Bachelor Thesis

Degree Project Geology 15hp

Investigation of the metamorphic environment conditions of Persholmen, NE Utö, with SEM generated data.

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Abstract:

This geothermobarometric investigation of St Persholmen, Utö, in the south central part of Sweden presents an attempt at determining the metamorphic conditions of this important part of the Svecofennian province. Belonging to the geology of the Bergslagen area, Utö historically represent part of Sweden's vast ore resources with concentrations of iron, copper and sulfides. Rock types from this area are around 1.91-1.89 Ga old (Stephens et al. 2009) and as such Paleoproterozoic in age. The rocks on Utö are considered representative of Bergslagen and record the closing of an ocean starting with subduction followed by volcanic episodes and orogeny (Talbot 2008). The bedrock we observe at Persholmen is thought to represent the remains of the aforementioned orogeny where greywackes from the oceanic stage have been preserved at the base of the mountain range (Stålhös 1982).

The two rock types of interest at Persholmen which have been evaluated in this study are 1) normal greywackes and 2) greywackes which have been migmatised either because of the influence of fluids, reworking in an accretionary prism or melted at the base of a mountain range. In this project the area of study has been mapped and samples have been retrieved in order to distinguish the mineralogy and metamorphic history of the bedrock. After petrographic analysis I have determined mineral chemistry by the use of a SEM (Scanning Electron Microscope). These chemical data have then been entered into the computer programs AX and THERMOCALC for determination of temperature and pressure. For the normal/migmatised greywackes a temperature of 538±36/756±133°C and a pressure of 3.1±1.3/3.8±3.2 kbars respectively have been estimated. Two generations of muscovite provide evidence of fluid-rock interactions and at the north coast of Persholmen the occurrence of sillimanite indicates a high grade of metamorphism.

Aim:

This thesis is part of a national project called ”The Metamorphic Map of Sweden” which is an attempt led by Professor Alasdair Skelton and funded by SGU at understanding the metamorphic evolution of our country. The goal of this thesis was to constrain the temperature and pressure environment in which the rock type at the island Persholmen, Utö, where formed and also investigate related geology at Ängsholmen constructing maps of both areas. This area is part of the Bergslagen region and belongs to the Svecofennian province. To achieve the required information petrographic analysis and SEM data was used in combination with the computer programs AX and THERMOCALC to gather details regarding chemistry, activity, temperature and pressure of the host rocks.

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1.0 Method:

Fieldwork and Mapping:
The first two weeks of the project was spent in the field on Utö where the bedrock of the area was mapped. This was done foremost in order to become familiar with the area but also because some of the available maps were lacking certain detail. A set of samples (points 1-5 in figure 3.0) was taken all over Persholmen for use in petrographic analysis of later taken thin sections.

Preparing and Analyzing Thin sections:
After visiting St. Persolmen and St. Ängsholmen, samples were chosen from the acquired rocks to try to gather the most representative analysis while still taking into account the different rock types. Rock sections were prepared at Stockholm University and then sent to Vancouver, Canada, to make the thin sections themselves. The samples for this analysis were chosen because they were thought to be representative of the area or seemed to contain clues for the geological history of the rocks (see page 11, Petrographic analysis, for further detail). The thin sections were then used in a petrographic analysis by microscopy to determine the mineralogy and metamorphic processes affecting the rock.

Determination of mineral chemistry by SEM:
Following petrographic analysis the thin sections were analyzed at Gothenburg University (Department of Earth Sciences) where it was placed into a scanning electron microscope to gather data on the mineral chemistry of the host rock. The samples were polished and carbon coated in a vacuum before being placed in the SEM. This coating was made to increase electrical conductivity and prevent the accumulation of electrostatic charge at the surface of the sample.

The SEM operates by sending a beam of electrons onto the sample causing interaction with the sample atoms (by exciting their electrons). By quantifying the electrons released from the sample one can generate a view of different properties such as composition, topography and electric conductivity. The type of SEM used was a Hitachi S-400N scanning electron microscope with simple oxide and metal standards for calibration which was further linked to a cobalt reference standard and checked with Smithsonian Institution mineral standards. The analytical properties at the time of operation were: 20 kV at a working distance of 10 mm with a specimen current of the electron beam of 3.5 nA. The error range of the SEM analysis is found in the Appendix represented by the Weight% sigma: the counting error (standard deviation in absolute %) of the measurement of the element. An error of the element oxide can be calculated as follows: Weight% sigma*(compound%/Weight%). A relative % error can be estimated using: 100*(Weight% sigma/Weight%)

Generating P/T conditions of metamorphim using the computer programs THERMOCALC and AX:
The acquired mineral chemistry data was then transferred to AX to determine activity and composition before being used in THERMOCALC to calculate the pressure and temperature that the rocks of Utö had experienced during metamorphism.

2.0 Introduction

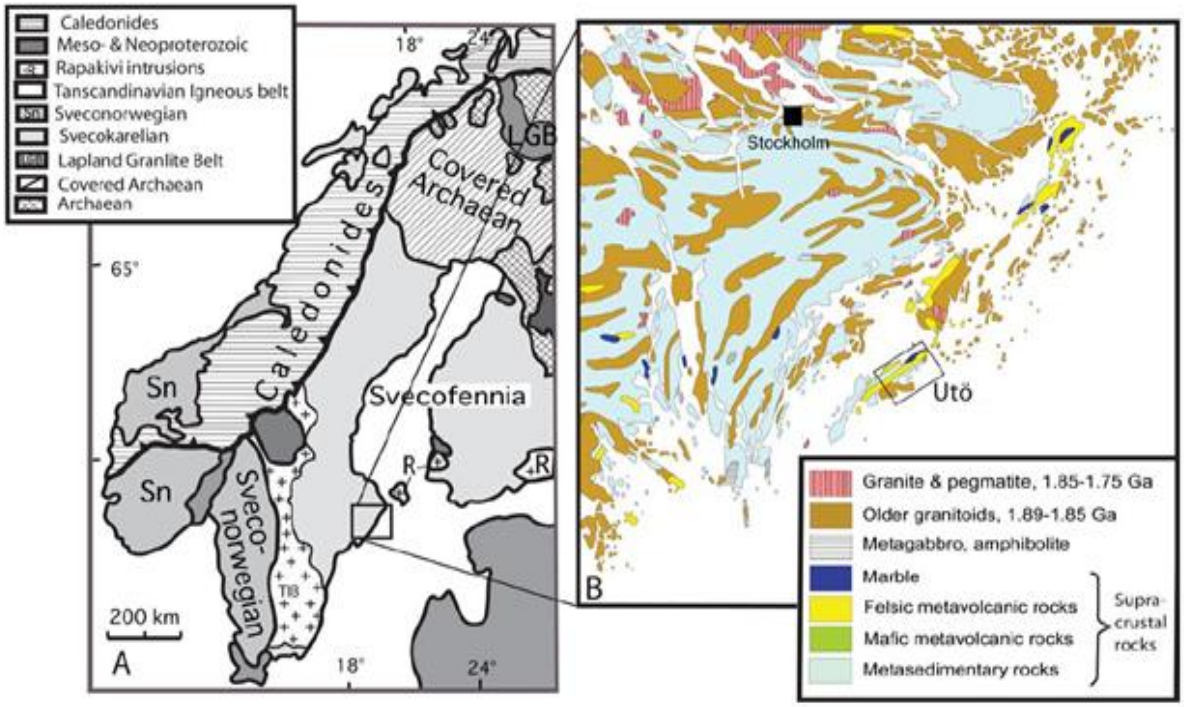

Figure 2.0. **(A)** *Tectonic map of Baltica displaying the location of Utö* ***(B)*** *in relation to surrounding geology (as modified from Talbot 2008).*

Utö, the geological site featured and analyzed in this study, is located in an especially well-preserved area in the Bergslagen region at the east coast of the central parts of Sweden (see figure 2.0). Bergslagen is part of the Baltic shield located within a felsic magmatic region and its rocks exhibits overall medium-high grade of metamorphism (Allen et al. 1996). The area is dominated by rocks with ages around 1.91-1.89 Ga (determined with radiometric dating on zircon with the U-Pb technique, Stephens et al. 2009) formed during the Svecofennian orogen with minor overprint from the Sveconorwegian orogeny in the far west (occurring in between 1.0-0.9 Ga, Stephens et al. 2009). As Bergslagen is intensely mineralized it has been host to major mining activities for around 1000 years (Allen et al. 1996) with scientific exploration at Utö starting 200 years ago (Lundström & Koyi 2003). Historically speaking, Bregslagen has counted for 38% of the world's iron production during the sixteenth century and produced 2/3 of the world's copper during the following century (Allen et al. 1996). The reason for choosing Utö was based on the fact that the Island with surrounding archipelago is very representative of the Bergslagen area providing insight into around 80 million years of the areas geological history (Lundström & Koyi 2003). It is furthermore a unique geological site with a lot of informative rock types spatially close to each other.

2.1 The environment of formation:

Utö features the remains of an old orogen (most often referred to the as the Svecofennian orogen but by some older sources called the Svecokarelian) and has during its formation been exposed to deposition of sediments and explosive volcanism at an active continental margin (Stålhös 1982). Around 2000 million years ago at the initial stage of orogeny, thick stratigraphic layers of sedimentary and volcanic successions were deposited atop an unknown surface predating the orogen (Lundström et al. 1998). During this time Scandinavia was located south of the equator in a different environment from the one we experience today (Lundström & Koyi 2003). The first geological clue to the history of Utö begins with clay-rich turbidites representing deposition in a calm deep ocean environment. With time these turbidites came to display an increase of sand content further up in the stratigraphy indicating a more disturbed sedimentary environment closer to the shore. Possibly this could have occurred as a result of magmatic-related land uplift and thermal doming (Talbot 2008). In this shelf-like environment the turbidites became interlayered with porphyr sheets at 1904±4 Ma (age determined on a metavolcanic rock at Utö (Lundström et al. 1998)) representing volcanism originating from a subduction zone. At the top of these layers carbonate banks settled and it was these accumulations along with associated metavolcanic rocks that later became extremely folded and host to sought-after ore deposits (Allen et al. 1996). Both iron from and sulphide ore has been mined at Utö, the iron hailing from banded iron formations representing calm water deposit.

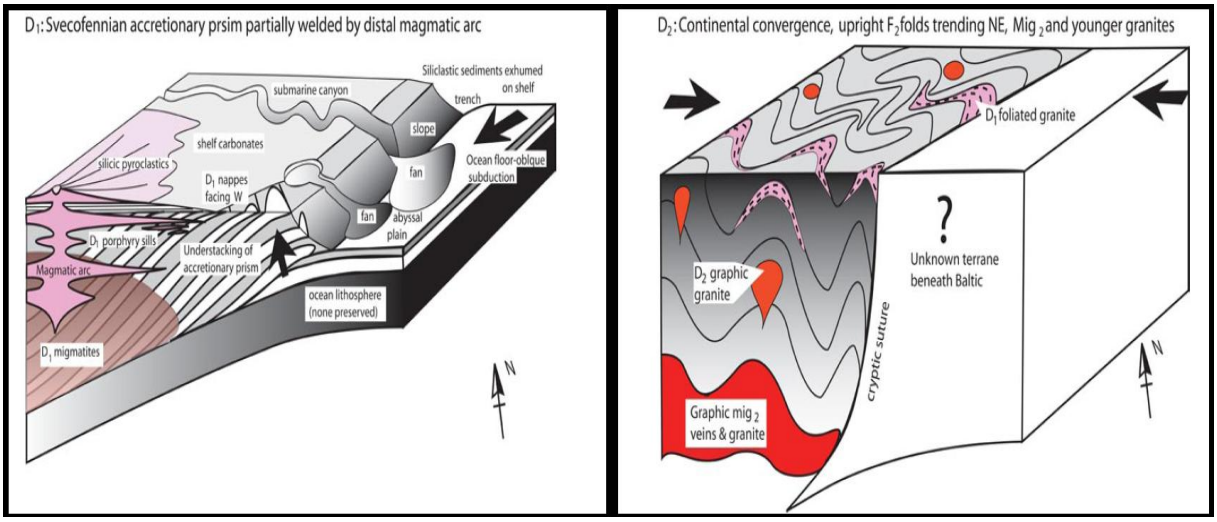

Figure 2.1. *The two main tectonic events of Bergslagen, subduction and orogeny, leaving imprints on the geology of Utö (as modified from Talbot 2008).*

Further indications regarding the environment of formation can be found in the geological structures of the rock types at Utö. Talbot (2008) argues that the low angle thrusts faults found at Utö possibly represents smaller variants of imbricate slices associated with subduction zone accretionary prisms (see figure 2.1). In the turbidite sequence remains of old river channels can be found and two generations of diagenetic concretions represents reworking in the accretionary prism (Talbot 2008). Metavolcanic rocks found elsewhere in the Bergslagen region have an analyzed chemistry which displays characteristics of rocks formed at a volcanic arc above a subduction zone (Lagerblad 1988). In relation to this subduction zone

and volcanic activity a large mountain range was created which became reflected in the east parts of Sweden as the temperature and pressure parameters were shifted to accommodate several kilometers of rock coverage (Stålhös 1982). The Orogeny is then estimated to have continued between 1950-1850 Ma years ago which is marked by several intrusions related to the crustal building (Stephens et al. 2009). What we can see in the outcrop today are the remains from beneath this mountain range that through erosion has been brought to the surface (Lundström & Koyi 2003).

At Utö a pegmatite with a radiometric age dating of 1821 Ma is found which is thought to represent a later stage in the Svecofennian/Svecokarelian orogeny (Lundström & Koyi 2003). Most of the earlier mentioned ore deposits were formed at this stage when volcanic activities started to calm (Stålhös 1982). After the orogeny came brittle deformation and faults during the post-orogenic phase which took place in between 1700-1200 Ma (Stålhös 1982).

3.0 Results and Discussion

This section of the thesis will present and discuss the results of my survey. It is important to note that except for the generated results, such as the map, the SEM results and the various data found in the appendix, everything in this section is of my own interpretation based on observations made in the field, from structural data from microscopy or chemical data.

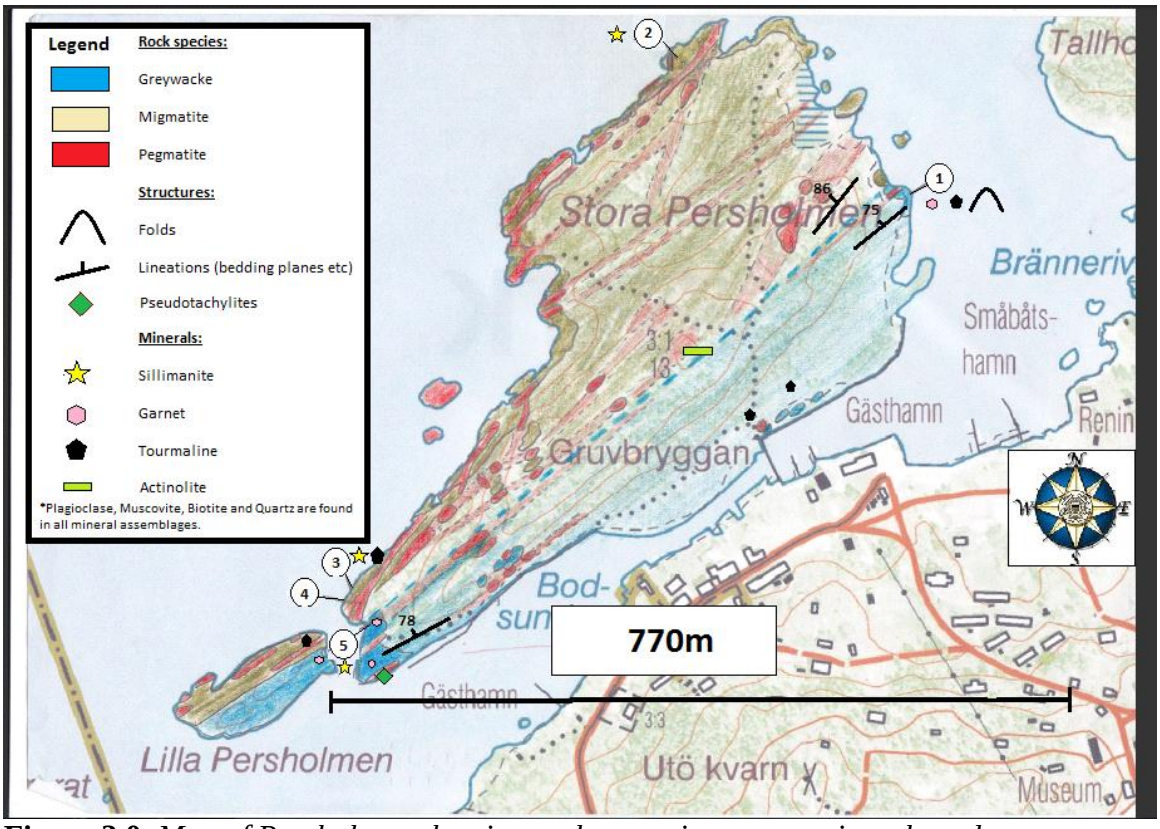

Figure 3.0. *Map of Persholmen showing rock types, important minerals and structures. Numbered in this picture are the sampling sites 1-5.*

The area of focus in this study includes two locations situated at the north part of Utö. Here Persholmen and Ängsholmen (fig 3.0 and 3.1 respectively) represent a part of the earlier described sequence of greywackes with migmatisation occurring down sequence. A lot of deformation has affected the area, making it very complex, and further south strongly folded

carbonates can be found which were once part of carbonate banks capping the greywackes in a shallow ocean. At the south end of the island another sequence of greywackes appear which seems to have many similarities with the one found at Persholmen and might have the same origin. The mineralogy of Persholmen displays fairly similar mineral assemblages with only slight deviation represented by differences in key minerals and mineral ratios (see fig 3.0). Above in figure 3.1 the sample locations of petrographic analysis are listed from 1-5. These samples are representative of the area and cover the three rock types present: greywackes, migmatites and pegmatites.

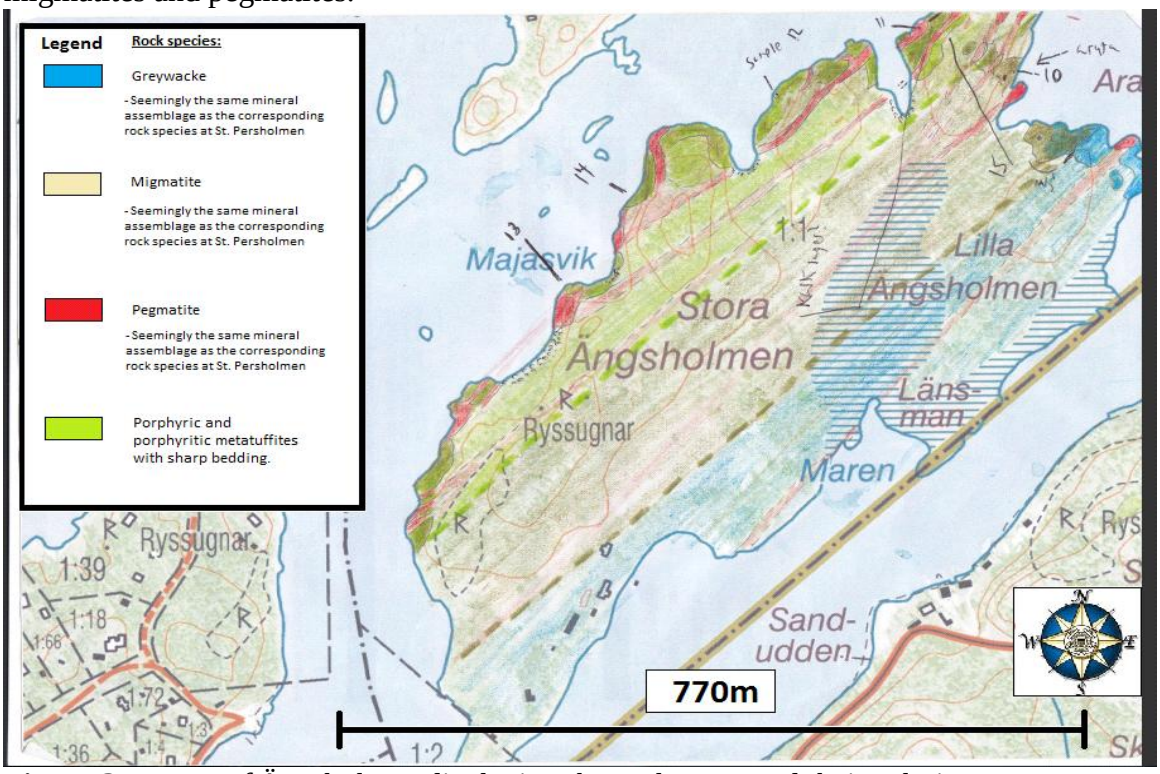

Figure 3.1. *Map of Ängsholmen displaying the rock types and their relations.*

Persholmen and Ängsholmen contain a lot of structural evidence recording their complex history of formation which are made further complicated by a shear zone crossing the north side of the islands. Signs of the Utö shear zone (Talbot 2008) can be found at the southwest coast of Persholmen in the form of psuedotachylites. At the same location, in close vicinity, kinking can be observed through the greywacke layers. Conjugate fractures and folds recording the orogeny of the area are common features on both islands. The pegmatites which are more pronounced in the north are likely to be part of the late orogenic processes and have in many cases been subjected to extensive boudinage. Quartz veins associated with these pegmatites also display pinch and swell structures.

The presence of tourmaline, often in close association with pegmatites and quartz veins, suggest that seawater has played a part as a fluid in the metamorphism of the rocks at Utö. The mineral contains boron which is an indicator of the fluids saline origin (commonly related to a subduction environment). The bedding plane of the rock types at Utö has, since deposition at a surface environment, been rotated 90 degrees to display a fine sequence when walking across the island. Contrasting structural data which in the south indicate younging of the sedimentary layers towards the north and in the north younging towards the south helps to identify that the area is heavily folded. At a locality called Soptippen near the center of the island high rates of deformations and fold interference patterns helps identify this site as a fold hinge explaining the contrasting data on up-direction.

Petrographic Analysis

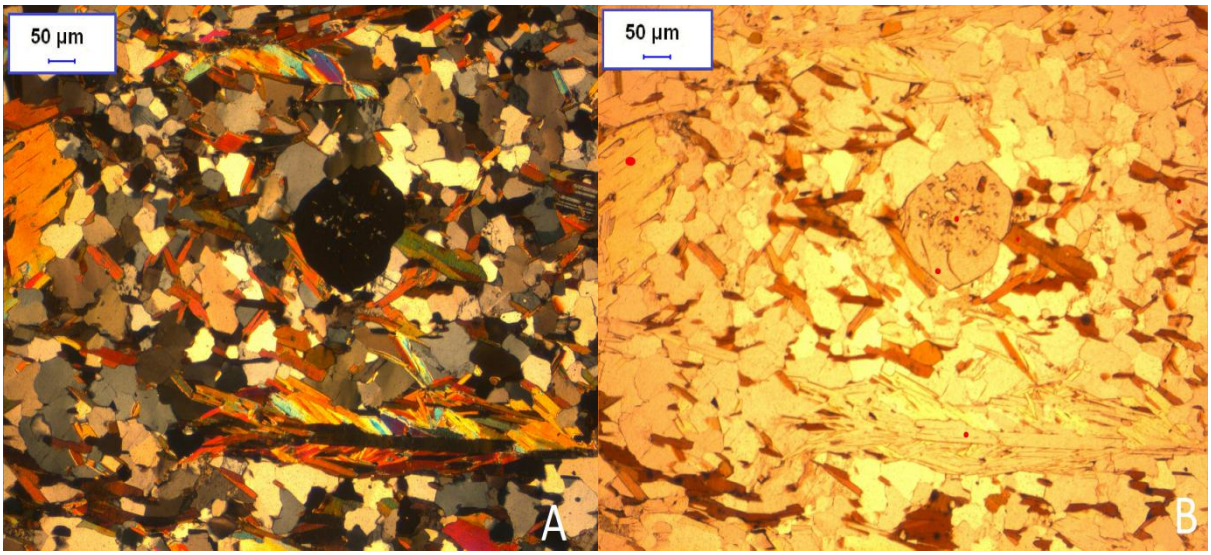

Figure 3.2. *Photomicrograph from thin sections taken from Persholmen, Utö* **A**, *Sample 18 in crosspolarized light* **B**, *Same location in sample 18 showed in polarized light.*

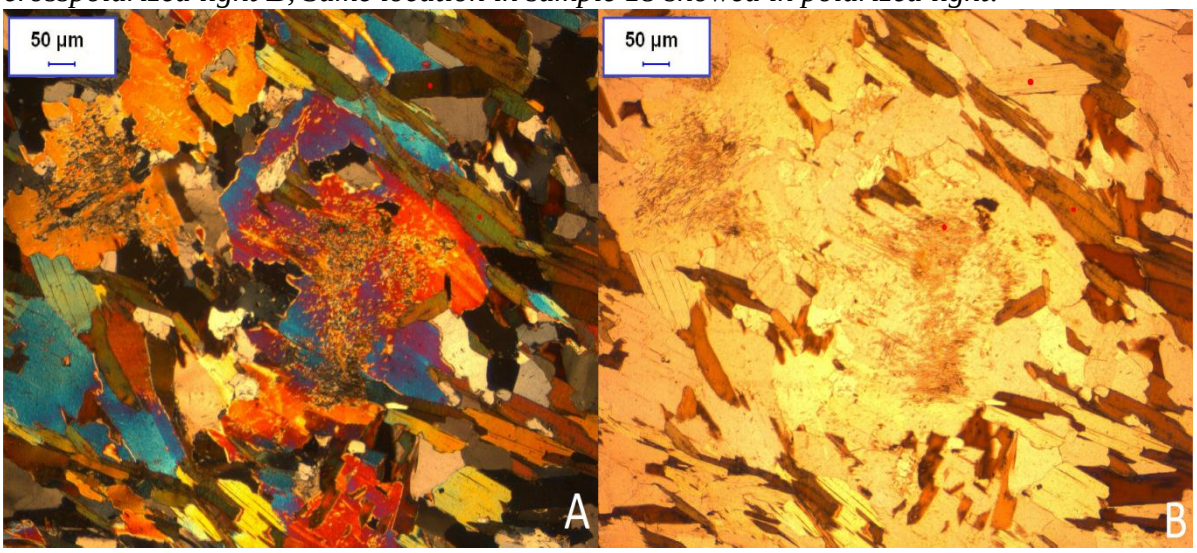

Figure 3.3. *Photomicrograph from thin sections taken from Persholmen, Utö* **A**, *Sample 19 in crosspolarized light* **B**, *Same location in sample 19 showed in polarized light.*

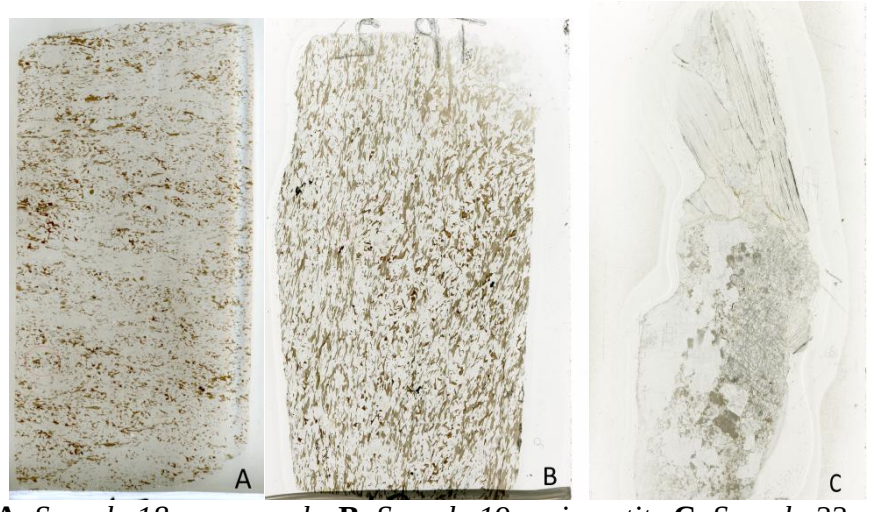

Figure 3.4. **A**, *Sample 18 - greywacke* **B**, *Sample 19 - migmatite* **C**, *Sample 22 - pegmatite*

3.1 Petrographic Analysis

Below are descriptions of points of interest in the individual thin sections. The mineral percentages are approximate estimations and as such do not represent the actual ratios.

Sample 18 – Greywacke

This sample was taken from the east coast of Persholmen (point 1 in figure 3.0). It represents one of the few available outcrops of greywacke type and displays folds. All grains seem to be equigranular and poikiloblastic garnets display inclusions of biotite, quartz and plagioclase. Porphyroblasts of muscovite ("muscovite books") are especially noteworthy (as will be discussed later). Feldspar can also be observed breaking down into a type of mica, probably serecite.

Quartz	Biotite	Muscovite	Feldspar	Garnet	Tourmaline
~40%	~30%	~20%	~10%	~5%	>1%

Sample 19 – Migmatite

This rock was sampled at the north end of Utö (point 2) where the greywackes have reached sufficient depth to melt creating migmatites. Rock types of this kind form when part of the rock is preferentially molten creating a leucosome (new material from the melt) and a mesosome (material that resisted the melting event). The grain size in this sample is larger than sample 18 but maintains an equigranular characteristic. It was chosen for SEM analysis as it was believed to be the greatest contrast to sample 18. Feldspar breakdown is present of the same type as seen in sample 18.

Quartz	Muscovite	Biotite	Feldspar	Sillimanite	Opaque
~15%	~30%	~40%	~10%	~5%	>1%

Sample 20 – Migmatite

At the south eastern coast of Persholmen three samples were chosen with the motive of investigating the reoccurring appearance of muscovite porphyroblasts scattered all across the island. Point 3 in figure 3.0 represent a migmatite displaying muscovite books in its matrix. When viewed with a microscope it becomes apparent that the second generation muscovite is in fact replacing biotite giving us a clue to the chemical processes behind the "Muscovite books". As biotite is replaced iron oxides are released to balance the reaction. Feldspar breakdown is also observed.

Quartz	Muscovite	Biotite	Feldspar	Tourmaline	Opaque
~50%	~25%	~20%	~5%	>1%	>1%

Sample 21 – Borderline of Migmatite and Greywacke.

This sample represents point 5 in figure 3.0 and lies on the border between migmatite and greywacke and was believed to contain no muscovite books. More extensive breakdown of feldspars takes place here.

Quartz	Muscovite	Biotite	Breakdown material (feldspar)	Feldspar	Garnet	Tourmaline
~20%	~35%	~15%	~20%	~10%	~5%	>1%

Sample 22 – Pegmatite with muscovite books

At point 4 in figure 3.0 this sample is found. It is a pegmatite and was taken in order of comparing the muscovite books in it with the other samples.

Quartz	Muscovite	Feldspar
~20%	~30%	~50%

3.2 Analysis with Scanning Electron Microscope (SEM)

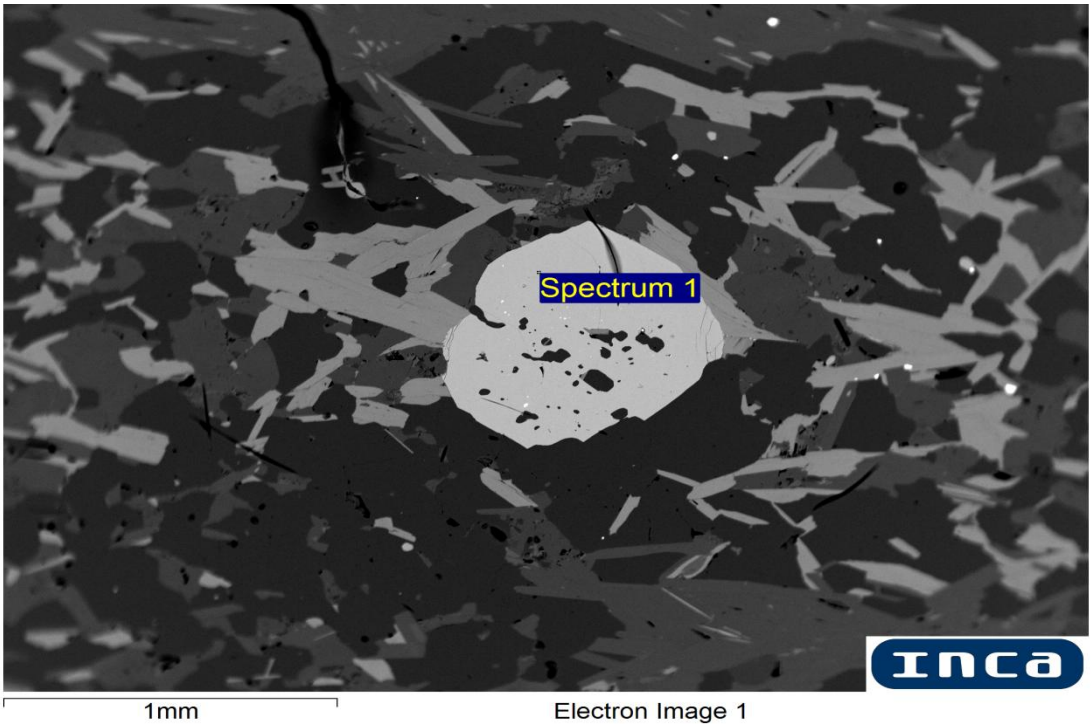

Figure 3.5. *SEM view of sample 18 – Greywacke.*

The determination of chemistry was, as earlier mentioned, performed with the use of a scanning electron microscope. Samples 18 and 19 were determined to represent the two most different environments of formation on Persholmen and as such were chosen for analysis. For a better understanding of the formation parameters and for covering of all rock types, sample 22 was also analyzed. An interesting characteristic that appeared during the study of the petrographic thin section was the aforementioned curious alignment of certain grains of muscovite. Throughout all of the analyzed samples a specific type of muscovite can be distinguished aligned almost 90 degrees to the foliation. It is usually larger than the surrounding muscovite grains and has a slightly blurry outline. All the grains of this type seem to have experienced compression and in places display microscopic versions of kink bands.

Sample 18	Biotite	Garnet	Biotite inclusion in Garnet	First generation Muscovite aligned to foliation	Second generation Muscovite aligned ~90 degrees to foliation	Plagioclase
Element	Compound%					
Na2O	0,26	0,22	0,27	0,58	0,58	6,54
MgO	7,66	1,91	9,19	0,65	0,63	0
Al2O3	18,99	21,03	19,69	35,44	35,67	26,1
SiO2	33,69	35,82	34,63	44,1	44,5	54,47
K2O	9,04	0	9,25	10,41	10,41	0,13
CaO	0,16	1,7	0,24	0,14	0,12	8,68
TiO2	1,8	0	1,48	0,57	0,48	0
MnO	0,41	10,86	0,53	0	0,06	0
FeO	22,27	30,26	19,44	1,06	1,02	0,1

Table 1.0. *Chemistry of sample 18 taking special note of 2 generations of muscovite.*

This would mean that they were formed after the 1st generation muscovite but not before shear activity had finished. Tough chemically much alike (see diagram 1.0) the muscovite in the

matrix and the larger porphyroblasts are likely to be quite different in origin, not only because of its difference in orientation. The muscovite porphyroblasts can in some places, such as in sample 20, be seen replacing biotite confirming the idea based on structural relationships that they are of a second generation. The "muscovite book" crystal habit is most likely caused by the pegmatites affecting the other rock types at Persholmen by adding fluids to the surrounding rocks. The presence of tourmaline in the matrix of some of the rock types not in direct contact with the pegmatites also suggests this relation (although quartz veins also could be responsible for the transport of fluids). The "book" appearance is a common site in pegmatites and is created through nucleation processes where a crystal forms around an initiated nucleation point. As such the pegmatites seem to be exerting more influence on the other rock types than is first observed in the field.

Another common reaction that occurs in almost all samples is the breakdown of feldspar. Though the level of breakdown is different in each sample the process of feldspar breaking down into mica can be readily observed. In places where breakdown is extensive, such as in sample 21, it becomes apparent that the newly formed mica is "radiating". This appearance is most likely due to the mineral having difficulties to nucleate and is a sign of a later stage retrogression process.

Sample 19	First generation Muscovite aligned to foliation	Second generation Muscovite aligned ~90 degrees to foliation	Sillimanite	Feldspar breaking down in high T environment	Mica material created by feldspar breakdown	Biotite
Element	Compound%					
MgO	0,53	0,56	0,12	2,62	4,9	8,16
Al2O3	35,67	35,86	62,03	27,71	27,47	19,16
SiO2	43,9	44,09	34,66	48,11	40,98	33,79
K2O	9,78	9,8	0,02	8,74	9,1	8,9
CaO	0,1	0,06	0	0,37	0,13	N/A
TiO2	0,65	0,59	0	0,13	0,05	2
MnO	0	0	0	0	0,08	0,23
FeO	0,83	0,89	0,14	3,58	8,82	22,37

Table 1.1. *Chemistry of sample 19 taking special note of 2 generations of muscovite.*

3.3 The calculated temperature and pressure:

The temperature and pressure for the samples was calculated using AX on the chemistry data received from the SEM to determine composition and activity. This produced a file which was run in THERMOCALC to create an estimation of the T and P parameters for the different samples. For the greywacke (sample 18) a temperature of 538±36 °C and a pressure of 3.1±1.3 kbars were generated (see figure 3.5). Such environment parameters correspond quite well to the imagined tectonic setting. The sample 19 gave a temperature of 756±133 °C and a pressure of 3.8±3.2 kbars representing the increased temperature due to migmatisation.

Sample 22	Big Muscovite "Book"	Small Muscovite not present as "Books"	Feldspar
Element	Compound%		
Na2O	0,66	0,56	0,47
MgO	0,51	0,67	0,07
Al2O3	35,82	35,4	18,79
SiO2	44,25	44,62	63,93
K2O	10,41	10,43	16,29
CaO	0,14	0,14	0,22
TiO2	0,04	0,13	0,08
MnO	0	0	0
FeO	1,07	1,2	0,04

Table 1.2. *Chemistry of sample 22 which shows the origin of the "muscovite books"*

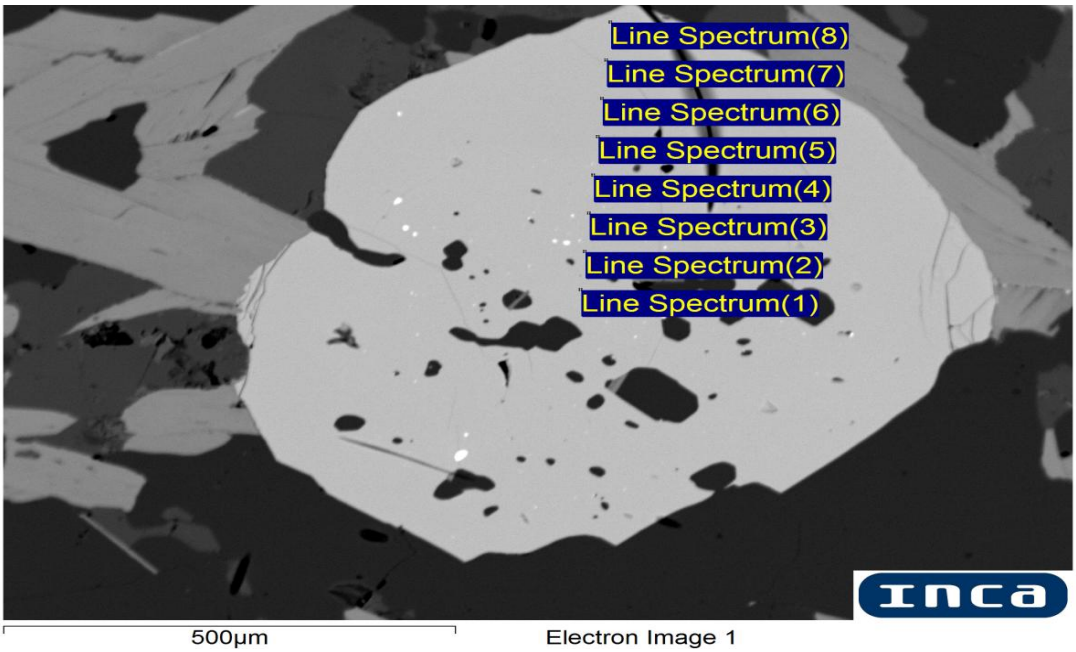

Figure 3.6. *This figure displays the cross section of a garnet in sample 18 with sampling points 1-8 corresponding to table 1.3 displayed below.*

When analyzing the garnets in thin section 18 with SEM further examination of the profile across the mineral reveal the true form of its chemical evolution. Due to its poikiloblastic characteristics garnets are often able to record change in chemistry as they trap so called "armored relics". In addition to this the garnet itself may display zoning which gives clues as to whether different stages of evolution have occurred. In the particular case of this sample the garnet chemistry varies little when travelling from the center of the mineral to its rim (see table 1.3). When comparing the biotite in the matrix and the inclusions (table 1.0) one can see that the two are similar to each other with the exception of iron which is more abundant in the matrix and magnesium which is more abundant in the inclusions.

Spectrum	Na	Mg	Al	Si	K	Ca	Ti	Mn	Fe	Sr	O
	Weight %										
Line Spectrum(1)	0,15	1,12	10,49	15,93	0	1,05	0	8,26	22,46	2,54	37,99
Line Spectrum(2)	0,23	0,94	10,51	16,02	0	1,13	0	8	22,77	2,38	38,03
Line Spectrum(3)	0	0,97	10,43	15,9	0	1,14	0	8,07	23,07	2,51	37,91
Line Spectrum(4)	0	1,04	10,47	15,91	0	1,23	0	7,91	23,13	2,32	37,98
Line Spectrum(5)	0	1,17	10,48	16,15	0	1,21	0	7,7	22,81	2,3	38,18
Line Spectrum(6)	0,25	1,26	10,59	15,73	0	1,12	0	7,76	23,09	2,23	37,98
Line Spectrum(7)	0,39	1,12	10,25	16	0	1,22	0	8,36	22,42	2,26	37,97
Line Spectrum(8)	0,28	0,97	10,63	16,02	0	1,35	0	8,11	22,45	2,04	38,15

Table 1.3. *Displayed in this table is the chemistry of the above garnet in sample 18*

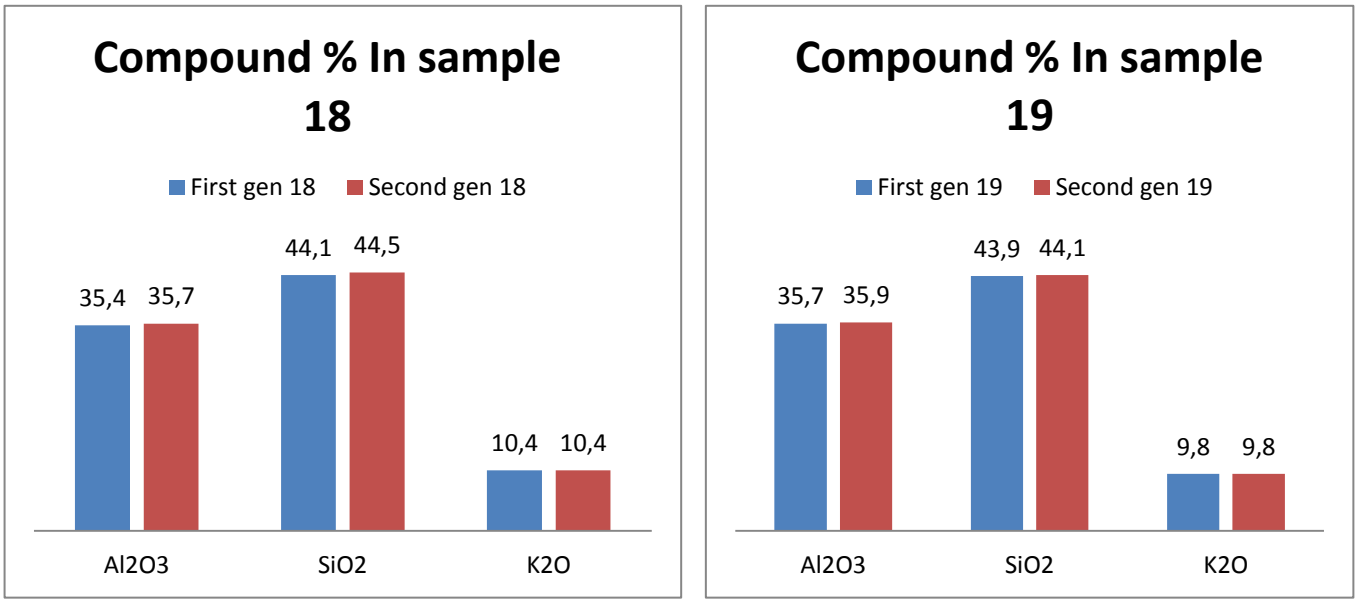

Diagram 1.0 *This diagram displays the chemical composition of the different generations of muscovite in sample 18 and 19 showing the similarity they share.*

3.4 Sources of errors:

When working with data of any kind it is not uncommon to encounter problems and errors in the process. As there is a risk of these errors affecting the interpretation of the observation and magnifying further along the data processing it is important to be aware of them in order to appropriately counter their influence. The first step of possible errors is data collection of this thesis starting in the field when the area was first observed and interpreted and the geological maps where made. As observations and interpretations in the field often vary with the observer the first chance of errors appears. In the case of this thesis the risk of errors was reduced as several peoples were operating in the field and arriving at the same conclusions. To a certain degree the risk of error remained for the mapping of Ängsholmen as it was not possible to transport people to the island within the give time frames. In this project the risk was reduced by focusing on the interpretations and data found at Persholmen. The same problem of observation arrives when analysis of the petrographic thin sections begin. Again the risk was reduced by the aid of several observers.

When the project arrives at the task of generating real measurements and data with THERMOCALC, AX and SEM the risk of technical errors arise. One example of uncertainties that became apparent in this survey was the high standard deviation of sample 19 as seen in box 1.0.

List of temperature and pressure for sample 19 and 18 with standard deviations.

19	T = 756°C, sd = 133, P = 3.8 kbars, sd = 3.2
18	T = 538°C, sd = 36, P = 3.1 kbars, sd = 1.3

Box 1.0 *T and P of samples 19 and 18 with standard deviations.*

In this sample the pressure is estimated to 3.8 kbars but has a high standard deviation of 3.2. This large range of error is caused because of a missing phase that is seemingly containing iron that was not accounted for in the THERMOCALC calculations. Thankfully the estimated temperature has not been disturbed as much and the pressure can be confirmed from sample

18 instead. In the SEM itself measures can go wrong if the working distance and other parameters are not set correctly or accounted for. The stability of the electron current registering the analyzed data along with use of correct standards is also important.

4.0 Conclusions:

The rock types found at Persholmen and Ängsholmen represent a glimpse of the geological history of Bergslagen which Utö itself record. The migmatised and non-migmatised greywackes of Persholmen records different depths of the metasedimentary accumulation on a shelf environment above a subduction zone. The volcanic phase representing later stage orogeny is found in the form of metatuffites at the north coast of Ängsholmen. When studied using petrographic thin sections peak metamorphism at the north end of Persholmen has managed to produce sillimanite indicating a high T medium-low P environment. The retrograde path created by resurfacing of the rock is recorded by the formation of secondary mica from feldspar which in the thin sections shows difficulty of nucleating.

Through SEM analysis the temperature and pressure of the greywackes and their migmatised counterpart at Persholmen can be estimated. Analysis shows that the greywackes of Persholmen have experienced a moderate temperature (538±36°C), moderate pressure (3.1±1.3 kbars) environment in around low-medium amphibolite facies. The migmatites display similar moderate P conditions (3.8±3.2 kbars) with an increase to a high temperature environment (756±133 °C) around granulite or hornfels facies. Overall the temperatures and pressures correspond well to the orogeny stage of formation and the structures and rock types found correspond to the older subduction zone environment.

Although the profile across the garnet in sample 18 shows little change in chemistry a deviation of iron and magnesium content in matrix/inclusion biotite remains as a testimony that the chemistry of the surrounding rock has been slightly altered. This could possibly be because of the addition of fluids recorded by the formation of secondary muscovite which is a manifestation of its counterpart mineral in pegmatites forming a “book-like” appearance. These muscovite books contain signs of shearing and as such must have formed before tectonic processes ended.

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This bachelor thesis is the result of many peoples combined efforts apart from my own. Because of this I would like to thank first and foremost my supervisors Alasdair Skelton and Joakim Mansfeld at Stockholm University for all the time they spent helping me and their unfailing support. Secondly I would like to express my gratitude to Magnus Ripa and The Geological Survey of Sweden (SGU) for presenting me with the opportunity of being part of such an interesting project. Furthermore I would like to thank David Cornell and all the other wonderful people at Göteborg University for helping me with the SEM analysis and patiently answering my questions. Lastly I would like to thank Oskar Bergkvist and Linnéa Lundin for their company to Utö, discussions and comments that helped improve this Thesis.

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6.0 Appendix

6.1. SEM data tables:

Biotite

Element	Line	App. Conc	k ratio	Intensity corrn.	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Na	K_SERIES	0,14	0,00059	0,6975	0,2	0,04	0,21	0,26	Na2O	0,04
Mg	K_SERIES	3,12	0,0207	0,6753	4,62	0,05	4,75	7,66	MgO	0,9
Al	K_SERIES	7,46	0,0536	0,7428	10,05	0,06	9,31	18,99	Al2O3	1,76
Si	K_SERIES	12,34	0,09296	0,7833	15,75	0,06	14,02	33,69	SiO2	2,64
K	K_SERIES	7,87	0,06323	1,0486	7,51	0,04	4,8	9,04	K2O	0,9
Ca	K_SERIES	0,11	0,00098	0,9577	0,11	0,02	0,07	0,16	CaO	0,01
Ti	K_SERIES	0,99	0,00906	0,9168	1,08	0,03	0,56	1,8	TiO2	0,11
Mn	K_SERIES	0,26	0,00262	0,8336	0,31	0,03	0,14	0,41	MnO	0,03
Fe	K_SERIES	14,75	0,14767	0,852	17,31	0,09	7,75	22,27	FeO	1,46
O					37,34	0,11	58,37			11
Totals					94,28					
									Cation sum	7,85

Garnet

Element	Line	App. Conc	k ratio	Intensity corrn.	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Na	K_SERIES	0,1	0,00043	0,6095	0,16	0,04	0,17	0,22	Na2O	0,03
Mg	K_SERIES	0,7	0,00462	0,6036	1,15	0,03	1,15	1,91	MgO	0,23
Al	K_SERIES	8,01	0,05753	0,7196	11,13	0,06	9,98	21,03	Al2O3	2,01
Si	K_SERIES	12,83	0,0967	0,7665	16,74	0,06	14,42	35,82	SiO2	2,9
K	K_SERIES	0	0	1,0606	0	0	0	0	K2O	0
Ca	K_SERIES	1,23	0,01108	1,0124	1,22	0,02	0,73	1,7	CaO	0,15
Ti	K_SERIES	0	0	0,9668	0	0	0	0	TiO2	0
Mn	K_SERIES	7,19	0,07188	0,8549	8,41	0,06	3,7	10,86	MnO	0,74
Fe	K_SERIES	20,51	0,20539	0,872	23,52	0,1	10,19	30,26	FeO	2,05
O					39,47	0,11	59,66			12
Totals					101,81					
									Cation sum	8,11

Biotite inclusion in Garnet

Element	Line	App. Conc	k ratio	Intensity corrn.	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Na	K_SERIES	0,14	0,00062	0,7226	0,2	0,04	0,21	0,27	Na2O	0,04
Mg	K_SERIES	3,85	0,02554	0,6951	5,54	0,05	5,59	9,19	MgO	1,05
Al	K_SERIES	7,8	0,05599	0,7482	10,42	0,06	9,47	19,69	Al2O3	1,78
Si	K_SERIES	12,67	0,0955	0,783	16,19	0,06	14,13	34,63	SiO2	2,66
K	K_SERIES	8,01	0,06436	1,0433	7,68	0,04	4,82	9,25	K2O	0,91
Ca	K_SERIES	0,16	0,00147	0,9519	0,17	0,02	0,11	0,24	CaO	0,02
Ti	K_SERIES	0,81	0,00742	0,9102	0,89	0,03	0,45	1,48	TiO2	0,09
Mn	K_SERIES	0,34	0,00344	0,8302	0,41	0,03	0,18	0,53	MnO	0,03
Fe	K_SERIES	12,82	0,12838	0,8485	15,11	0,08	6,63	19,44	FeO	1,25
O					38,11	0,11	58,4			11
Totals					94,72					
									Cation sum	7,83

First generation Muscovite aligned to foliation

Element	Line	App. Conc	k ratio	Intensity corrn.	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Na	K_SERIES	0,39	0,00168	0,9129	0,43	0,03	0,43	0,58	Na2O	0,08
Mg	K_SERIES	0,33	0,00218	0,8382	0,39	0,03	0,37	0,65	MgO	0,07
Al	K_SERIES	17,47	0,12544	0,9315	18,76	0,06	15,85	35,44	Al2O3	2,86
Si	K_SERIES	16,56	0,12477	0,803	20,61	0,07	16,73	44,1	SiO2	3,01
K	K_SERIES	8,7	0,06991	1,0067	8,64	0,04	5,04	10,41	K2O	0,91
Ca	K_SERIES	0,09	0,0008	0,9122	0,1	0,02	0,06	0,14	CaO	0,01
Ti	K_SERIES	0,29	0,0027	0,8681	0,34	0,02	0,16	0,57	TiO2	0,03
Mn	K_SERIES	0	0	0,808	0	0	0	0	MnO	0
Fe	K_SERIES	0,68	0,00681	0,826	0,82	0,03	0,34	1,06	FeO	0,06
O					42,84	0,1	61,04			11
Totals					92,94					
									Cation sum	7,02

Second generation Muscovite aligned ~90 degrees to foliation

Element	Line	App. Conc	k ratio	Intensity corrn.	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Na	K_SERIES	0,4	0,00169	0,9135	0,43	0,03	0,43	0,58	Na2O	0,08
Mg	K_SERIES	0,32	0,00213	0,8386	0,38	0,03	0,36	0,63	MgO	0,06
Al	K_SERIES	17,59	0,12633	0,9321	18,88	0,06	15,85	35,67	Al2O3	2,86
Si	K_SERIES	16,71	0,12591	0,8031	20,8	0,07	16,78	44,5	SiO2	3,02
K	K_SERIES	8,69	0,06983	1,0063	8,64	0,04	5	10,41	K2O	0,9
Ca	K_SERIES	0,08	0,00069	0,9122	0,08	0,02	0,05	0,12	CaO	0,01
Ti	K_SERIES	0,25	0,00229	0,8681	0,29	0,02	0,14	0,48	TiO2	0,02
Mn	K_SERIES	0,04	0,00035	0,8081	0,04	0,03	0,02	0,06	MnO	0
Fe	K_SERIES	0,66	0,00657	0,826	0,79	0,03	0,32	1,02	FeO	0,06
O					43,12	0,1	61,06			11
Totals					93,46					
									Cation sum	7,01

Plagioclase

Element	Line	App. Conc	k ratio	Intensity corrn.	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Na	K_SERIES	4,52	0,0194	0,9328	4,85	0,05	4,48	6,54	Na2O	0,59
Mg	K_SERIES	0	0	0,7876	0	0	0	0	MgO	0
Al	K_SERIES	12,39	0,08898	0,8967	13,82	0,06	10,87	26,1	Al2O3	1,42
Si	K_SERIES	21,6	0,1628	0,8484	25,46	0,07	19,25	54,47	SiO2	2,52
K	K_SERIES	0,11	0,0009	0,9993	0,11	0,02	0,06	0,13	K2O	0,01
Ca	K_SERIES	5,86	0,05273	0,945	6,21	0,04	3,29	8,68	CaO	0,43
Ti	K_SERIES	0	0	0,8686	0	0	0	0	TiO2	0
Mn	K_SERIES	0	0	0,81	0	0	0	0	MnO	0
Fe	K_SERIES	0,06	0,00063	0,828	0,08	0,03	0,03	0,1	FeO	0
Sr	L_SERIES	2,42	0,02246	0,7287	3,32	0,11	0,8	3,92	SrO	0,11
O					46,11	0,11	61,21			8
Totals					99,95					
									Cation sum	5,07

Setup

Processing option :	Oxygen by stoichiometry	Element	Standard
		Na	jadeite mac 20-Jan-2010 04:04 PM
Sample is polished.		Mg	MgOMAC 20-Jan-2010 04:09 PM
		Al	al2o3 mac 20-Jan-2010 04:14 PM
Sample is coated with Carbon - thickness (nm): 25.0, density (g/cm3): 2.25		Si	Wollastonite 13-Nov-2009 10:15 PM
		K	k-feldspar mac 13-Nov-2009 06:30 PM
Thresholding has been selected : All quantitative results below 1 sigma have been set to zero		Ca	Wollastonite 13-Nov-2009 10:15 PM
		Ti	Rutile2 13-Nov-2009 10:14 PM
Detector efficiency : Calculation		Mn	Mn 13-Nov-2009 06:29 PM
		Fe	Fe met nov09 13-Nov-2009 06:28 PM
Pulse pile up correction performed.		Sr	SrF2 1-Jun-1999 12:00 AM

Table 1.4. *Chemistry data of sample 18 acquired by SEM.*

First generation Muscovite aligned to foliation

Element	Line	App. Conc	k ratio	Intensity corrn	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Mg	K_SERIES	0,27	0,00181	0,8488	0,32	0,02	0,3	0,53	MgO	0,04
Al	K_SERIES	17,78	0,12767	0,9419	18,88	0,06	16,05	35,67	Al2O3	2,09
Si	K_SERIES	16,6	0,12505	0,8084	20,52	0,07	16,76	43,9	SiO2	2,19
K	K_SERIES	8,15	0,06544	1,0032	8,12	0,04	4,76	9,78	K2O	0,62
Ca	K_SERIES	0,07	0,00059	0,9132	0,07	0,02	0,04	0,1	CaO	0,01
Ti	K_SERIES	0,34	0,00312	0,8696	0,39	0,02	0,19	0,65	TiO2	0,02
V	K_SERIES	0	0	0,7961	0	0	0	0	V2O5	0
Mn	K_SERIES	0	0	0,8099	0	0	0	0	MnO	0
Fe	K_SERIES	0,53	0,00534	0,8281	0,64	0,03	0,26	0,83	FeO	0,03
Sr	L_SERIES	0,92	0,00851	0,6971	1,31	0,1	0,34	1,55	SrO	0,04
O					42,76	0,11	61,29			8
Totals					93,02					
									Cation sum	5,05

Second generation Muscovite aligned ~90 degrees to foliation

Element	Line	App. Conc	k ratio	Intensity corrn	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Mg	K_SERIES	0,28	0,00189	0,8482	0,34	0,02	0,32	0,56	MgO	0,04
Al	K_SERIES	17,85	0,12823	0,9411	18,98	0,06	16,06	35,86	Al2O3	2,1
Si	K_SERIES	16,64	0,12541	0,8074	20,61	0,07	16,76	44,09	SiO2	2,19
K	K_SERIES	8,17	0,0656	1,0033	8,14	0,04	4,75	9,8	K2O	0,62
Ca	K_SERIES	0,04	0,00034	0,9132	0,04	0,02	0,02	0,06	CaO	0
Ti	K_SERIES	0,31	0,00284	0,8697	0,36	0,02	0,17	0,59	TiO2	0,02
V	K_SERIES	0,03	0,00032	0,7961	0,04	0,02	0,02	0,07	V2O5	0
Mn	K_SERIES	0	0	0,8098	0	0	0	0	MnO	0
Fe	K_SERIES	0,57	0,00572	0,8279	0,69	0,03	0,28	0,89	FeO	0,04
Sr	L_SERIES	0,82	0,00766	0,6963	1,18	0,1	0,31	1,4	SrO	0,04
O					42,94	0,11	61,31			8
Totals					93,31					
									Cation sum	5,05

Sillimanite

Element	Line	App. Conc	k ratio	Intensity corrn	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Mg	K_SERIES	0,06	0,00042	0,8899	0,07	0,02	0,06	0,12	MgO	0,01
Al	K_SERIES	31,96	0,22955	0,9736	32,83	0,07	25,28	62,03	Al2O3	3,25
Si	K_SERIES	11,38	0,08578	0,7027	16,2	0,07	11,98	34,66	SiO2	1,54
K	K_SERIES	0,02	0,00016	0,9838	0,02	0,02	0,01	0,02	K2O	0
Ca	K_SERIES	0	0	0,9386	0	0	0	0	CaO	0
Ti	K_SERIES	0	0	0,8825	0	0	0	0	TiO2	0
V	K_SERIES	0	0	0,8038	0	0	0	0	V2O5	0
Mn	K_SERIES	0	0	0,8137	0	0	0	0	MnO	0
Fe	K_SERIES	0,09	0,00088	0,8298	0,11	0,03	0,04	0,14	FeO	0,01
Sr	L_SERIES	0,83	0,00771	0,612	1,36	0,1	0,32	1,6	SrO	0,04
O					47,99	0,11	62,31			8
Totals					98,57					

Feldspar breaking down in high T environment

Element	Line	App. Conc	k ratio	Intensity corrn	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Mg	K_SERIES	1,3	0,00862	0,8224	1,58	0,03	1,51	2,62	MgO	0,27
Al	K_SERIES	13,21	0,09491	0,901	14,67	0,06	12,59	27,71	Al2O3	2,26
Si	K_SERIES	18,7	0,14095	0,8318	22,49	0,07	18,54	48,11	SiO2	3,32
K	K_SERIES	7,28	0,05847	1,0038	7,25	0,04	4,29	8,74	K2O	0,77
Ca	K_SERIES	0,25	0,00221	0,9182	0,27	0,02	0,15	0,37	CaO	0,03
Ti	K_SERIES	0,07	0,0006	0,8742	0,08	0,02	0,04	0,13	TiO2	0,01
V	K_SERIES	0	0	0,8012	0	0	0	0	V2O5	0
Mn	K_SERIES	0	0	0,8124	0	0	0	0	MnO	0
Fe	K_SERIES	2,31	0,02316	0,8303	2,79	0,05	1,16	3,58	FeO	0,21
Sr	L_SERIES	0,99	0,00916	0,7158	1,38	0,11	0,36	1,63	SrO	0,07
O					42,39	0,12	61,36			11
Totals					92,88					
									Cation sum	6,93

Mica material created by feldspar breakdown

Element	Line	App. Conc	k ratio	Intensity corrn	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Mg	K_SERIES	2,31	0,0153	0,7807	2,96	0,04	2,89	4,9	MgO	0,38
Al	K_SERIES	12,31	0,08841	0,8469	14,54	0,06	12,8	27,47	Al2O3	1,7
Si	K_SERIES	15,38	0,11587	0,8026	19,16	0,06	16,21	40,98	SiO2	2,16
K	K_SERIES	7,67	0,06163	1,016	7,55	0,04	4,59	9,1	K2O	0,61
Ca	K_SERIES	0,09	0,00078	0,928	0,09	0,02	0,06	0,13	CaO	0,01
Ti	K_SERIES	0,03	0,00025	0,8862	0,03	0,02	0,02	0,05	TiO2	0
V	K_SERIES	0	0	0,8142	0	0	0	0	V2O5	0
Mn	K_SERIES	0,05	0,0005	0,8193	0,06	0,03	0,03	0,08	MnO	0
Fe	K_SERIES	5,74	0,05749	0,8374	6,86	0,06	2,92	8,82	FeO	0,39
Sr	L_SERIES	0,85	0,00788	0,693	1,22	0,1	0,33	1,45	SrO	0,04
O					40,51	0,11	60,17			8
Totals					92,97					
									Cation sum	5,3

Biotite

Element	Line	App. Conc	k ratio	Intensity corrn	Weight%	Weight% sigma	Atomic%	Compound%	Formula	Number of ions
Mg	K_SERIES	3,35	0,02221	0,6803	4,92	0,05	5,04	8,16	MgO	1,98
Al	K_SERIES	7,54	0,05412	0,7431	10,14	0,06	9,35	19,16	Al2O3	3,68
Si	K_SERIES	12,36	0,09313	0,7826	15,79	0,06	13,99	33,79	SiO2	5,5
K	K_SERIES	7,74	0,0622	1,0479	7,39	0,04	4,7	8,9	K2O	1,85
Ti	K_SERIES	1,1	0,01008	0,9171	1,2	0,03	0,62	2	TiO2	0,24
Mn	K_SERIES	0,15	0,00147	0,8335	0,18	0,03	0,08	0,23	MnO	0,03
Fe	K_SERIES	14,82	0,14834	0,8519	17,39	0,09	7,75	22,37	FeO	3,05
O					37,6	0,11	58,47			23
Totals					94,61					
									Cation sum	16,34

Setup

Processing option :	Oxygen by stoichiometry	Element	Standard
		Na	jadeite mac 20-Jan-2010 04:04 PM
Sample is polished.		Mg	MgOMAC 20-Jan-2010 04:09 PM
		Al	al2o3 mac 20-Jan-2010 04:14 PM
Sample is coated with Carbon - thickness (nm): 25.0, density (g/cm3): 2.25		Si	Wollastonite 13-Nov-2009 10:15 PM
		K	k-feldspar mac 13-Nov-2009 06:30 PM
Thresholding has been selected : All quantitative results below 1 sigma have been set to zer		Ca	Wollastonite 13-Nov-2009 10:15 PM
		Ti	Rutile2 13-Nov-2009 10:14 PM
Detector efficiency : Calculation		Mn	Mn 13-Nov-2009 06:29 PM
		Fe	Fe met nov09 13-Nov-2009 06:28 PM
Pulse pile up correction performed.		Sr	SrF2 1-Jun-1999 12:00 AM

Table 1.5. *Chemistry data of sample 19 acquired by SEM.*

Big Muscovite "Book"										
Element	**Line**	**App. Conc**	**k ratio**	**Intensity corrn.**	**Weight%**	**Weight% sigma**	**Atomic%**	**Compound%**	**Formula**	**Number of ions**
Na	K_SERIES	0,45	0,00193	0,9159	0,49	0,03	0,49	0,66	Na2O	0,05
Mg	K_SERIES	0,26	0,0017	0,8394	0,31	0,03	0,29	0,51	MgO	0,03
Al	K_SERIES	17,7	0,12712	0,9338	18,96	0,06	16	35,82	Al2O3	1,57
Si	K_SERIES	16,59	0,12502	0,8019	20,68	0,07	16,77	44,25	SiO2	1,65
K	K_SERIES	8,69	0,06983	1,0055	8,64	0,04	5,04	10,41	K2O	0,5
Ca	K_SERIES	0,09	0,00082	0,9111	0,1	0,02	0,06	0,14	CaO	0,01
Ti	K_SERIES	0,02	0,00017	0,8675	0,02	0,02	0,01	0,04	TiO2	0
Mn	K_SERIES	0	0	0,8081	0	0	0	0	MnO	0
Fe	K_SERIES	0,69	0,00688	0,826	0,83	0,03	0,34	1,07	FeO	0,03
O					42,86	0,1	61,01			6
Totals					92,9					
									Cation sum	3,83
Small Muscovite not present as "Books"										
Element	**Line**	**App. Conc**	**k ratio**	**Intensity corrn.**	**Weight%**	**Weight% sigma**	**Atomic%**	**Compound%**	**Formula**	**Number of ions**
Na	K_SERIES	0,38	0,00164	0,9133	0,42	0,03	0,41	0,56	Na2O	0,04
Mg	K_SERIES	0,34	0,00223	0,8387	0,4	0,03	0,38	0,67	MgO	0,04
Al	K_SERIES	17,45	0,12536	0,9318	18,74	0,06	15,78	35,4	Al2O3	1,55
Si	K_SERIES	16,77	0,12637	0,8037	20,86	0,07	16,88	44,62	SiO2	1,66
K	K_SERIES	8,71	0,06998	1,0058	8,66	0,04	5,03	10,43	K2O	0,49
Ca	K_SERIES	0,09	0,00083	0,9114	0,1	0,02	0,06	0,14	CaO	0,01
Ti	K_SERIES	0,07	0,00061	0,8678	0,08	0,02	0,04	0,13	TiO2	0
Mn	K_SERIES	0	0	0,8082	0	0	0	0	MnO	0
Fe	K_SERIES	0,77	0,00769	0,8261	0,93	0,03	0,38	1,2	FeO	0,04
O					42,97	0,1	61,04			6
Totals					93,16					
									Cation sum	3,83
Feldspar										
Element	**Line**	**App. Conc**	**k ratio**	**Intensity corrn.**	**Weight%**	**Weight% sigma**	**Atomic%**	**Compound%**	**Formula**	**Number of ions**
Na	K_SERIES	0,31	0,00135	0,8988	0,35	0,03	0,33	0,47	Na2O	0,03
Mg	K_SERIES	0,03	0,00023	0,83	0,04	0,02	0,04	0,07	MgO	0
Al	K_SERIES	9,3	0,06682	0,9353	9,95	0,05	7,89	18,79	Al2O3	0,77
Si	K_SERIES	27,42	0,2066	0,9174	29,88	0,07	22,78	63,93	SiO2	2,22
K	K_SERIES	13,63	0,10952	1,0081	13,52	0,05	7,41	16,29	K2O	0,72
Ca	K_SERIES	0,14	0,00124	0,8936	0,15	0,02	0,08	0,22	CaO	0,01
Ti	K_SERIES	0,04	0,00036	0,8561	0,05	0,02	0,02	0,08	TiO2	0
Mn	K_SERIES	0	0	0,803	0	0	0	0	MnO	0
Fe	K_SERIES	0,02	0,00024	0,8218	0,03	0,03	0,01	0,04	FeO	0
O					45,91	0,1	61,44			6
Totals					99,89					
									Cation sum	3,77

Setup			
Processing option :	Oxygen by stoichiometry	**Element**	**Standard**
		Na	jadeite mac 20-Jan-2010 04:04 PM
Sample is polished.		Mg	MgOMAC 20-Jan-2010 04:09 PM
		Al	al2o3 mac 20-Jan-2010 04:14 PM
Sample is coated with Carbon - thickness (nm): 25.0, density (g/cm3): 2.25		Si	Wollastonite 13-Nov-2009 10:15 PM
		K	k-feldspar mac 13-Nov-2009 06:30 PM
Thresholding has been selected : All quantitative results below 1 sigma have been set to zero		Ca	Wollastonite 13-Nov-2009 10:15 PM
		Ti	Rutile2 13-Nov-2009 10:14 PM
Detector efficiency : Calculation		Mn	Mn 13-Nov-2009 06:29 PM
		Fe	Fe met nov09 13-Nov-2009 06:28 PM
Pulse pile up correction performed.		Sr	SrF2 1-Jun-1999 12:00 AM

Table 1.6. *Chemistry data of sample 22 acquired by SEM.*

6.2 THERMOCALC output files:

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THERMOCALC 3.21 running at
15.09 on Thu 9 Jun,2011 with thermodynamic dataset
produced at

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	mu
a	0.000920	0.000130	0.180	0.0257	0.0870	0.0300	0.780
sd(a)/a	0.73345	0.81113	0.17060	0.44719	0.29825	0.42759	0.10000

	pa	cel	an	ab	q	H2O
a	0.596	0.0150	0.670	0.590	1.00	1.00
sd(a)/a	0.10000	0.66667	0.10000	0.05043	0	

Independent set of reactions
1) gr + 2pa + 3q = 3an + 2ab + 2H2O
2) 3east + 6q = py + phl + 2mu
3) phl + east + 6q = py + 2cel
4) ann + 3an = gr + alm + mu
5) phl + 3an = py + gr + mu

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	1.8	0.75	143.75	0.71	-0.26153	7.718	7.726	0.893
2	6.7	4.16	45.52	10.06	-0.02421	-3.411	-0.630	1.557
3	9.1	2.86	65.33	3.70	0.02960	-3.907	-8.223	1.643
4	1.8	0.84	-47.78	1.21	0.13837	-7.317	-7.268	0.936
5	3.2	1.12	6.22	0.74	0.11456	-7.034	-11.325	1.223

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.38, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	3.1	1.3	538	36	0.786	1.30

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	2.70	1.22	523	36	0.813	1.17	0.92	0.23
gr	4.11	1.66	549	34	0.780	1.16	-0.69	0.71
alm	3.21	1.28	544	37	0.800	1.26	-0.36	0.08
phl	2.92	1.24	531	35	0.793	1.24	-0.56	0.07
ann	3.40	1.28	553	39	0.816	1.20	0.63	0.24
east	2.96	1.26	536	35	0.788	1.26	-0.46	0.02
mu	3.13	1.30	541	38	0.795	1.29	-0.20	0.05
pa	3.10	1.27	544	41	0.729	1.28	0.22	0.24
cel	2.76	1.06	534	29	0.786	1.05	1.45	0.07
an	3.24	1.37	540	36	0.778	1.28	0.25	0.10
ab	3.07	1.28	539	37	0.767	1.30	-0.11	0.06
q	3.06	1.28	538	36	0.786	1.30	0	0
H2O	3.06	1.28	538	36	0.786	1.30	0	0

T = 538°C, sd = 36,

P = 3.1 kbars, sd = 1.3, cor = 0.786, sigfit = 1.30

****

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THERMOCALC 3.21 running at
14.35 on Mon 20 Jun,2011 with thermodynamic dataset
produced at

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	east	mu	cel	sill	q	mic
a	0.0292	0.0320	0.770	0.00590	1.00	1.00	1.00
sd(a)/a	0.41246	0.41925	0.10000	0.51137	0	0	0

	H2O
a	1.00
sd(a)/a	

Independent set of reactions
1) 3east + 5q = 2phl + mu + 2sill
2) 2east + 5q = phl + cel + 2sill
3) 2cel + sill = east + 4q + mic + H2O

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.8	8.01	9.97	10.05	-0.02020	-1.744	2.998	1.507
2	6.8	4.81	19.88	6.74	0.00675	-1.998	-1.782	1.065
3	1.7	2.14	21.67	3.66	-0.09162	3.740	6.824	1.105

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.38, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.96
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	3.8	3.2	756	133	0.993	0.58

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	3.90	3.23	758	133	0.993	0.45	0.28	0.00
east	3.34	3.44	735	142	0.994	0.41	-0.34	0.10
mu	3.87	3.25	759	139	0.975	0.58	0.05	0.94
cel	5.11	5.35	807	218	0.997	0.50	-0.20	0.80
sill	3.84	3.22	756	133	0.993	0.58	0	0
q	3.84	3.22	756	133	0.993	0.58	0	0
mic	3.84	3.22	756	133	0.993	0.58	0	0

H2O	3.84	3.22	756	133	0.993	0.58	0	0

T = 756°C, sd = 133,
P = 3.8 kbars, sd = 3.2, cor = 0.993, sigfit = 0.58
==========