

DETERMINING QUANTITATIVE MINERALOGY USING A MODIFIED MODAN APPROACH ON THE QUESTA ROCK PILE MATERIALS, NEW MEXICO

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ABSTRACT

Petrographic analysis of rocks is traditionally performed with optical microscopy using thin sections and point counting. However, this does not provide accurate mineral proportions for sedimentary, volcanic, and soil-like material, because rock fragments, groundmass, and matrix are not identified as specific minerals. In addition, groundmass phases in volcanic rocks can be too fine to identify individually, and making thin sections of intact soil-like material is difficult because much of the material is not well cemented. ModAn is a normative calculation that estimates modes "...by applying Gaussian elimination and multiple linear regression techniques to simultaneous mass balance equations" (Paktunc, 2001) and allows location-specific mineral compositions to be used. One of the features of ModAn that makes it appropriate for this study is that it can model one of several sulfide minerals. Mineral compositions for Questa minerals were determined from electron microprobe analysis and entered into ModAn. Then by combining and normalizing results, bulk quantitative mineralogy can be determined using ModAn, petrographic observations, electron microprobe analysis, clay mineral analysis, and the whole-rock chemistry of the sample.

INTRODUCTION

Petrographic analysis of rocks has been traditionally performed with optical microscopy using thin sections and point counting thereby providing a quantitative modal mineralogy (van der Plas and Tobi, 1965; Delvigne, 1998). However, these methods do not always provide accurate mineral proportions for sedimentary, volcanic, and soil-like material, because rock fragments, groundmass, and matrix are typically identified as separate phases, not as specific minerals. In addition, groundmass phases in volcanic rocks can be too fine to identify individually by these methods, and making thin sections of intact soil-like material can be difficult because much of the material is not well cemented. In addition, variable modal analyses can be obtained by different petrographers.

Quantitative mineral abundance determination by whole rock X-ray diffraction analysis can be difficult, because the effects of mineral crystallinity, preferential orientation in the sample mount, differential absorption of X-rays, and overlapping peaks by different minerals, affect the diffractogram patterns and makes their interpretation difficult. For example, some minerals, such as hematite and other iron oxides, have poor crystallinity and are not always detected by X-ray diffraction. The Rietveld method attempts to overcome some of these issues (Bish and Howard, 1988; Bish and Post, 1993; Young, 1993; Oerter et al., 2007).

Another approach that can be used to determine quantitative mineralogy is to calculate a normative mineralogy from the whole-rock chemical composition. A normative mineralogy is the quantity of idealized minerals that are calculated from a whole-rock chemical analysis, although not all calculated minerals are necessarily actually present in the sample (Neuendorf et al., 2005). Normative mineralogy

is usually calculated for volcanic rocks that have glass and/or very small crystals, for which it is difficult to determine a modal mineralogy. A normative mineralogy also is calculated for altered or metamorphosed igneous rocks that no longer have the original igneous mineralogy. One of the most widely used normative calculations is the CIPW norm. Another normative method involves the combination of X-ray diffraction and whole-rock chemical analysis and attempts to provide a better quantitative mineralogy (SEDNORM; Cohen and Ward, 1991; Ward et al., 1999).

ModAn is a normative calculation that estimates modes "...by applying Gaussian elimination and multiple linear regression techniques to simultaneous mass balance equations" (Paktunc, 1998, 2001) and allows location-specific mineral compositions to be used. Representative mineral compositions for minerals in the Questa samples were determined from electron microprobe analysis and used in ModAn for this study (Appendix 1). A feature of ModAn that makes it appropriate for this study is that it can model one of several sulfide minerals.

In 2002, Chevron Mining Inc. (formerly Molycorp Inc.), the owner of the Questa molybdenum mine, initiated an extensive study by an independent consortium of academicians and consultants to examine the effects of weathering on the present and future stability of the mine rock piles. As part of this investigation, geologic, geochemical and geotechnical characterization of rock-pile and other materials was conducted from 2004 through 2008. Changes due to weathering are of interest with respect to predicting long-term geotechnical slope stability of the rock piles at the Questa molybdenum mine. Quantitative mineralogy is an important parameter and part of the characterization of samples used in the Questa project and is required for the humidity cell studies, modeling, and for understanding the geochemical, mineralogical, and geotechnical changes due to weathering. One purpose of the Questa project is to determine the quantitative mineralogy along with characterizing the textures and paragenesis of weathering in order to distinguish between post-mining weathering and pre-mining hydrothermal alteration and understand the weathering processes in the rock piles and other materials. Using a modified ModAn method, the quantitative mineralogy can be determined using ModAn, petrographic observations, electron microprobe analysis, clay mineral analysis, and the whole-rock chemistry of the sample. The purpose of this paper is to describe this method and present a case study for the Questa rock piles.

SITE DESCRIPTION

Chevron Mining, Inc. (formerly Molycorp, Inc.) operates a molybdenum mine on the western slope of the Taos Range of the Sangre de Cristo Mountains, Taos County, at Questa, northern New Mexico (Fig. 1). During the period of open-pit mining (1965-1983), approximately 350 million tons of overburden rock were removed and deposited onto mountain slopes and into tributary valleys forming nine rock piles around the area of the open pit (URS Corporation, 2003). Rock piles, the preferred term by many in the metal mining industry

today, refer to the man-made structures consisting of piles of non-ore material that had to be removed in order to extract the ore. This material, referred to as mine waste, overburden, subore, or proto-ore in older literature, does not include the tailings material, which consists of non-ore material remaining after milling. The Questa rock piles are up to 1600 feet high and hundreds of feet wide, and one of them, Goathill North (GHN), experienced some movement due to a weak foundation (URS Corporation, 2003; Norwest Corporation, 2004). The final goal of the Questa investigation is to develop a procedure that will assess the potential for gravitational instability of existing mine rock piles over time (100 yrs and 1000 yrs) based on the physical, chemical, mineralogical, biological, and geotechnical characteristics as well as the weathering of the rocks in the rock piles. Mineralogy is a key in understanding the post-mining weathering, because the predominant weathering system in the Questa rock piles is the oxidation of pyrite and dissolution of calcite to precipitate gypsum, jarosite, soluble efflorescent salts, and Fe oxide/hydroxide minerals.

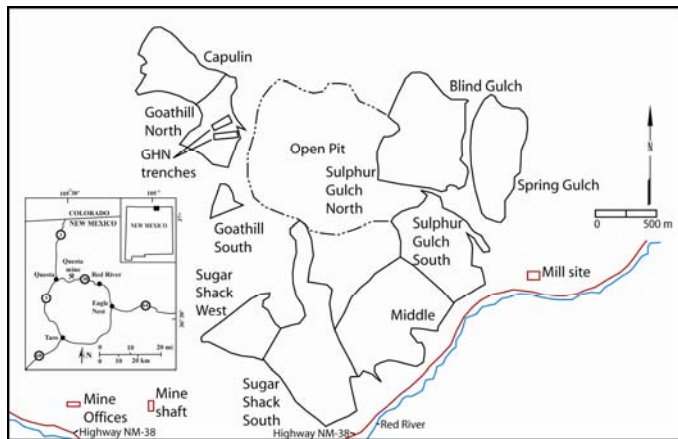


Figure 1. Location of the Questa mine, Taos Range, north-central New Mexico showing rock piles and other mine features.

TECHNICAL APPROACH

Introduction

The purpose of any study must be stated and understood in order to collect the proper samples and perform the needed field and laboratory analyses. Field observations and petrographic analysis are critical in understanding the composition, especially mineralogy, of the rocks and the processes the samples were subjected to (i.e. alteration, weathering, etc.). This modified ModAn technique described in this paper relies on more information to determine the mineralogy than typical modal techniques. Is the modified Modan technique required for the study, or can modal analysis provide the required data. Furthermore, the modified ModAn technique does not provide any specific information on the sample or mineral textures; petrographic analysis, including examination with a binocular microscope, thin section analysis, and electron microprobe analysis is required. In summary, quantitative mineralogy is only one of many data sets required to address the problem.

Sample collection

Several different types of samples were collected for the Questa project that required determination of quantitative mineralogy:

- Rock-pile material that includes both the soil matrix and rock fragments of mixtures of different lithologies and alteration assemblages
 - Samples collected from the surface and from test pits throughout the rock piles
 - Samples of the rock-pile material collected from trenches in GHN (5 ft channel or composite of selected layers)
- Residual soil profiles of colluvium/weathered bedrock, alteration scar, and debris flows
- Outcrop samples of unweathered (or least weathered) igneous rocks representative of the mined rock (overburden)

(includes all predominant lithologies and alteration assemblages at various hydrothermal alteration and weathering intensities)

- Sections of drill-core samples of the mined rock (overburden) and ore deposit before mining
- Splits of drill cuttings from holes drilled into the rock piles and underlying colluvium/bedrock.

The collected samples from the rock piles consisted of a heterogeneous mixture of rock fragments ranging in size from boulders (0.5 m) to <1 mm in diameter within a fine-grained soil matrix. Most rock fragments were hydrothermally altered before mining occurred and could have undergone oxidization and weathering since emplacement in the rock pile.

Mineralogical analysis

Mineralogical data was obtained from several different techniques in the Questa project, including:

- Petrographic analysis of a bulk grab sub-sample using a binocular microscope (van der Plas and Tobi, 1965)
- Petrographic analysis of thin sections of the rock fragments using a petrographic microscope (including both transmitted and reflected light microscopy; van der Plas and Tobi, 1965; Delvigne, 1998)
- Electron microprobe analysis of both the fine-grained soil matrix and the rock fragments
- Clay mineral determination of a bulk sample split using clay separation techniques and X-ray diffraction analysis (Moore and Reynolds, 1989; Hall, 2004)
- Rietveld analysis of heavy mineral separates (Oerter et al., 2007)
- Other methods of determining mineralogy (spectral analysis, X-ray diffraction, fizz test)

Figure 2 is a flow chart of the characterization procedure for a typical sample collected for the Questa study.

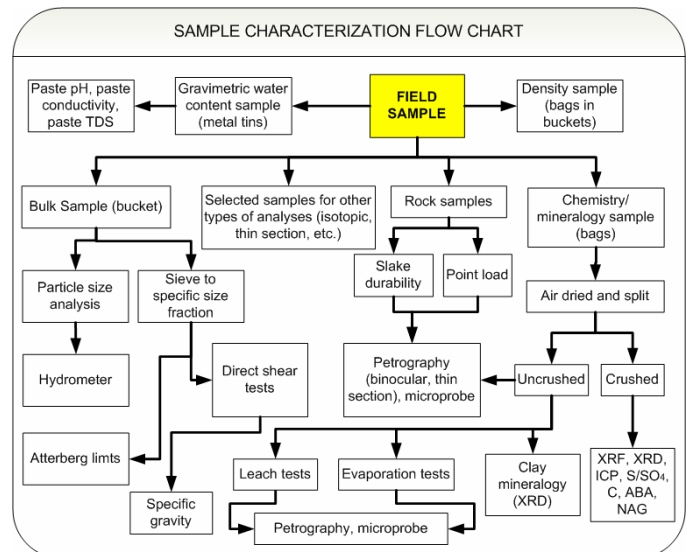


Figure 2. Flow chart showing characterization analyses of selected samples in the Questa project. Not all analyses are performed on every sample. Bucket, metal tin, and bags refers to size of sample collected. XRF–X-ray fluorescence analyses, XRD–X-ray diffraction analysis, ICP–Induced-coupled plasma spectrographic analysis, NAG–net acid producing tests, ABA–acid base accounting tests.

Steps in determination of quantitative mineralogy using ModAn and other data (Fig. 3) are below.

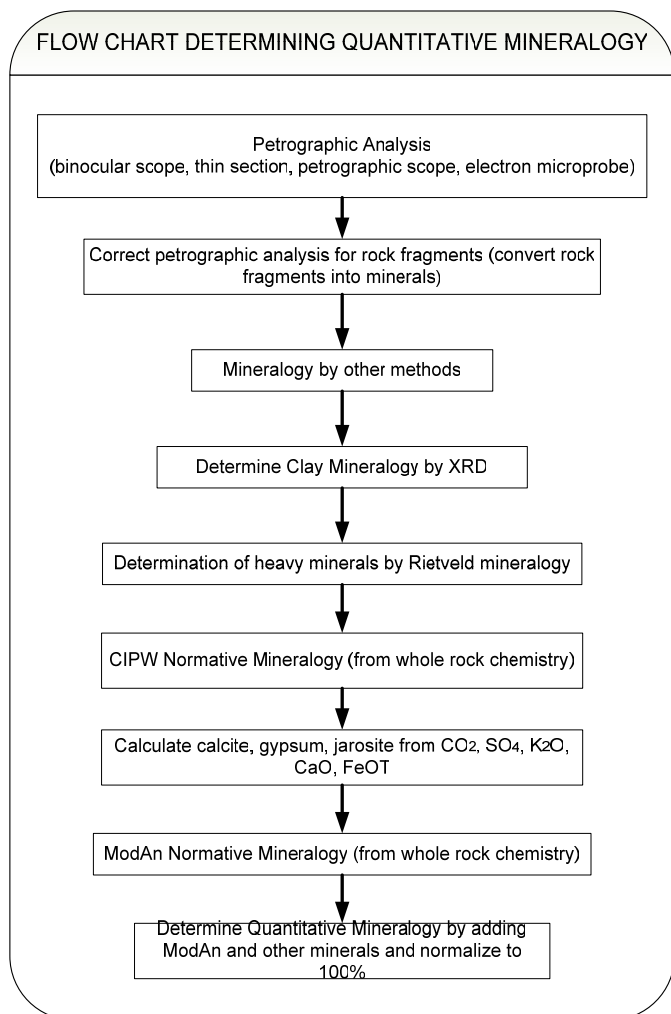


Figure 3. Flow chart for determining quantitative mineralogy using ModAn, petrographic observations, electron microprobe analysis, clay mineral analysis, and the whole-rock chemistry of the sample.

- Complete the petrographic analysis (soil petrography using a binocular microscope and/or more detailed petrography using thin sections and petrographic scope on selected samples as described above).
- Complete the electron microprobe analysis on selected samples.
- Complete the clay mineral analysis by X-ray diffraction (XRD) analysis (Hall, 2004; Moore and Reynolds, 1989).
- Complete the Rietveld mineralogy on heavy mineral separates of select samples (Oerter et al., 2007).
- Complete the whole-rock chemical analysis, including sulfide, sulfate, and carbon analyses.
- Calculate the amount of carbonate minerals using CaO and C (and MgO, MnO, FeO if other carbonate minerals are present), gypsum using CaO and SO₄ and jarosite using FeO, K₂O, and SO₄. ModAn does not model sulfate minerals, so the chemical analysis of the sample to be input into ModAn must be adjusted by subtracting the amount of CaO, SO₄, FeO, and K₂O to reflect the presence of gypsum and jarosite. These mineral abundances will be added to the mineralogy modeled by ModAn.
- Constrain ModAn with minerals observed in petrographic and other mineralogical analyses. This method allows the mineralogy to be consistent with the petrographic and other mineralogical observations and allows ModAn to model the appropriate mineral abundances.

- Input adjusted chemical analysis (corrected for the presence of gypsum and jarosite).
- Select from the ModAn list of minerals the observed minerals in the Questa sample obtained from petrography and other mineralogical analysis.
- If ModAn responds with an error message, then that mineral is deleted from the selection. If a mineral contained a negative value, it is removed from the selection. Typically only one or two clay minerals can be modeled.
- Different combinations of minerals and mineral compositions can be selected and modeled until the residual sum of squares of the remaining, unused oxides is less than 0.5, preferably less than 0.01 (A.D. Paktunc, personal communication, April 2008).
- Some Questa samples contain more MnO and P₂O₅ than is utilized by ModAn and results in larger residual sum of squares of the remaining, unused oxides. In these samples, a larger residual sum is acceptable because electron microprobe analysis does indicate that Mn-oxide minerals and the presence of P-rich goethite and jarosite are relatively common.
- Calculate CIPW norm to compare to quantitative mineralogy and to determine amount of zircon and fluorite.
- Correct normative mineral abundances obtained with ModAn by adding calculated gypsum, jarosite, known clay mineral proportions, and other known minerals not determined by ModAn (ModAn can only model 11 minerals and typically can only model 2 clay minerals). Typically these additional minerals are minor (<5%) and trace (<0.1%) minerals and are added to the ModAn calculated minerals to provide a more complete quantitative mineralogy. Equations are in Appendix 2.
- Normalize the corrected normative mineralogy to 100% and round to one significant figure (1% for major minerals, 0.1% for minor minerals, and 0.01% for trace minerals).

Not all samples have all of these data, but ModAn can still be used if you know what minerals are present in the sample or if there is another similar sample from which the minerals can be implied. Field observations and petrographic analysis using a binocular microscope is suggested for all samples to ensure the proper minerals are selected in the ModAn program.

RESULTS AND DISCUSSION

Examples from Questa

Two sets of samples were used from the Questa project to illustrate this technique. Samples from the rock piles and outcrop samples of unweathered and weathered igneous rocks were selected for humidity cell experiments and this modified ModAn technique was used to determine their mineralogy. Graf (2008) used this technique on samples from residual soil profiles in the alteration scars near the mine. Mineral compositions for Questa minerals were determined from electron microprobe analysis and entered into ModAn. Then by combining results from the petrographic observations, electron microprobe analysis, clay mineral analysis, and the whole-rock chemistry of the sample, bulk quantitative mineralogy can be determined using ModAn (Tables 1 (see Appendix A), and 2). Appendices 2 and 3 include the modal analyses determined from petrographic analysis at NMT (by D. Sweeney and G. Graf).

Validity of the modified ModAn method

Three independent techniques were used to test the validity of the modified ModAn method to determine the quantitative mineralogy. Independent petrographic analysis and Rietveld analysis were determined on 14 samples that were used in the humidity cell experiments from Mineral Services Canada, Inc. (2008). Quantitative X-ray diffraction (QXRD) was determined on one set of samples from the Hansen alteration scar (Appendix 3, Graf, 2008). The mineralogies obtained from the modified ModAn method were compared to these separate analyses (Appendices 2, 3). Not all methods compared exactly, but all methods provided similar enough results that the

quantitative mineralogy method obtained by the modified ModAn method is reliable, to approximately <5% in most samples, with a maximum error in some samples of 10%.

Table 2. Mineralogy of samples from the residual soil profile in the Hansen alteration scar (Graf, 2008).

	HAS-GJG-0006	HAS-GJG-0007	HAS-GJG-0008	HAS-GJG-0009	HAS-GJG-0010
Albite	3.7	5	3	0	0
Biotite	0	0	0	0	0
Calcite	0	0	0	0	0
Chlorite	12.1	9	16	0	6
Epidote	0	0	0	0	0
Fe oxides	1.7	2.8	0	1	1
Gypsum	7.5	11.5	15	5	5
Orthoclase	20.5	9.2	6	0	0
Pyrite	4.2	5.1	0.4	0	0.2
Quartz	21.4	24.2	28	25	45
Smectite	9.6	8.3	0	0	5.4
Kaolinite	4.8	0	0	0	0
Illite	4.8	16.6	32	69	26.9
Mixed layered clays	9.6	6.9	0	0	10.8
Total	99.9	98.6	100.4	100	100.3

Some of the differences between the three techniques are due to the identification and amounts of clay minerals. Petrographic techniques are unable to accurately identify or quantify the clay minerals because of their fine-grain size. In the quantitative mineralogy technique presented in this paper, clay mineral analysis was performed using standard clay mineral separation techniques and X-ray diffraction analysis (Hall, 2004; Moore and Reynolds, 1989). Typically the entire uncrushed sample is used, but the clay minerals that are obtained by the clay mineral separation techniques are from the fine-grained matrix and not within the matrix of the rock fragments. Electron microprobe analysis was used to verify the clay minerals within the soil matrix and rock fragments. ModAn will only model two clay minerals; therefore the remaining two clay minerals were added to the mineralogy obtained by ModAn (typically <2% each as determined from the clay mineral analysis).

Additional reasons that the three techniques differ are related to the identification and quantification of trace minerals. Rutile and apatite are not always identified by petrographic techniques because of their low abundance and small size. However, these minerals have been identified by electron microprobe analysis and are the most likely minerals to account for the TiO₂ and P₂O₅ observed in the whole-rock chemical analysis. Magnetite is found in the unaltered igneous rocks in the Questa-Red River area, however in most of the Questa rock-pile samples, magnetite is absent or altered and is therefore identified as a Fe-oxide mineral. Electron microprobe analysis and reflectance spectroscopy analysis indicates that goethite is more prevalent than hematite, although both are present.

Uncertainties and assumptions

This modified procedure using ModAn and other mineralogical determination has underlying uncertainties and assumptions like most petrographic and normative determinations. These uncertainties and assumptions include:

- A maximum of 11 minerals can be modeled by ModAn and typically the program will only accept as many as two clay minerals.
- Only one sulfide mineral can be modeled in ModAn.
- Ti is assumed to be included only as rutile when actually Ti could be in other phases such as Ti oxides and ilmenite at Questa. These other Ti-bearing minerals are found only in trace amounts in the Questa samples.
- P is assumed to be included only as apatite, when actually P is found in goethite and jarosite at Questa.

- Mn is assumed to be included only in calcite, chlorite, epidote, and small amounts in other minerals, unless petrographic analysis identifies the rare occurrence of rhodochrosite. Mn oxides are likely common but are typically present in small amounts and are not included in the quantitative mineralogy.
- C is assumed to be included only in carbonate minerals (calcite, calcite with Mn or Mg), unless organic material is specifically identified. Only trace amounts of rhodochrosite and other carbonate minerals have been found in the Questa samples.
- Fe is assumed to be included mostly in Fe oxides. Some of the specific chemical analysis of Questa minerals, such as chlorite and illite, do include Fe as a constituent.
- ModAn will not model sulfate minerals. CaO is adjusted in order to make gypsum and FeOT (total iron calculated as FeO) and K₂O are adjusted to make jarosite. Other sulfate minerals are found in only trace amounts in the Questa samples.

This modified ModAn technique does not provide any information on sample and mineral textures, which must be obtained from the field observations and petrographic analysis.

CONCLUSION

The quantitative mineralogy is a normative mineralogy that makes use of and is consistent with the available petrographic observations, electron microprobe analysis, clay mineral analysis, other mineralogical determinations and the whole-rock chemistry of the sample. Unlike most normative mineral analyses, all of the minerals calculated for the quantitative mineralogy are in the actual sample. In some samples, only selected data are available. A combination of petrographic analyses and ModAn can be used to calculate the quantitative mineralogy. This technique provides a quantitative mineralogy that is consistent with the petrographic observations, electron microprobe analysis, clay mineral analysis, and the whole-rock chemistry of the sample. This technique can be modified for use at many mine sites where quantitative mineralogy is required and should be useful in determining mineralogical composition in most studies, especially in studies where the mineralogy of sediments, volcanic rocks, soils, rock piles, and tailings are required.

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APPENDIX A

Table 1. Mineralogy of samples selected for humidity cell experiments using the modified ModAn technique.

Sample	Quartz	K-spar/ orthoclase	Plagioclase	Biotite	Illite/ sericite	Chlorite	Smectite	Kaolinite	Epidote	Magnetite
BCS-VWL-0004-8	32	5	12	0.01	33	2	1	1	0.01	
GHN-JRM-0001-8	38	15	10	0.01	23	4	1	1	0.1	
GHN-JRM-0002-8	28	21	18		15	6	1	1	0.1	0.01
GHN-JRM-0009-8	44	14	5		26	3	1	1	0.01	
GHN-KMD-0057-8	27	19	25		8	7	1	1	7	
GHN-KMD-0088-8	30	26	19		13	4	1	1	0.01	
GHN-KMD-0096-8	51	24	0.01	0.01	19	1	1	1	0.01	
MIN-VTM-0021-8	34	13			40	4	1	1	0.01	
PIT-RDL-0005-8	48	33	0.9		13	0.7	1	1		
PIT-RDL-0006-8	51	25	1		18	1	1	1	0.01	
PIT-RDL-0007-8	54	19	0.3		21	1	1	1		
PIT-VTM-0600-8	27	18	16		18	6	1	1	0.01	0.01
ROC-NWD-0002-8	19	26	31		11	4	1	1		
SPR-JWM-0002-8	26	17	30	0.01	5	9	1	1	5	

Sample	Fe oxides	Rutile	Apatite	Pyrite	Calcite	Gypsum	Zircon	Jarosite	Chalco-pyrite	Organic carbon	Total
BCS-VWL-0004-8	10	0.01	1	0.1	0.2	0.4	0.03	2		0.5	100.26
GHN-JRM-0001-8	0.8	0.5	0.3	3	0.4	0.8	0.03	2			99.94
GHN-JRM-0002-8	7	0.5	0.7		0.3	1.5	0.03	0.01			100.15
GHN-JRM-0009-8	0.2	0.4	0.2	2	0.5	0.8	0.04	1.7			99.85
GHN-KMD-0057-8	2	0.6	0.8		1	0.2	0.03				99.63
GHN-KMD-0088-8	3	0.4	0.3	1	0.3	1	0.03				100.04
GHN-KMD-0096-8	0.4	0.2	0.01	0.1	0.2	0.5	0.06	1.4			99.9
MIN-VTM-0021-8	5.5	0.4	0.3		0.9	0.1	0.03	0.1			100.34
PIT-RDL-0005-8	1	0.1	0.01	0.01	0.3	0.08	0.06	0.7			99.86
PIT-RDL-0006-8	1	0.1	0.01	0.01	0.2	0.06	0.06	0.8			100.25
PIT-RDL-0007-8	0.01	0.1	0.01	1	0.2	0.02	0.06	1			99.7
PIT-VTM-0600-8	4	0.5	0.1	2	2	4	0.03		0.01		99.66
ROC-NWD-0002-8	1	0.7	0.6	4	0.1	0.1	0.03	0.6	0.01		100.14
SPR-JWM-0002-8	2	0.7	0.8	0.6	1	0.1	0.03	0.01	0.01		99.26

APPENDIX 1

Mineral compositions (in terms of number of cations and anions in unit formula) used in ModAn, including compositions already in the program, and representative mineral compositions using electron microprobe mineral data from Questa rock pile samples.

Mineral/element	Si	Ti	Al	Fe	Mn	Mg	Ca	Na	K	P	C	O	H
MODAN compositions													
actinolite	7.5	0	0.66	2.2	0	2.4	1.6	0.47	0	0	0	24	2
albite	3	0	1	0	0	0	0	1	0	0	0	8	0
amphibole	6.8	0	2.1	2.4	0	2.2	2.1	0.5	0	0	0	24	2
ankerite 1	0	0	0	0.25	0	0.25	0.5	0	0	0	1	3	0
ankerite 2	0	0	0	0.2	0.1	0.2	0.5	0	0	0	1	3	0
ankerite 3	0	0	0	0.15	0	0.35	0.5	0	0	0	1	3	0
ankerite 4	0	0	0	0.12	0.01	0.38	0.5	0	0	0	1	3	0
anorthite	2	0	2	0	0	0	1	0	0	0	0	8	0
anthophyllite	8	0	0	6	0	1	0	0	0	0	0	24	2
apatite	0	0	0	0	0	0	5	0	0	3	0	13	1
biotite 1	6	0.3	3	3.8	0	1.5	0	0	2	0	0	24	4
biotite 2	2.9	0.05	1.1	0	0	1.5	1.5	0	0	0	0	12	2
calcite	0	0	0	0	0	0	1	0	0	0	1	3	0
calcite-Mg	0	0	0	0.06	0.04	0.3	0.6	0	0	0	1	3	0
calcite-Mn	0	0	0	0.1	0.1	0	0.8	0	0	0	1	3	0
chlorite 1	6	0	4.7	5.2	0	3.38	0	0	0	0	0	44	16
chlorite 2	5	0	4.6	8.7	0	1.8	0	0.17	0	0	0	44	16
chlorite 3	3	0	2	2.5	0	2.5	0	0	0	0	0	14	4
chlorite 4	5.4	0	5.2	3.4	0	6	0	0	0	0	0	44	16
chlorite 5	5.8	0	4.7	5.8	0	3.4	0	0	0	0	0	44	16
chromite	0	0.025	0.488	0.943	0.01	0.392	0	0	0	0	0	4	0
clinopyroxene 1	1.91	0.01	0.14	0.15	0	0.91	0.84	0.02	0	0	0	6	0
clinopyroxene 2	2	0	0.1	0.4	0	0.8	0.8	0	0	0	0	6	0
diopside	1	0	0	0	0	0.5	0.5	0	0	0	0	3	0
dolomite	0	0	0	0	0	0.5	0.5	0	0	0	1	3	0
enstatite	1	0	0	0	0	1	0	0	0	0	0	3	0
epidote	3	0	0.75	2.25	0	0	2	0	0	0	0	13	1
ferrosilite	1	0	0	1	0	0	0	0	0	0	0	3	0
garnet-almandine	3	0	2	3	0	0	0	0	0	0	0	12	0
garnet-andradite	3	0	0	2	0	0	3	0	0	0	0	12	0
garnet-grossular	3	0	2	0	0	0	3	0	0	0	0	12	0
garnet-pyrope	3	0	2	0	0	3	0	0	0	0	0	12	0
garnet-spessartine	3	0	2	0	3	0	0	0	0	0	0	12	0
glaucofane	7.79	0	1.9	0.73	0	2.62	0.15	1.83	0.12	0	0	24	2
goethite	0	0	0	1	0	0	0	0	0	0	0	2	1
hedenbergite	1	0	0	0.5	0	0	0.5	0	0	0	0	3	0
hematite	0	0	0	2	0	0	0	0	0	0	0	3	0
hornblende 1	6	0.16	2.5	1.11	0	3.22	1.99	0.56	0.12	0	0	24	2
hornblende 2	7	0	1	2.5	0	2.5	2	1	0	0	0	24	2
hornblende 3	6.7	0	1.9	2	0	2.3	1.9	0.3	0.1	0	0	24	2
illite 1	7	0	5	0	0	0	0	0	1	0	0	24	4
illite 2	3.25	0	2.75	0	0	0	0	0	0.75	0	0	12	2
ilmenite	0	1	0	1	0	0	0	0	0	0	0	3	0
kaolinite	2	0	2	0	0	0	0	0	0	0	0	9	4
kuthnohorite	0	0	0	0	0.5	0	0.5	0	0	0	1	3	0
lepidolite	6.75	0	4	3	0	0.2	0	0.3	1.7	0	0	24	4
magnetite	0	0	0	3	0	0	0	0	0	0	0	4	0
muscovite 1	6	0	6	0	0	0	0	0	2	0	0	24	4
muscovite 2	6	0	5.8	0.1	0	0	0	0.2	1.7	0	0	24	4
oligonite	0	0	0	0.5	0.5	0	0	0	0	0	1	3	0
olivine-Fo10	1	0	0	1.8	0	0.2	0	0	0	0	0	4	0
olivine-Fo60	1	0	0	0.8	0	1.2	0	0	0	0	0	4	0
olivine-Fo70	1	0	0	0.6	0	1.4	0	0	0	0	0	4	0
olivine-Fo80	1	0	0	0.4	0	1.6	0	0	0	0	0	4	0

Mineral/element	Si	Ti	Al	Fe	Mn	Mg	Ca	Na	K	P	C	O	H
olivine-Fo81	1	0	0	0.33	0	1.66	0	0	0	0	0	4	0
olivine-Fo82	1	0	0	0.36	0	1.64	0	0	0	0	0	4	0
olivine-Fo84	1	0	0	0.32	0	1.68	0	0	0	0	0	4	0
olivine-Fo86	1	0	0	0.28	0	1.72	0	0	0	0	0	4	0
olivine-Fo88	1	0	0	0.24	0	1.76	0	0	0	0	0	4	0
olivine-Fo90	1	0	0	0.2	0	1.8	0	0	0	0	0	4	0
orthoclase	3	0	1	0	0	0	0	0	1	0	0	8	0
orthopyroxene 1	1.94	0.01	0.06	0.32	0.01	1.64	0.05	0	0	0	0	6	0
orthopyroxene 2	2	0	0	0.15	0	1.85	0	0	0	0	0	6	0
orthopyroxene 3	2	0	0	0.6	0	1.4	0	0	0	0	0	6	0
pargasite	6.7	0	1.8	0.26	0	4.31	1.88	0.69	0.22	0	0	24	2
phlogopite	5.7	0	2.8	0.5	0	4.78	0	0	1.7	0	0	24	4
pigeonite	1.96	0	0.04	0.55	0	1.3	0.15	0	0	0	0	6	0
plagioclase-An20	2.8	0	1.2	0	0	0	0.2	0.8	0	0	0	8	0
plagioclase-An40	2.6	0	1.4	0	0	0	0.4	0.6	0	0	0	8	0
plagioclase-An5	2.95	0	1.05	0	0	0	0.05	0.95	0	0	0	8	0
plagioclase-An60	2.4	0	1.6	0	0	0	0.6	0.4	0	0	0	8	0
plagioclase-An80	2.2	0	1.8	0	0	0	0.8	0.2	0	0	0	8	0
plagioclase-An85	2.15	0	1.85	0	0	0	0.85	0.15	0	0	0	8	0
plagioclase-An88	2.12	0	1.88	0	0	0	0.88	0.12	0	0	0	8	0
plagioclase-An90	2.1	0	1.9	0	0	0	0.9	0.1	0	0	0	8	0
plagioclase-An95	2.05	0	1.95	0	0	0	0.95	0.05	0	0	0	8	0
quartz	1	0	0	0	0	0	0	0	0	0	0	2	0
rhodochrosite	0	0	0	0	1	0	0	0	0	0	1	3	0
richterite	7.75	0.01	0.23	0.21	1.06	3.96	0.84	1.57	0.31	0	0	24	2
rutile	0	1	0	0	0	0	0	0	0	0	0	2	0
siderite 1	0	0	0	0.95	0.05	0	0	0	0	0	1	3	0
siderite 2	0	0	0	0.8	0.1	0.1	0	0	0	0	1	3	0
siderite 3	0	0	0	0.6	0.1	0.3	0	0	0	0	1	3	0
siderite 4	0	0	0	0.5	0	0.5	0	0	0	0	1	3	0
siderite 5	0	0	0	0.5	0.1	0.4	0	0	0	0	1	3	0
siderite 6	0	0	0	1	0	0	0	0	0	0	1	3	0
siderite-Ca	0	0	0	0.55	0.1	0.15	0.2	0	0	0	1	3	0
siderite-Mg	0	0	0	0.38	0	0.62	0	0	0	0	1	3	0
siderite-Mn	0	0	0	0.65	0.25	0.1	0	0	0	0	1	3	0
sillimanite	1	0	2	0	0	0	0	0	0	0	0	5	0
spinel	0	0	2	0	0	1	0	0	0	0	0	4	0
stilpnomelane 1	8	0	1.3	5	0.1	0.65	0.04	0	0.3	0	0	25	6
stilpnomelane 2	8	0	1.3	4.8	0	1.13	0	0	0.6	0	0	25	6
talc	4	0	0	0	0	3	0	0	0	0	0	12	2
tremolite	8	0	0	0	0	5	2	0	0	0	0	24	2
vermiculite	2.81	0	1.47	0.5	0	1.95	0	0	0.62	0	0	12	2
biotite KZK	6	0.19	3.38	3.14	0.03	2.38	0	0.03	1.97	0	0	24	4
ankerite KZK	0	0	0	0.24	0.02	0.23	0.5	0	0	0	1	3	0
montmorillonite1	7.81	0	3.56	0.09	0	0.73	0.27	0.03	0.01	0	0	26	8
montmorillonite2	4	0	1.8	0	0	0.2	0.15	0.15	0	0	0	13	4
dol UM				0.09		0.43	0.48				1	3	0
dol BS				0.13		0.36	0.51				1	3	0
serpentine	2					3						9	4
anthophyllite-Mg (Weber)	8.27	0	0.11	0.03	0.01	6.25	0.01	0.01	0			24	2
tremolite (Weber)	8.01	0	0.08	0.11	0.01	4.77	1.96	0.05	0.02			24	2
Questa compositions													
Moly ksp 1	2.95	0	1.06	0.01	0	0	0	0.26	0.72	0	0	8	0
Moly ksp 2	2.97	0	1.03	0	0	0	0	0.04	0.99	0	0	8	0
Moly Na-spar 1	2.8	0	1.22	0	0	0	0.18	0.78	0.03	0	0	8	0
Moly Na-spar 2	2.82	0	1.23	0	0	0	0.01	1	0.01	0	0	8	0
Moly chlorite 1	2.67	0	1.67	1.83	0.24	6.16	0.01	0.17	0.03	0	0	18	

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Mineral/element	Si	Ti	Al	Fe	Mn	Mg	Ca	Na	K	P	C	O	H
Moly chlorite 2	2.32	0	1.6	2	0	0.13	6.81	0.1	0	0	0	18	
Moly ave. clay	3.848	0.004	2.561	0.288	0.01	0.61	0.068	0.048	0.334	0	0	13	
Moly illite 1	3.84	0.01	2.56	0.21	0.02	0.52	0.02	0.05	0.94	0	0	13	
Moly illite 2	3.88	0.01	2.44	0.23	0.01	0.57	0.01	0.08	0.95	0	0	13	
Moly kaolinite 1	2.58	0	2	0.11	0	0.28	0.04	0.01	0.01	0	0	9	
Moly kaolinite 2	2.38	0	2.05	0.31	0.01	0.46	0.6	0	0.04	0	0	9	
Moly smectite 1	4.16	0	2.15	0.27	0	0.77	0.11	0.01	0.04	0	0	13	
Moly smectite 2	4.07	0	2.11	0.39	0.01	0.7	0.11	0.13	0.02	0	0	13	
Moly epidote 1	2.74	0	1.82	1.47	0.02	0.02	1.82	0	0	0	0	13	
Moly epidote 2	2.8	0	2.11	1.17	0.04	0.03	1.84	0	0	0	0	13	
Moly Fe oxides 1	0	0.05	0	0.9	0	0.08	0	0	0	0	0	2	
Moly Fe oxides 2	0	0.02	0	0.97	0	0	0	0	0	0	0	2	
Moly Fe oxides 3	0.02	0	0	0.97	0	0	0	0	0	0	0	2	

APPENDIX 2

Equations used to adjust the chemical composition before inputting into ModAn.

$$\text{Sulfate (weight \%)} = (\text{amount of sulfur in sulfate} \times 96) / 32$$

$$\text{Gypsum (weight \%)} = (\text{SO}_4\% / 0.557)$$

$$\text{Ca in gypsum} = (\text{amount of gypsum} / 0.233)$$

$$\text{CaO in gypsum} = (56.078 \times \text{Ca} \% / 40.078)$$

APPENDIX 3

Comparison of QXRD, modal petrography and ModAn modeling results from the Hansen profile (Graf, 2008).

Sample	HAS-GJG-0006 (Q)	HAS-GJG-0006 (M)	HAS-GJG-0006 (P)	HAS-GJG-0007 (Q)	HAS-GJG-0007 (M)	HAS-GJG-0007 (P)	HAS-GJG-0008 (Q)	HAS-GJG-0008 (M)	HAS-GJG-0008 (P)
Albite	5	3.7	5-10%	8	5.0	2-5%	3	3.0	2-5%
Biotite	1	0.0	-	2	0.0	*	4	0.0	*
Calcite	-	0.0	2-3%	-	0.0	*	-	0.0	*
Chlorite	25	12.1	15-20%	24	9.0	10-15%	28	16.0	25-30%
Epidote	-	0.0	-	-	0.0	*	-	0.0	*
Fe-Oxides	-	1.7	-	-	2.8	10-15%	-	0.0	*
Gypsum	9	7.5	-	16	11.5	5-10%	15	15.0	-
Orthoclase	25	20.5	18-25%	11	9.2	7-10%	6	6.0	4-8%
Pyrite	2	4.2	2-3%	3	5.1	-	0	0.4	1-2%
Quartz	28	21.4	25-30%	29	24.2	20-30%	36	28.0	30-35%
Total Clay	-	28.9	15-20%	-	33.2	20-25%	-	32.0	20-25%
TOTAL	95	100.0			100.0		22	100.0	
Smectite		9.6			8.3			0.0	
Kaolinite		4.8			0.0			0.0	
Mixed Layer		9.6			6.9			0.0	
Illite		4.8			16.6			32.0	

Sample	HAS-GJG-0009 (Q)	HAS-GJG-0009 (M)	HAS-GJG-0009 (P)	HAS-GJG-0010 (Q)	HAS-GJG-0010 (M)	HAS-GJG-0010 (P)
Albite	-	0.0	-	-	0.0	-
Biotite	-	0.0	*	-	0.0	*
Calcite	-	0.0	-	-	0.0	-
Chlorite	-	0.0	-	8	6.0	10-15%
Epidote	-	0.0	*	-	0.0	*
Fe-Oxides	-	1.0	2-3%	-	1.0	2-3%
Gypsum	3	5.0	-	6	5.0	-
Orthoclase	-	0.0	*	-	0.0	*
Pyrite	-	0.0	<1%	-	0.2	Tr
Quartz	17	25.0	15-20%	41	45.0	35-40%
Total Clay	80	69.0	75-80%	40	43.0	40-45%
TOTAL		100.3		97	100.0	
Smectite		0.0			5.4	
Kaolinite		0.0			0.0	
Mixed Layer		0.0			10.8	
Illite		69.0			26.9	

(Q) = QXRD
(M) = ModAn
(P) = Petrography
(*) = suppressed in ModAn simulation

APPENDIX 4

Comparison of the modified ModAn method to modal analysis and Rietveld method by Mineral Services Canada, Inc. 2008) for 14 samples used in the weathering (humidity) cells.

Sample	method	quartz	K-spar/ orthoclase	plagioclase	biotite	illite/sericite (muscovite)	chlorite	smectite	kaolinite	epidote	magnetite
BCS-VWL-0004-8	NMT modified ModAn	32	5	12	0.01	33	2	1	1	0.01	
BCS-VWL-0004-8 NMT											
BCS-VWL-0004min_ser	Mineral Services petrography	35	15	15	2	15	0.01		3	0.01	
BCS-VWL-0004Reit	Mineral Services Reitveld	41.4	14.2	16.8	2.4	15.9	3.7				
GHN-JRM-0001-8	NMT modified ModAn	38	15	10	0.01	23	4	1	1	0.1	
GHN-JRM-0001min_ser	Mineral Services petrography	15	15	10	1	15	3		1	2	
GHN-JRM-0001Reit	Mineral Services Reitveld	42.8	12.9	13.8	5	14	4				
GHN-JRM-0002-8	NMT modified ModAn	28	21	18		15	6	1	1	0.1	0.01
GHN-JRM-0002-min_ser	Mineral Services petrography	20	25	30		5	10			3	0.01
GHN-JRM-0002Reit	Mineral Services Reitveld	29.6	20.8	26.6		8	10.6			1.6	0.7
GHN-JRM-0009-8	NMT modified ModAn	44	14	5		26	3	1	1	0.01	
GHN-JRM-0009-min_ser	Mineral Services petrography	20	15	35		15	5		0.01	1	
GHN-JRM-0009Reit	Mineral Services Reitveld	48.4	13.5	8.6		17.1	5.2				0.2
GHN-KMD-0057-8	NMT modified ModAn	27	19	25		8	7	1	1	7	
GHN-KMD-0057-min_serv	Mineral Services petrography	15	30	40			10			5	tr-1
GHN-KMD-0057Reit	Mineral Services Reitveld	26.4	27.2	28.7			11.1			6.3	
GHN-KMD-0088-8	NMT modified ModAn	30	26	19		13	4	1	1	0.01	
GHN-KMD-0088-8min_serv	Mineral Services petrography	30	25	25		5	3			3	0.01
GHN-KMD-0088-8Reit	Mineral Services Reitveld	31.2	23.4	28.9		5.9	7.3			1.1	
GHN-KMD-0096-8	NMT modified ModAn	51	24	0.01	0.01	19	1	1	1	0.01	
GHN-KMD-0096-8 min_serv	Mineral Services petrography	15	20	0.01		15			2	0.01	
GHN-KMD-0096-8Reit	Mineral Services Reitveld	56.7	21.2	4.2		12.9			2.3		
MIN-VTM-0021-8	NMT modified ModAn	34	13			40	4	1	1	0.01	
MIN-VTM-0021-8min_ser	Mineral Services petrography	10	1			26	3				
MIN-VTM-0021-8Reit	Mineral Services Reitveld	42.7				53.7	3.1				
PIT-RDL-0005-8	NMT modified ModAn	48	33	0.9		13	0.7	1	1		
PIT-RDL-0005min_ser	Mineral Services petrography	15	25			15			1		
PIT-RDL-0005Reit	Mineral Services Reitveld	55.3	26.6	1.3		11.4			3.5		
PIT-RDL-0006-8	NMT modified ModAn	51	25	1		18	1	1	1	0.01	
PIT-RDL-0006-8min_ser	Mineral Services petrography	15	20			5			1	0.01	
PIT-RDL-0006-8Reit	Mineral Services Reitveld	57	24.7	2.3		11.5			3		
PIT-RDL-0007-8	NMT modified ModAn	54	19	0.3		21	1	1	1		
PIT-RDL-0007-8min_serv	Mineral Services petrography	20	15	0.01		25			1		
PIT-RDL-0007-8Reit	Mineral Services Reitveld	56.2	16.5			26.2					
PIT-VTM-0600-8	NMT modified	27	18	16		18	6	1	1	0.01	0.01

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Sample	method	quartz	K-spar/ orthoclase	plagioclase	biotite	illite/sericite (muscovite)	chlorite	smectite	kaolinite	epidote	magnetite
	ModAn										
PIT-VTM-0600-8min_serv	Mineral Services petrography	20	15	0.01		10	10			2.5	0.5
PIT-VTM-0600-8Reit	Mineral Services Reitveld	31	16.9	25.2		10	10.1			1.8	1
ROC-NWD-0002-8	NMT modified ModAn	19	26	31		11	4	1	1		
ROC-NWD-0002-8min_serv	Mineral Services petrography	10	20	35	1	12	5				
ROC-NWD-0002-8Reit	Mineral Services Reitveld	17.5	17.3	40.7			5.3				0.2
SPR-JWM-0002-8	NMT modified ModAn	26	17	30	0.01	5	9	1	1	5	
SPR-JWM-0002-8min_serv	Mineral Services petrography	35	10	30	10	0.01	5			1	1
SPR-JWM-0002-8Reit	Mineral Services Reitveld	27.5	10.1	43	4.4	4	9.1				0.9

Sample	Fe oxides	rutile	apatite	pyrite	calcite	gypsum	zircon	jarosite	Chalco-pyrite	Vermicu-lite	organic carbon	Ground-mass	Total
BCS-VWL-0004-8	10	0.01	1	0.1	0.2	0.4	0.03	2			0.5		100.26
BCS-VWL-0004min_ser	3	0.01		0.01		0.01		3			1		92.05
BCS-VWL-0004Reit	1.8							2.6		1.1			99.9
GHN-JRM-0001-8	0.8	0.5	0.3	3	0.4	0.8	0.03	2					99.94
GHN-JRM-0001min_ser	2	1		5		0.01		0.01				20	90.02
GHN-JRM-0001Reit				3.9	0.4	1.7		1.6					100.1
GHN-JRM-0002-8	7	0.5	0.7		0.3	1.5	0.03	0.01					100.15
GHN-JRM-0002min_ser	3	2		0.01				0.01					98.03
GHN-JRM-0002Reit	0.9					0.8		0.3					99.9
GHN-JRM-0009-8	0.2	0.4	0.2	2	0.5	0.8	0.04	1.7					99.85
GHN-JRM-0009min_ser	0.01	0.01		3	0.01			<2					94.04
GHN-JRM-0009Reit				2.9	0.5	2		1.7					100.1
GHN-KMD-0057-8	2	0.6	0.8		1	0.2	0.03						99.63
GHN-KMD-0057min_serv	tr-1	0.01		0.01	1								101.02
GHN-KMD-0057Reit					0.4								100.1
GHN-KMD-0088-8	3	0.4	0.3	1	0.3	1	0.03						100.04
GHN-KMD-0088-8min_serv	0.01	tr-1		<2					0.0001				91.0201
GHN-KMD-0088-8Reit				2.2									100
GHN-KMD-0096-8	0.4	0.2	0.01	0.1	0.2	0.5	0.06	1.4					99.9
GHN-KMD-0096-8_min_serv	0.01	0.01		0.01				3				40	95.05
GHN-KMD-0096-8Reit						1		1.6					99.9
MIN-VTM-0021-8	5.5	0.4	0.3		0.9	0.1	0.03	0.1					100.34
MIN-VTM-0021-8min_ser	2	0.01								1	3	50	46.01
MIN-VTM-0021-8Reit		0.5											100
PIT-RDL-0005-8	1	0.1	0.01	0.01	0.3	0.08	0.06	0.7					99.86
PIT-RDL-0005min_ser	2	0.01		0.01				1.5				35	59.52
PIT-RDL-								1.9					100

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Sample	Fe oxides	rutile	apatite	pyrite	calcite	gypsum	zircon	jarosite	Chalco-pyrite	Vermicu-lite	organic carbon	Ground-mass	Total
0005Reit													
PIT-RDL-0006-8	1	0.1	0.01	0.01	0.2	0.06	0.06	0.8					100.25
PIT-RDL-0006-8min_ser	3	0.01						2				50	46.02
PIT-RDL-0006-8Reit								1.5					100
PIT-RDL-0007-8	0.01	0.1	0.01	1	0.2	0.02	0.06	1					99.7
PIT-RDL-0007-8min_serv	0.01	1		2				0.01	0.01			30	64.04
PIT-RDL-0007-8Reit				1.2									100.1
PIT-VTM-0600-8	4	0.5	0.1	2	2	4	0.03		0.01				99.66
PIT-VTM-0600-8min_serv	0.01	0.01		2.5	2.5				0.01			35	63.04
PIT-VTM-0600-8Reit				2	1.9								99.9
ROC-NWD-0002-8	1	0.7	0.6	4	0.1	0.1	0.03	0.6	0.01				100.14
ROC-NWD-0002-8min_serv	0.02	1		4					0.01				88.03
ROC-NWD-0002-8Reit		0.9		5.4									87.3
SPR-JWM-0002-8	2	0.7	0.8	0.6	1	0.1	0.03	0.01	0.01				99.26
SPR-JWM-0002-8min_serv	0.02	0.01		1	3			0.01	0.01				96.06
SPR-JWM-0002-8Reit				0.7	0.3								100