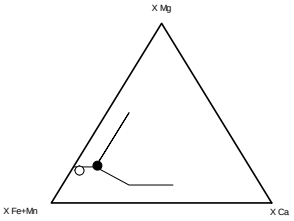

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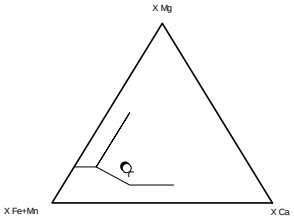

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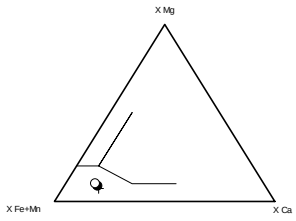

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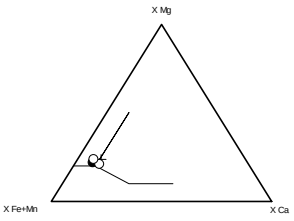

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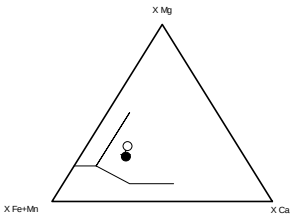

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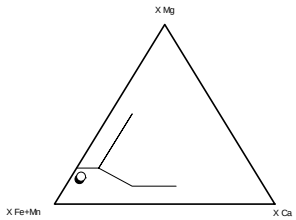

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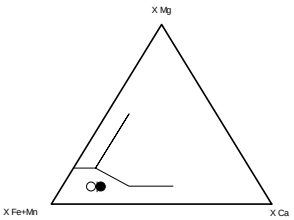

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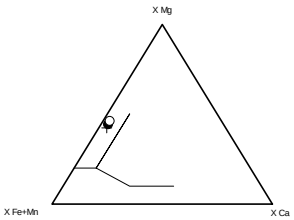

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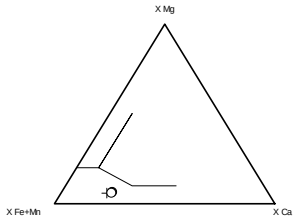

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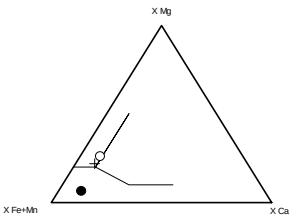

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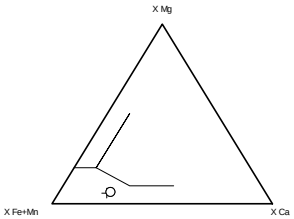

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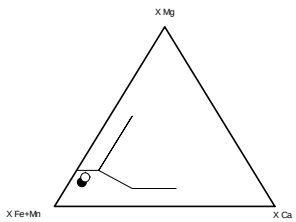

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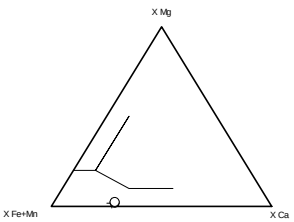

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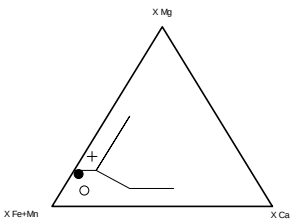

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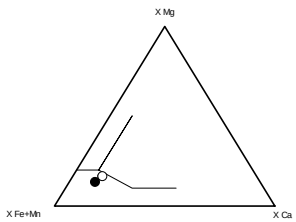

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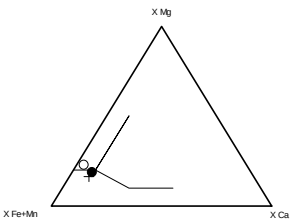

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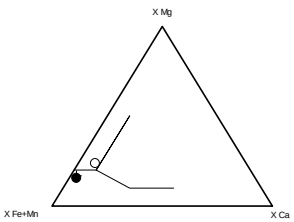

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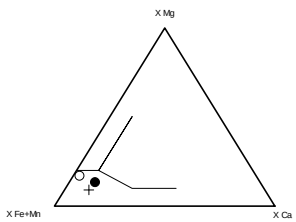

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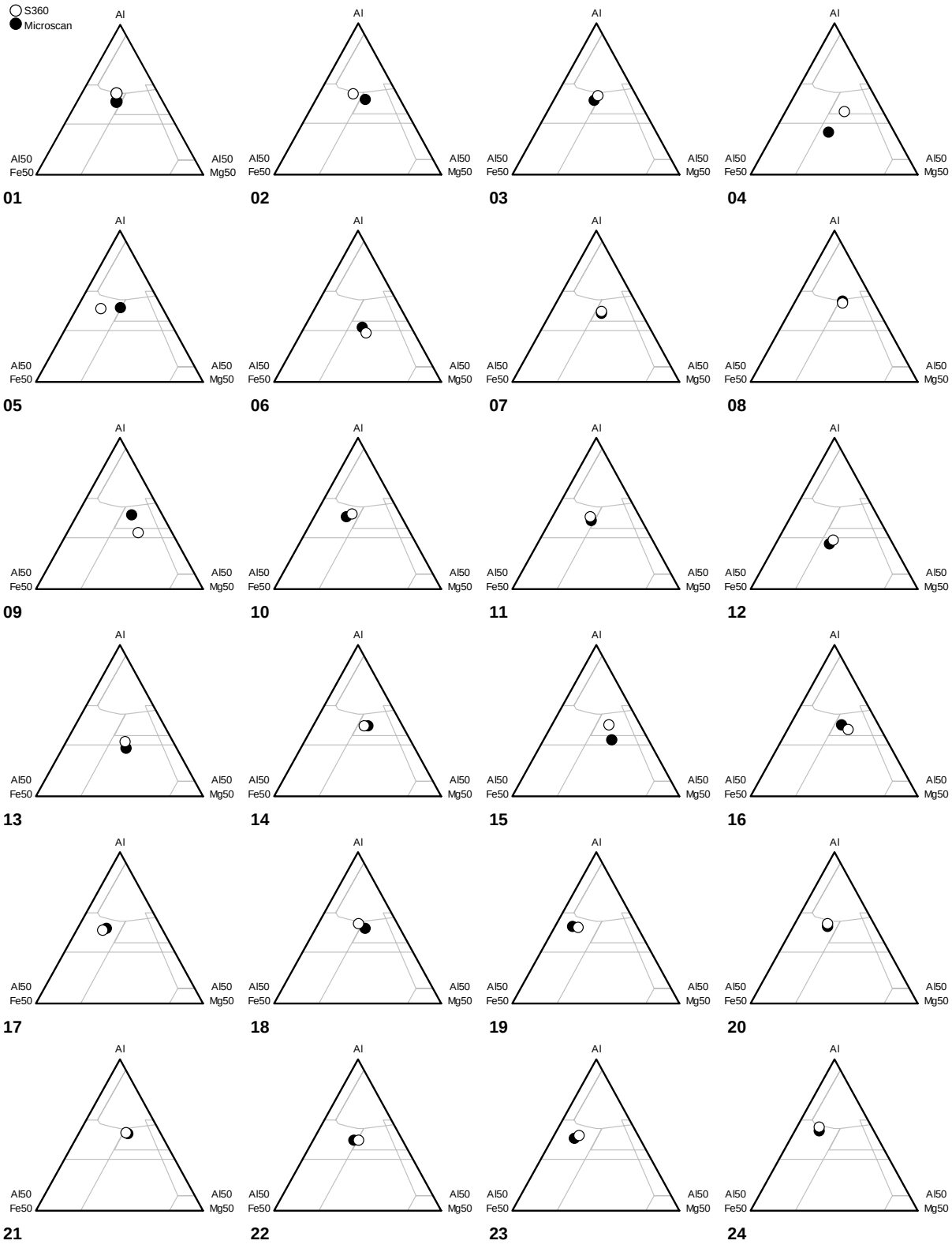
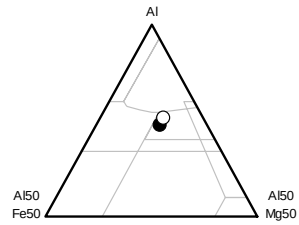
Appendix 3 Tourmaline Triangular Diagrams





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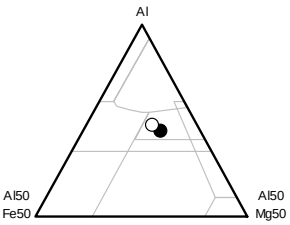

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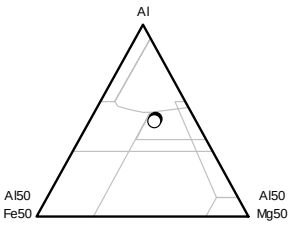

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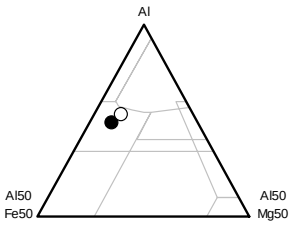

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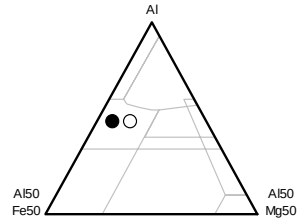

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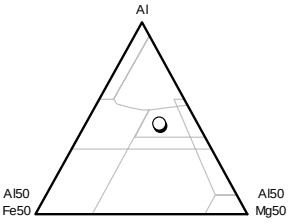

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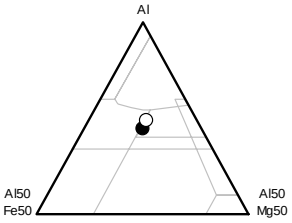

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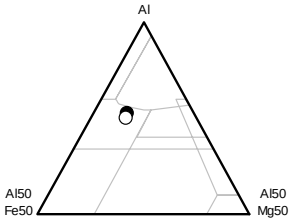

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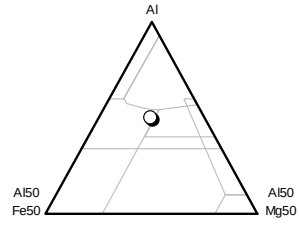

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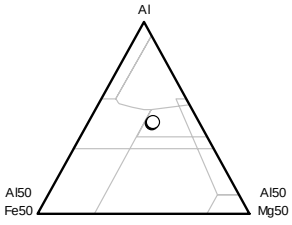

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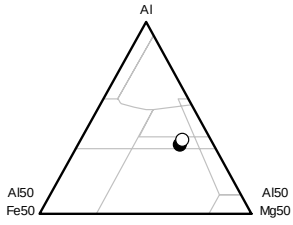

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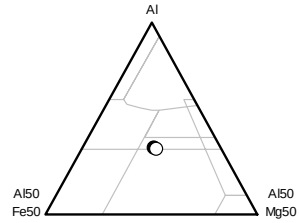

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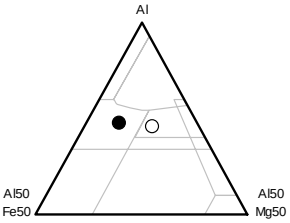

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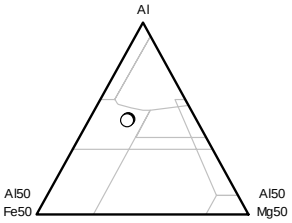

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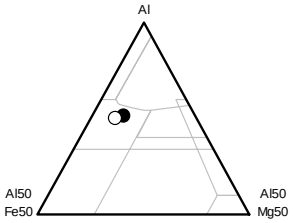

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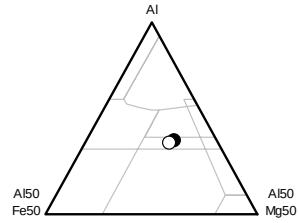

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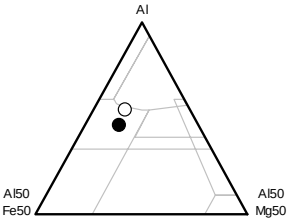

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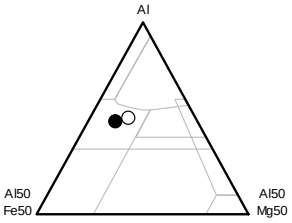

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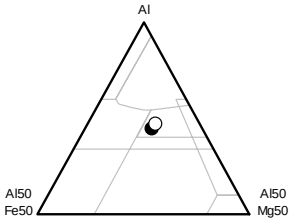

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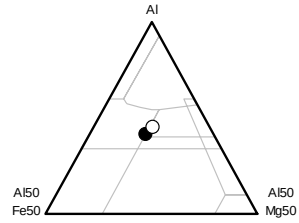

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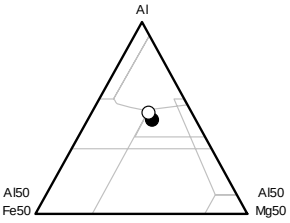

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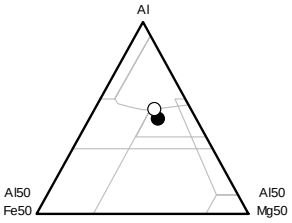

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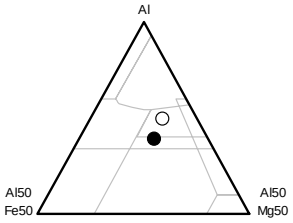

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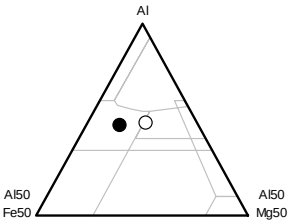

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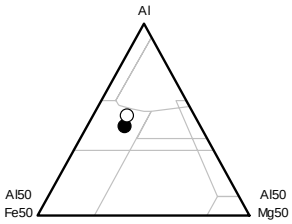

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