Stockholm University

Bachelor Thesis

Degree Project in
Geology 15 hp

Pressure-Temperature-time path model of Fårskär-Rävstavik greywacke formation, NE Utö, with EPMA generated data

Oskar Bergkvist

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Department of Geological Sciences
Stockholm University
SE-106 91 Stockholm

Abstract

This thesis attempts to determine the formation conditions of the greywackes at Fårskär , Utö. A Pressure-temperature-time path model is made to describe the pressure and temperature evolution of formation. The rocks at Fårskär represent the oldest parts of the 80 million year rock suite exposed at Utö, in bergslagen. Bergslagen is mainly situated in the SW part of the Svecokarelian (Svecofennian) orogen in the Fennoscandian shield (Baltic shield) (Stephens, M. et al. 2009), the middle part of the Svecofennian province in Finland and Sweden (Gavelin, S. 1976). Rocks dominating this area were typically formed during Palaeoproterosoic ages, between 1.9 and 1.8 Ga. In this time period during Svecokarelian orogenic activity these rocks were variably influenced by deformation and metamorphism (Stephens, M. et al. 2009).

Greywackes at Fårskär and NE of Fårskär towards Stora sillsvik at Utö, are likely formed in the transition between greenshist and amphibolite facies conditions. The greywacke NE of Fårskärsudd towards Stora sillsvik likely recorded part of a retrograde path.

Aim

In May 2011 the Swedish Geological survey financed project *"Metamorphic map of Sweden"* was started. Its goal of which is to compile a pressure-temperature-fluid compression data from metamorphic rocks in Sweden. This thesis is part of this project.

This thesis aim is to find out the pressure and temperature at which the metapelite schist (greywacke) at Rävstavik/Fårskärsudd Utö formed by thermodynamic modelling using the computer programs AX_2 and Thermocalc 3.23 with data extracted from thin sections using an electron microprobe (EPMA) and to model a PTt path. Prior to this a map was made in order to find suitable sampling sites and to attain adequate local geological knowledge.

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1.0 Introduction

Utö is an island in Bergslagen located in the southern part of Stockholm archipelago, about 40 km SSE of Stockholm.

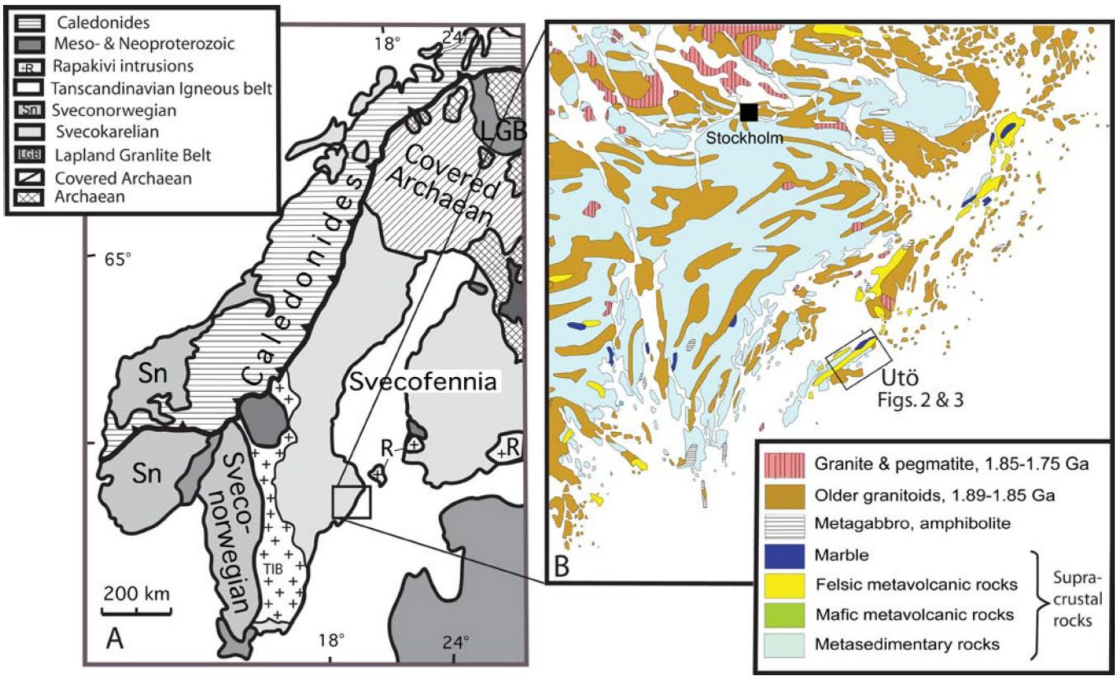

Figure 1. *Map of Utö in relation to regional geology (Talbot 2008).*

1.1 Regional geology

The rock suite found on Utö is representative for typical supra crustal rocks in central Sweden (Gavelin, S. 1976). Bergslagen is mainly situated in the SW part of the Svecokarelian (Svecofennian) orogen in the Fennoscandian shield (Baltic shield) (Stephens, M. et al. 2009), the middle part of the Svecofennian province in Finland and Sweden (Gavelin, S. 1976). Rocks dominating this area were typically formed during Palaeoproterosoic ages, between 1.9 and 1.8 Ga. In this time period during

Svecokarelian orogenic activity these rocks were variably influenced by deformation and metamorphism, the western parts were also to some extent affected and tectonically overprinted by Sveconorwegian orogeny at 1.0-0.9 Ga (Stephens, M. et al. 2009).

Outcrops on Utö are well exposed and preserve a unique archive over geological events that have affected Bergslagen and the eastern parts of middle Sweden during these almost hundred million years (Talbot, C. et.al. 2008). The archive consists of mineralogical, structural and tectonic information that is very representative for Bergslagen. The well exposed mineralogy, structures and the fact that the bedrock on Utö is tilted to a somewhat upright position makes it easy to put in a time perspective. Outcrops expose 80 million years of time, easily accessed and studied (Lundström. 2003).

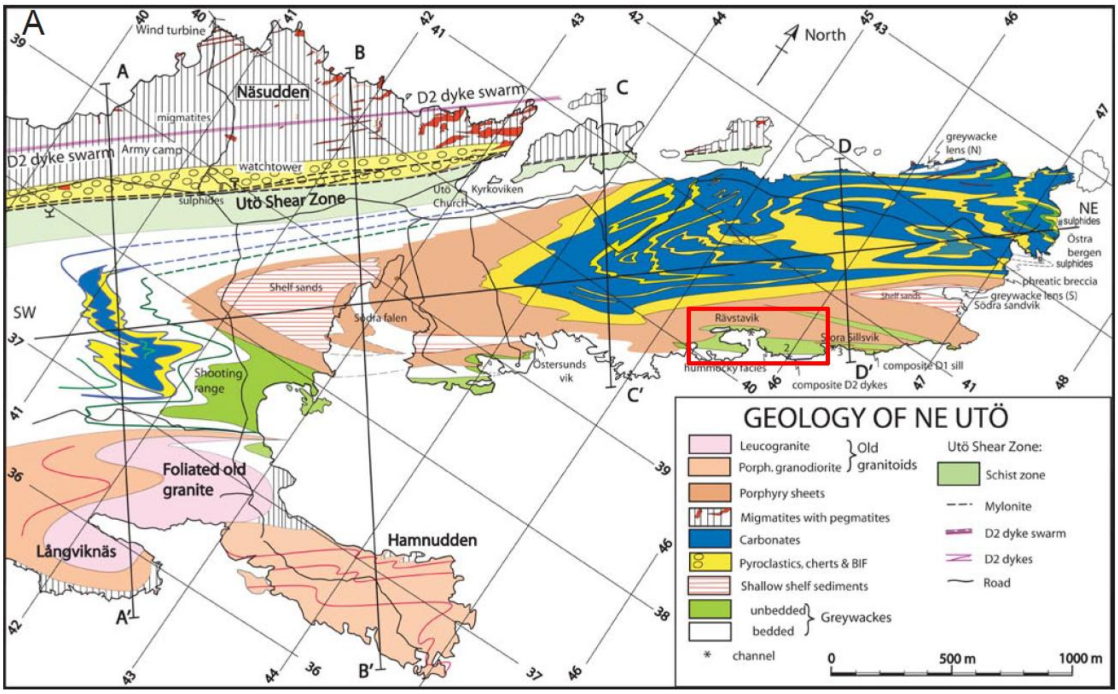

Figure 2. *Study area in red box, Rävstavik and Fårskär. Modified from Talbot 2008.*

1.2 The stratigraphy

Utö has a complicated stratigraphy due to deformation and metamorphism but many parts correlates well with rest of Bergslagen. In the northern parts of Utö the layers highest up in the stratigraphy is visible, the youngest layers. The top layer mainly consist of leptites (Felsic metavolcanoclastics) interlayered by crystalline limestone (skarn) and iron ore. Next in the column to the south east is a quartzite formation and dacitic and rhyolitic volcanites (also called ignimbrites, medium-K composition) Further south east argillite's and greywackes (greywacke meaning metagreywacke). represent the oldest and lowest part of the stratigraphy (Lindquist, J. 2011) (Stephens, M. et al. 2009). (Greywacke meaning metagreywacke).

1.3 Formation conditions

1.3.1 Tectonic setting

Utö exposes the remnants of an old orogen, the Svekofennian orogen. The orogenic belts formed at an active continental margin, a subduction zone where an open ocean floor to the east is obliquely subducted, building an accretionary prism. The shelf like prism was built up by siliclastic sediments and was recycled by mass flows, carbonate banks which were later flattened by falls of silicic pyroclastic rocks, and then as the follow up magmatic arc began to form a mix of andesitic to rhyolitic melts intruded the prism. Magmatic arc began to crystallize the accretionary prism to crystalline Svekofennia at about 1904 Ma. The Greywackes making the accretionary prism were tectonized in two major faces of orogeny, first during open ocean crustal building and then when the ocean closed continental convergence continued to tectonize and thicken the Greywackes, making two metamorphic($M_1$and M_2) and structural (D_1 and D_2) generations (Talbot, C. et.al. 2008).

Evidence for combined tectonic and sedimentary reworking in an accretionary prism is found in two generations of concretions. $M_1$and M_2 most likely accompanied and outlived the two clearly distinguishable deformational phases at Utö (D_1 and D_2), probably also contemporaneous with the two phases of regional metamorphism in Bergslagen dated to 1.87 and 1.76 Ga. The two metamorphic phases are visible in the field, in the mudstones of the greywacke as macroscopic zoning of the porphyroblasts of andalusite, cordierite and garnet. (Talbot, C. et.al. 2008).

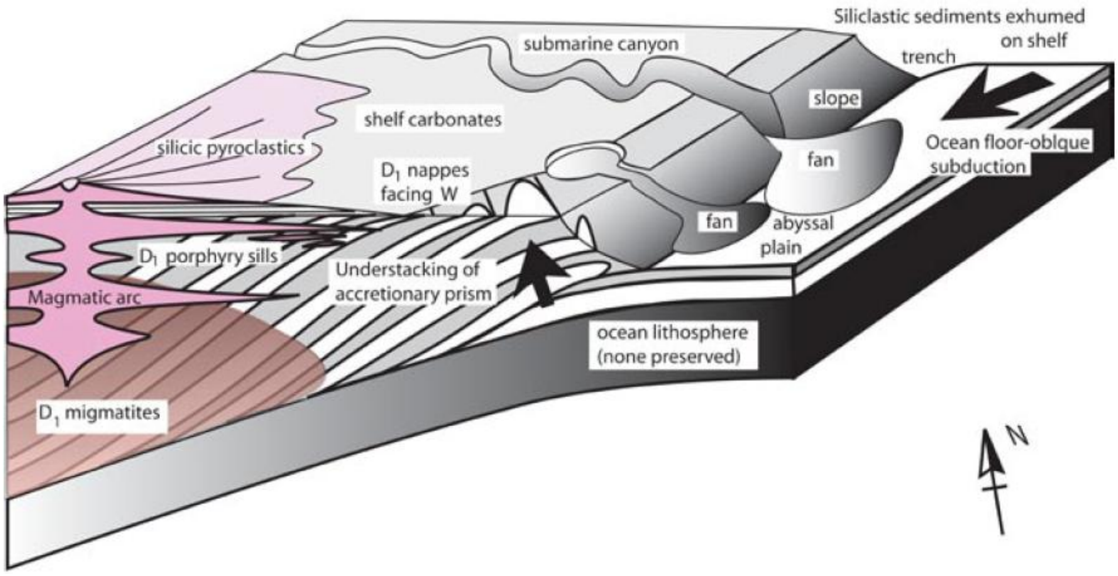

Figure 3. *Svecofennian accretionary prism partially welded by distal magmatic arc (Talbot 2008)*.

Metavolcanic rocks like those seen on Utö are found in other localities in Bergslagen and show a very typical chemical signature, the chemical signature of a subduction zone (Lagerblad, B., 1988) at the time of formation Scandinavia was situated south of the equator, experiencing environment conditions very different from present conditions. What we see today is the rock that was ones metamorphosed by the pressure and heat of the orogen, the orogen itself is since long weathered and eroded away (Lundström & Koyi 2003).

The sediments making up the stratigraphy can be related to different sedimentation environments, four different sedimentation phases can be identified (Lundström, et al 1998. p 2.). (1) A pre volcanic phase, sedimentation prior to arc magmatism. (2) An intense volcanic phase started around 1.9 Ga (Stephens, M. et al. 2009), volcanic related sedimentation. (3) A late volcanic phase, waning volcanic phase (Lundström, et.al 1998. p 2.) sedimentation related to distal arc volcanism (Lundström & Koyi 2003). (4) An overlying sediment succession phase, deposited in context of hemipelagic suspension and dilute turbidity currents (Lundström, et.al 1998), on top of an accreting prism. The first three phases are the most relevant, especially the very first, in the context of this thesis aim.

1.3.2 Pre volcanic phase

The oldest parts of the rock suite are the greywackes on Fårskärsudd, younging to the NW, towards Rävstavik which is the next part of the rock suite. Continuous younging towards NW (Talbot, C. et.al. 2008). The fine grained Greywackes at Fårskärsudd clearly indicates a calm deep sea depositional environment, typical for the pre volcanic phase (Lundström & Koyi 2003). The greywacke is built up in layers ranging from centimetre to meter in thickness and mostly consisting of sand and clay rich sediments (Talbot, C. et.al. 2008), on Fårskärsudd typically around 10 cm in thickness and deposited on the shelf (Lundström & Koyi 2003). Graded beds are common within these layers, deposited by turbidity currents. In dark clay rich layers the metamorphic minerals andalusite, cordierite and garnet are typical. Graded beds indicates way up, in this case NW (Lundström & Koyi 2003).

In Rävstavik just north of Fårskärsudd, a sign of a future volcanic phase is evident. Calm deep water sedimentation conditions were interrupted 1.9 Ga by the onset of the volcanic phase (Stephens, M. et al. 2009). In Rävstavik sediments are coarsening to sand and gravel size, lenses of conglomerate are exposed, layers are more variable in thickness and cross bedding is common. These features clearly indicates a higher energy environment, likely signs of a shallower deposition environment, closer to land, beach like conditions(Lundström & Koyi 2003). The shallower conditions are argued to be the consequence of uplift by thermal doming, caused by a rising magma body in the crust (Stephens, M. et al. 2009) (Lundström & Koyi 2003).

1.3.3 Intense volcanic phase

The rocks at Nasknäsudd are the oldest examples from the volcanic phase, pyroclastic mass flows deposited in a shallow sea or on land, around 1904 Ma (Lundström & Koyi 2003). Deposition of mostly juvenile volcanoclastics, emplacement of cryptodomes and subvolcanic intrusions are typical markers for the intense volcanic phase. The kind of pyroclastic flow deposits found at Nasknäsudd make up the majority of the rocks from this phase and marks deposition ages with precision (Lundström, et.al 1998).

1.3.4 Late volcanic phase, overlying sediment succession phase

The waning volcanism mainly produced planar bedded volcanic silt- and sandstones, according to (Lindquist, J. 2011) quartzite and rhyolitic to dacitic volcanites or ignimbrites. Sediments were deposited below wave base by suspension and dilute turbidity currents (Lundström, et.al 1998). This calmer phase made ore formation possible, the ores on Utö are found in the carbonate rich layers stretching from Krokarna down over the mining area (Lundström & Koyi 2003). During The "overlying sediment succession phase" the deposition environment is roughly the same as earlier with respect to a hemi pelagic component. Argillitic rocks, clay slates and shists are typical for this phase (Lundström, et.al 1998).

2.0 Methods

2.1 Methods overview

- Mapping metamorphic terrain of 1,5x0.5 km, collecting rock samples from geothermobarometrically adequate localities at Utö.
- Preparing rock samples for making thin sections. Sending cut rock samples to Vancouver Petrographic Ltd.
- Petrographic analysis. Preparation for SEM and EPMA analysis.
- EPMA analysis on thin sections at Uppsala University.
- Geothermobarometry, AX_2 and Thermocalc modelling on EPMA data.
- Literature studies.
- Compilation of collected data.

2.2 Mapping

In order to understand the geology and to find adequate sampling sites the project started out in the field making a geological rock map over the hole 1.5x0.5 km area on a roughly 1-10 meter scale, scale depending on importance of feature. The main objective was to find sampling sites were the rock contained minerals suitable for geothermobarometric analysis and to be able to fit data from the samples into a wider geological context. Mapping also included measurement of strike/dip direction, angle on features like sedimentary/metamorphic layering and brief descriptions of ductile and brittle structures. Structural data is useful for correlation and comparison with older published maps and data. Ductile and brittle structures also give a rough estimate of past metamorphic conditions, temperature pressure and deformation.

2.3 Thin section preparation

Before rock samples were sent to Canada for thin section making they were prepared with a rock cutting tool to obtain the right size and shape. In the cutting process the samples were made to represent the bigger initial samples with respect to composition and grain size.

After preparation samples were sent to; Vancouver Petrographic Ltd.

2.4 Petrographic analysis

Thin section samples were analysed to determine mineral composition and rock type, samples were also photographed partly as an important preparation for SEM and EPMA analysis but also for presentational purposes. Identifying suitable mineral grain couples and their position on the thin section sample is vital for effective SEM and EPMA analysis. For microscopy analysis a Nikon OPTIPHOT2-POT mounted with a Leica EC3 camera and a Leica DMPL mounted with DFC320 camera was used.

2.5 EPMA analysis

Geothermobarometric modelling requires bulk composition data from suitable neighbouring mineral grains, in this case a biotite /garnet/plagioclase trio and a Amphibole/garnet/plagioclase trio. Data from other neighbouring mineral grains is also useful. The EPMA instrument *Field Emission Electron Probe Microanalyzer Jeol JXA8530F Hyperprobe* measures bulk composition with very high accuracy. The Jeol JXA8530F Hyperprobe produced all data processed in Ax_2 and thermocalc 3.23.

A SEM analysis instrument, the Hitachi S-400N was first used but the data extracted was not used or presented. Data did not meet requirements for AX_2 and Thermocalc 3.21 modelling in terms of quality and a suitable mineral composition.

2.5.1 Preparation

Before analysis the samples were prepared with a carbon coating to prevent surface charging problems which would lower the resolution and the general quality of the analysis (Reed. S.J.B. 1993).

2.5.2 EPMA Theory

An EPMA instrument produces electrons by heating a tungsten filament to high temperatures. Those electrons are accelerated away from the filament and towards the sample. The electrons are directed and focused by electrostatic lenses, creating a beam. When the beam hits the sample surface it produces backscattered electrons, secondary electrons, cathodoluminescence, auger electrons and most importantly X-rays that can be analysed by spectrometers to determine the samples composition. The emitted X-rays have a characteristic wavelength and energy proportional to the atom from which they are produced. High energy backscattered and low energy secondary electrons are used by the instrument to make an image of the sample (Reed. S.J.B. 1997).

The instrument parameters set during analysis; acc. volt. 15kV, beam current 10nA, beam diameter - focused beam (less than 1 um) and
K alpha lines were measured.(Jarek maika)

2.6 Geothermobarometry

The main goal is to make a well supported estimation of the temperature and pressure of formation, at which the greywacke formed. The method is executed in two parts, geothermometry and geobarometry. Geothermometry is the evaluation of the temperature and geobarometry is the evaluation of the pressure of rock formation. Both methods rely on experimental data extracted from laboratory experiments with a relatively narrow range of common compositions and conditions combined with experimental data from natural systems and thermodynamics. To make applications beyond the experimental base, possible thermodynamic data is extracted. Combined with adequately fitted activity-composition (a-X) models to the mineral solutions it's possible to extract reliable P and T data. Since the method relies on extrapolation it's important to realise that the data becomes less reliable the more extrapolation is performed (winter).

The computer software used is AX_2 (Holland 2008) and Thermocalc. 3.21 (Powell and Holland, 1998). Thermocalc uses the experimental database and extrapolates when necessary to model phase diagrams and calculate P and T.

2.6.1 AX_2 and Thermocalc modelling

The EPMA data expressed in mineral oxide weight percent is first inserted in activity-composition AX_2 software for mineral end member activity calculations. AX_2 first recalculates the mineral oxides to mineral formulas and then determines the activities of mineral endmembers.

Each mineral in a solid solution chemical system has an activity composition (a-x) model that describes the distribution of elements on sites and interaction energies. A-x models used are macroscopic and describe the interaction between endmembers rather than sites. Different minerals have different complexity and characteristics with respect to distribution of elements on different sites and the ideal/non-ideal type of mixing between endmembers. Combinations of a number of A-x models are designed to compensate for these characteristics in order to make the most accurate activity composition model. Individual Mineral characteristics also change with Temperature and pressure, A-x_2 software were set to **P: 5.0 kbar** and **T: 550 °C**, considered normal metamorphic conditions which makes for accurate AX_2 models. (Holland, TJB, & Powell, R, 2003) In simple words an activity composition model describes the availability of a component to react, activities of mineral endmembers is described and not the modal proportion.

The created AX_2 output file was manually modified according to chemical equilibrium assumptions made from the petrographic analysis. Mineral grains showing clear signs of a non equilibrium state, like evident reaction textures, were not sampled. Andalusite and muscovite were set as stable phases. Muscovite is also added since its present in the rock, but it has not been analyzed with EPMA. The modified output file is then run in Thermocalc 3.21 for P and T modelling.

Geothermobarometry modelling would traditionally be manually calculated "by hand" using only a few phases and simple activity composition models.

The geothermometry part in both thin sections would then most likely be calculated as a Fe-Mg exchange reaction. The geobarometry part would be executed with a GASP continuous net transfer reaction. GASP stands for; G-garnet, A-aluminosilicate, S-silicate and P-plagioclase. The GASP reaction is commonly applied to high-grade pelitic schists such as the Greywackes at Rävstavik and Fårskärsudd containing garnet, plagioclase, aluminosilicate (Andalusite) and Quartz. The reaction can be simplified to;

Grossular (G) + 2 kyanite (A) + Qtz (S)= 3 Anorthite (P)

Thin sections analysed does not contain Kyanite but Andalusite, which would therefore be set as a stable phase and used instead.

Thermocalc 3.21 however, can model more accurately using more phases, sometimes all phases present in a sample. Simplified Thermocalc 3.21 calculations for current samples presented below.

Independent set of reactions sample OUF2.

1) gr + 2and + q = 3an
2) 5py + 3east + 4mu = 7phl + 12and
3) py + phl + 2mu = 3east + 6q
4) alm + mu = ann + 2and + q

Independent set of reactions sample OUF4.

1) gr + 2and + q = 3an
2) 10gr + 3cumm + 27and = 7py + 30an + 3H2O
3) 10gr + 3grun + 27and = 7alm + 30an + 3H2O

Gr-grossular, and-andalusite, q-quartz, an- anorthite, cumm-cummingtonite, py-pyrope, alm-almandine, grun-grunerite, mu-muscovite, phl-phlogopite, ann-annite and east-eastonite. From Thermocalc output file. Appendix ?

2.7 Literature studies

Earlier published literature on the subject is always important to study, to get an overview of previous research and knowledge gaps that needs to be filled in. Studied literature is listed under references.

3.0 Results

All results presented are my interpretations of collected data using previous stated methods.

3.1 Map

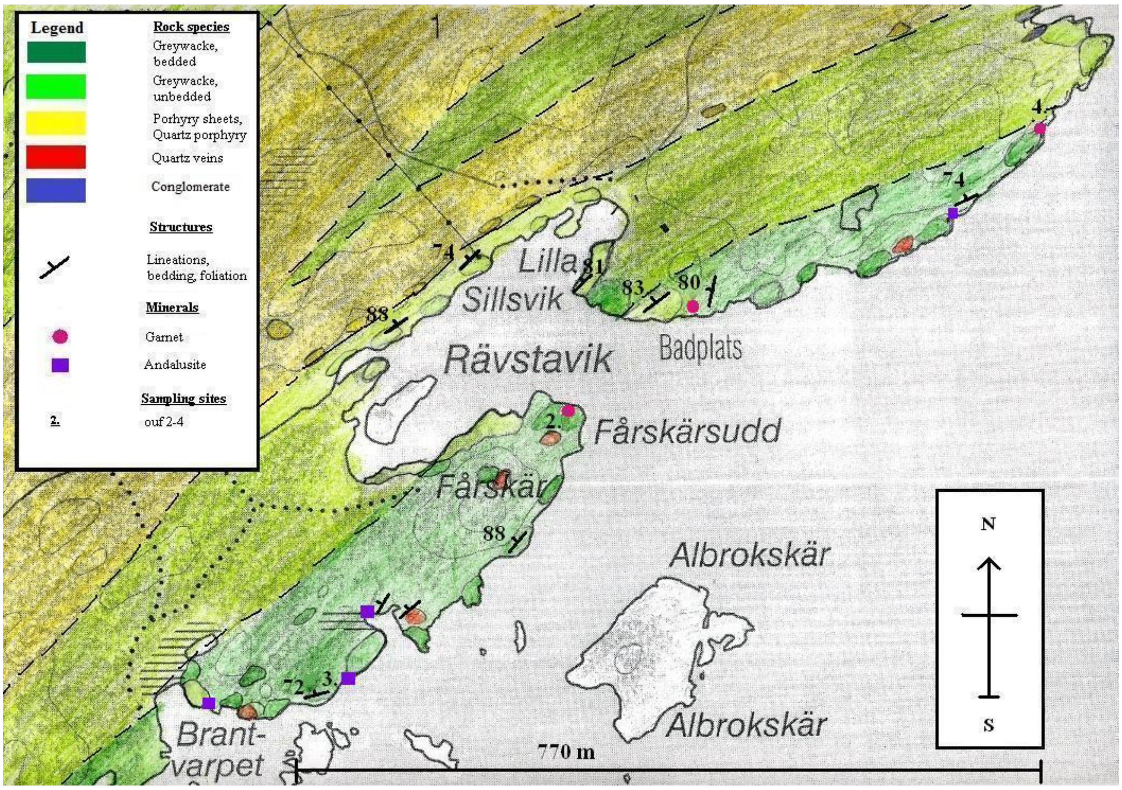

Figure 4. *Map over the area in focus, Fårskärsudd and Rävstavik. Map displaying rock types, sampling sites, important minerals and structural features.*

3.2 Field observations, along the coast from south to north

3.2.1 Bedded greywacke section, general description

In the southern parts of Fårskärsudd near Brantvarpet a greywacke is dominating, as described in earlier literature. It is Foliated and built up in layers by a more pelitic and a more psamitic component. The grain size varies from clay to gravel. Essentially sand and gravel sized grains in a clay matrix. Naturally the more psamitic layers contain less clay and vice versa. Psamitic layers contain Biotite and plagioclase besides Quartz. Pelitic layers contain Biotite, Quartz, Muscovite and Andalusite visible to the naked eye, besides clay matrix. Moving to the shoreline, furthest south east the oldest parts of the rock is visible, a more fine grained, more schist like, darker and more clay rich rock. Typically the oldest rock contains more mica. The more clay rich, finer grained rock corresponds well with the idea of a deep sea sedimentation environment. The oldest parts of the rock is visible from Brantvarpet in south to Stora sillsvik in the north, sometimes not visible on the shore but most likely just below the waterline. Sample 3 is a typical example from the older parts of the bedded greywacke section and sample 2 is typical for the younger parts of the bedded greywacke section. Along the coast from Lilla sillsvik to Stora sillsvik the greywacke is essentially of the younger bedded sort, in some places close to the water the older part can be seen. The Garnets however change their appearance compared to the ones across the bay at Fårskär, at a first glance they just look paler but at a closer look they seem broken up somehow. A petrographic analysis of the thin section clearly indicates that they are broken up, broken up into smaller garnet shaped grains but within the bigger Garnet. Sample 4 is also taken in the bedded greywacke section but near the boundary to the unbedded section. This sample clearly shows the broken up garnets.

3.2.2 Structures

The most eye catching structure is the foliation, about 227/80-90. Relict beds and relict graded beds (10-20 cm thick) are clearly visible, showing way up. Typical ductile features like tension gauges(20-60 cm, strike ca. 230-250. Facing E), tooth paste structures, folds, parasitic folds, delta clasts and boudines are side by side with more brittle structures like conjugate fractures (202/80 and 262/80. Facing N).

3.3 Unbedded greywacke section

Rävstavik clearly shows the next part of the geological history. Like some areas near Brantviken metapsamite and metapelite makes a cyclic composition banding, just by the shore line. Cross bedding and graded bedding is evident in both compositions. Compared to the greywacke on Fårskärsudd and Brantviken the greywacke in Rävstavik is coarser grained, even conglomerate are present. It's is easy to see that the sedimentation environment is changing, to a shallower higher energy environment, a shallow ocean. The conglomerate clasts have different compositions, mainly limestone, clay stone and quartz rich rocks.

3.3.1 Structures

The most typical structures in Rävstavik are the c-s/c-s structures, c-240/80 and s-214/74, s-212/80 and c-240/78. Structural features like foliation, folds, toothpaste structures, tension gauges and kink bands are also visible. A Conjugate fracture measuring 240/84, 276/88 (facing N). These structures have recorded the rocks ductile and brittle deformation history, past temperature, pressure, strain and shear domains. Ductile features imply sufficient heat for quartz plasticity but not sufficient to induce melt, an interval between 250 and 600 degree Celsius. Measurements of structures correspond with measurements of structures described by Talbot.

3.4 Quartz porphyry section

Just 50-100 meters up from the shoreline in Rävstavik the next section starts, the contact is fairly abrupt. A quartz- and feldspar porphyry rock deposited by pyroclastic mass flows, typically 0.5-5 mm grains of quartz and feldspar, rose quartz spotted in various locations near the contact.

3.5 Petrographic analysis

Thin sections were analysed in a petrographic microscope to find relevant spots for SEM an EPMA analysis and to determine the mineralogy and microstructure of the rock at hand. Below follows descriptions and pictures of representative and interesting spots on each thin section from the three sampling sites. The mineral percentages stated are approximate estimations and does not represent the true ratios. Estimations were based on microscopic observation of thin sections.

3.5.1 Photos of thin sections

OUF2

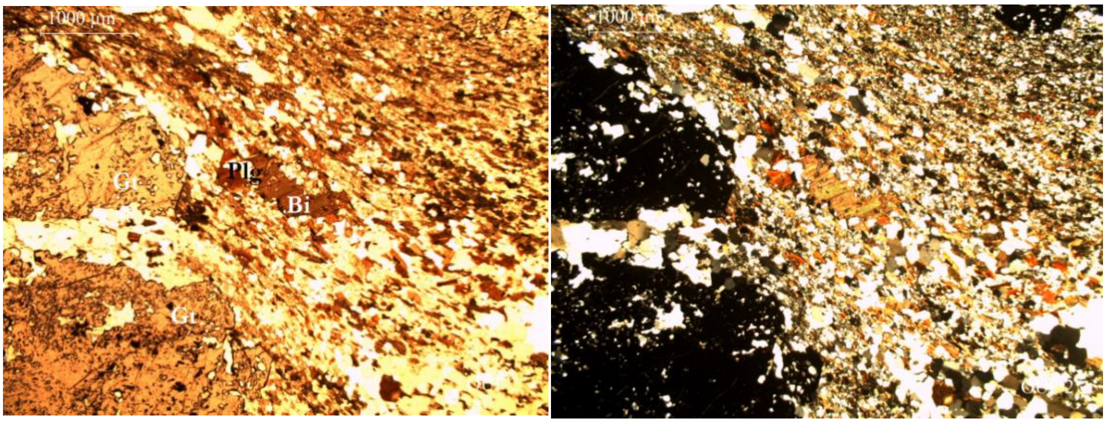

Figure 5. OUF2

Photomicrographs of thin section from sample 2 taken from Fårskärsudd. Left picture in polarized light. Right picture in cross polarized light.

OUF3

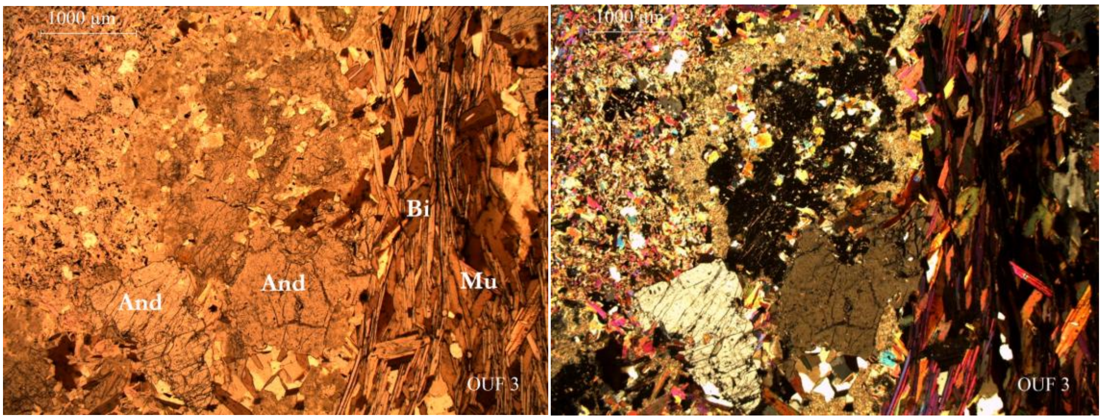

Figure 6. OUF3

Photomicrographs of thin section from sample 3 taken from Fårskär. Left picture in polarized light. Right picture in cross polarized light.

OUF4

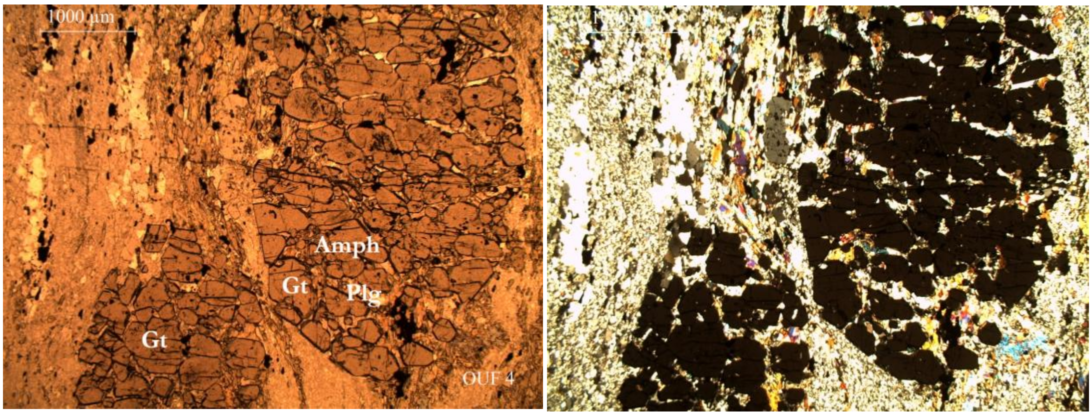

Figure 7. OUF4

Photomicrographs of thin section from sample 4 taken close to Sillsvik. Left picture in polarized light. Right picture in cross polarized light.

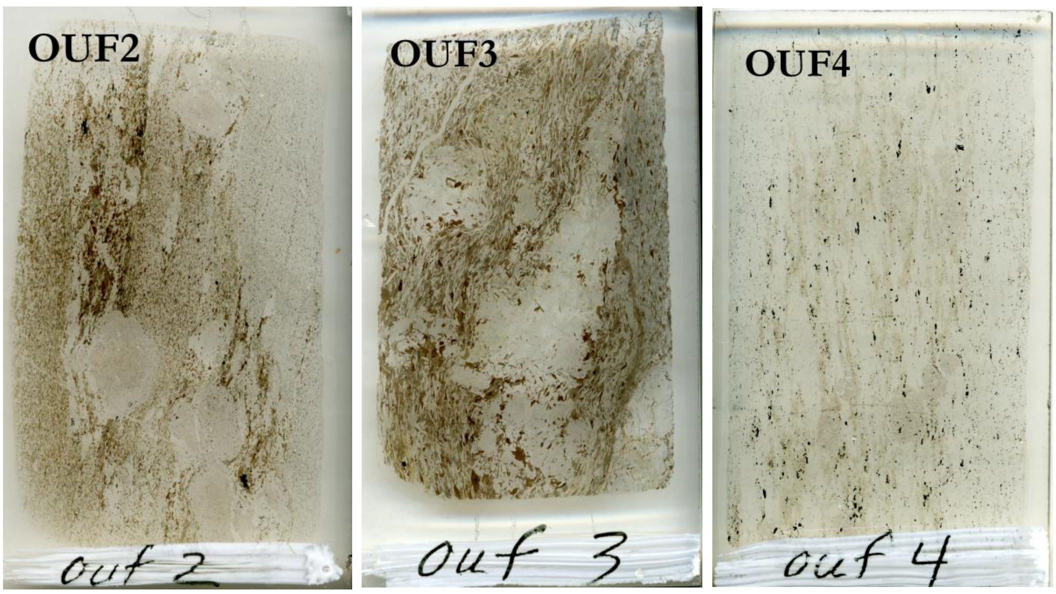

Figure 8. *Scanned thin sections*.

3.6 Macro- and microscopic petrographic analysis

3.6.1 Ouf 2, Fårskärsudd – Greywacke

The sample was taken near the shore line on the eastern cape of Fårskärsudd, point 2 on the map. A fine grained greywacke with garnets visible in hand specimen. Alignment of biotite and quartz show an evident foliation texture. Most grains are equigranular and poikiloblastic, especially porphyroblasts of garnet present a poikiloblastic texture. Garnets have inclusions of quartz, biotite and also but more rarely plagioclase. The garnets are broken up and show signs of disequilibrium, being replaced by biotite and quartz. Biotite and quartz grains generally appear greater in size close to the garnets. Plagioclase grains are hard to find and identify since twinnings in cross polarized light are very rare. The porphyroblasts of garnet show macroscopic zoning that might be a result of two metamorphic growth phases, M_1 and $M_{2,}$ visible in figure 8.

Quartz	Biotite	Muscovite	Garnet	Plagioclase	Chlorite
~50%	~20%	~10%	~10%	~9%	~1%

3.6.2 Ouf 3, Fårskärsudd – Greywacke

The sample was taken from the south western part of Fårskärsudd not far from Brant varpet, point 3 on the map. Andalusite crystals are visible in hand specimen and the sample rock easily falls apart along the foliation plane. Two foliations in almost the same direction are visible in thin section, both stated by biotite and quartz alignment, biotite show difference in grain size between the two foliations. Poikiloblastic porphyroblasts of Andalusite and also more rarely Cordierite is present and show inclusions of biotite, muscovite, quartz and plagioclase. Some sort of brake down or reaction rim is present around the probable cordierites, grain size is too small for identification in microscope.

Quartz	Biotite	Muscovite	Andalusite	Cordierite
~ 50%	~ 20%	~20%	~8%	~2%

3.6.3 Ouf 4, Stora Sillsvik – Greywacke

The sample was taken south east of Stora Sillsvik. Garnet crystals can be noted in hand specimen. A foliation texture is evident by alignment of muscovite and quartz. Grains are Subhedral in shape and show an equigranular texture. Poikiloblastic porphyroblasts of garnet are broken down to smaller subhedral grains, in between garnet grains muscovite, quartz and plagioclase are found.

Quartz	Muscovite	Garnet	Plagioclase	Amphibole
~ 50%	**~ 15%**	**~15%**	**~10%**	**~10%**

3.7 EPMA analysis, Ax_2 and Thermocalc 3.21 modelling

EPMA analyses were performed on all three thin sections but only OUF2 and OUF4 showed a suitable composition for geothermobarometry. Neighbouring grains of garnet, biotite and plagioclase or garnet, amphibole and plagioclase makes a suitable composition. Analyses of OUF3 bulk composition supported assumptions made during petrographic analyses performed in microscope.

3.7.1 OUF 2 – Fårskärsudd

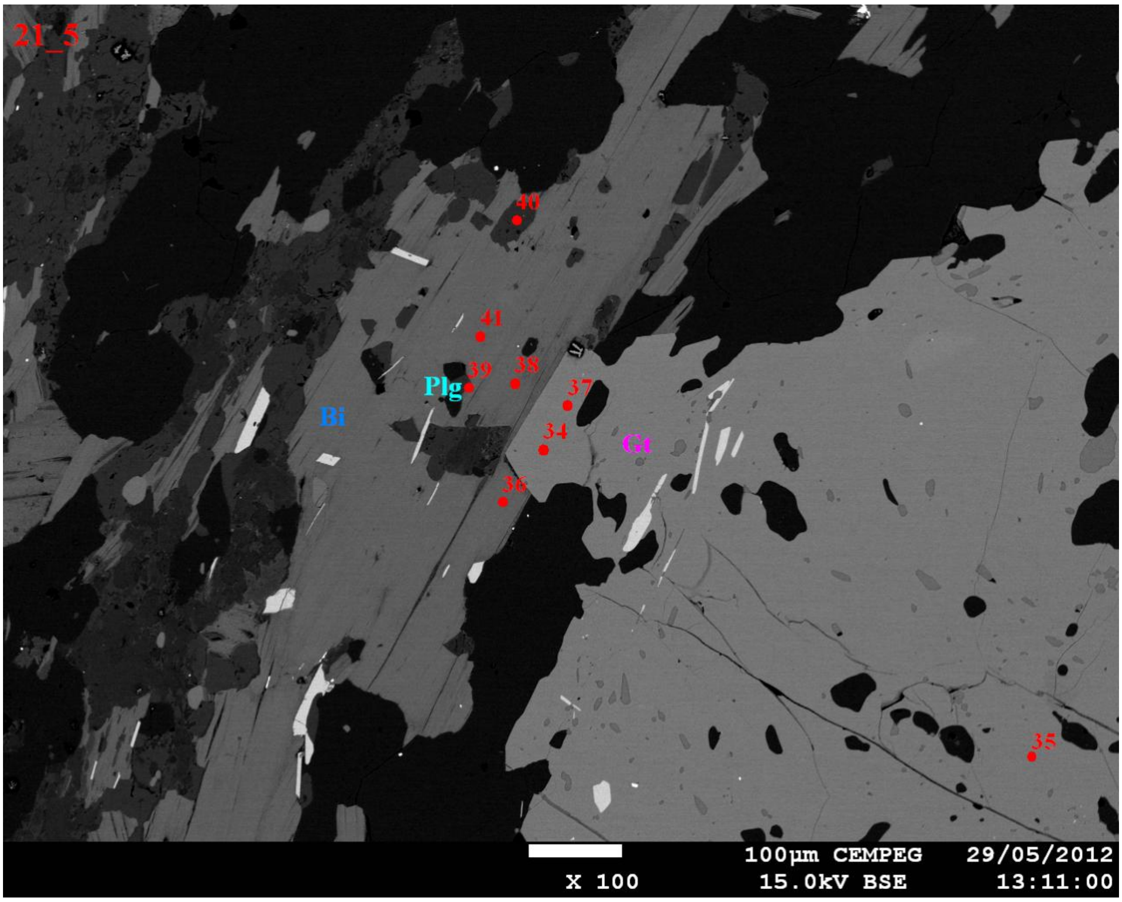

Figure 9. EPMA image of sample OUF 2, sample site 21_5

Thermocalc

21_51			
Mineral	**Point**	**T**	**P**
Garnet	34	490°C	4.1 kbars
Biotite	36	sd = 83	sd = 1.0
Plagioclase	39		

21_52			
Mineral	**Point**	**T**	**P**
Garnet	35	419°C	3.5 kbars
Biotite	38	sd = 115	sd = 1.4
Plagioclase	40		

21_52			
Mineral	**Point**	**T**	**P**
Garnet	37	508°C	4.1 kbars
Biotite	41	sd = 98	sd = 1.1
Plagioclase	40		

Table 1. Sample chemistry and calculated results sample site 41_1. OUF 2

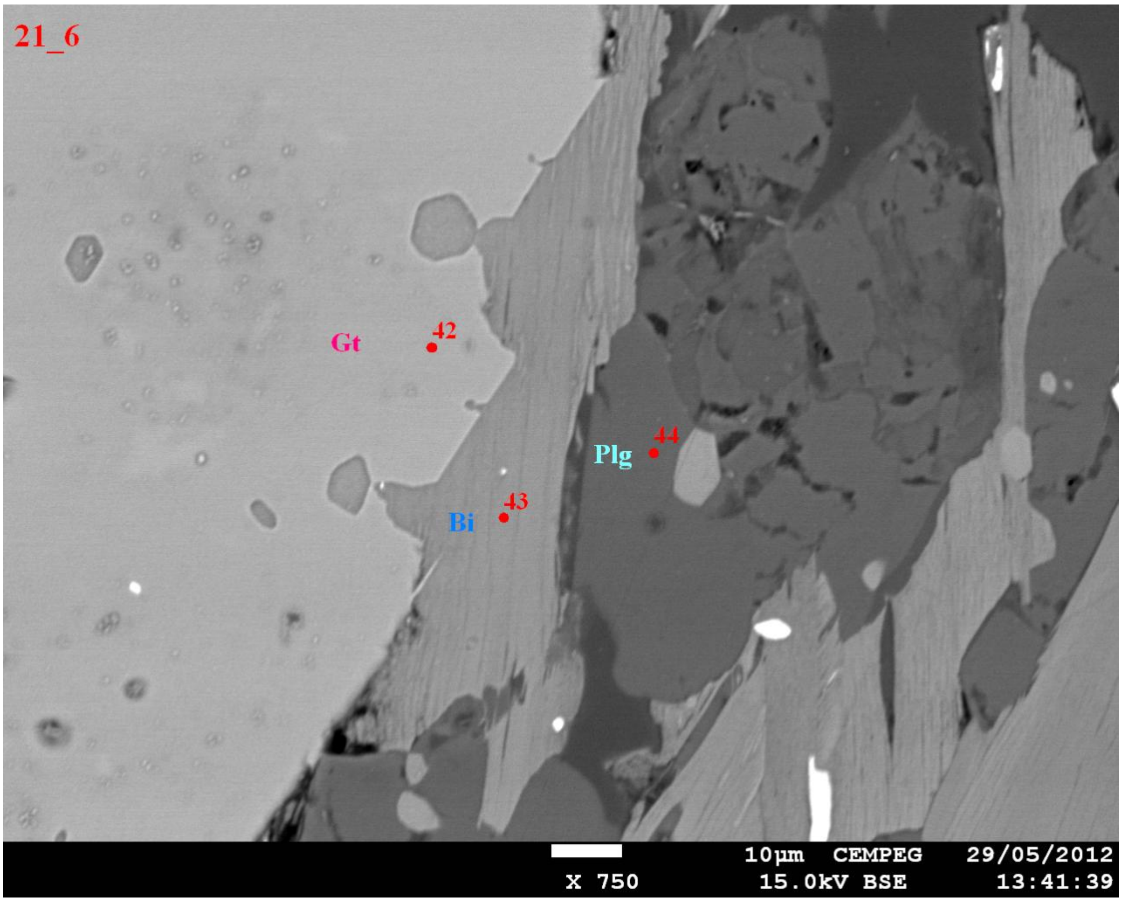

Figure 10. EPMA image of sample OUF 2, sample site 21_6

21_6			
Mineral	**Point**	**T**	**P**
Garnet	42	519°C	4.9 kbars
Biotite	43	sd = 92	sd = 1.1
Plagioclase	44		

Table 2. Sample chemistry and calculated results sample site 41_1. OUF 2

3.7.2 OUF 4 – Stora sillsvik

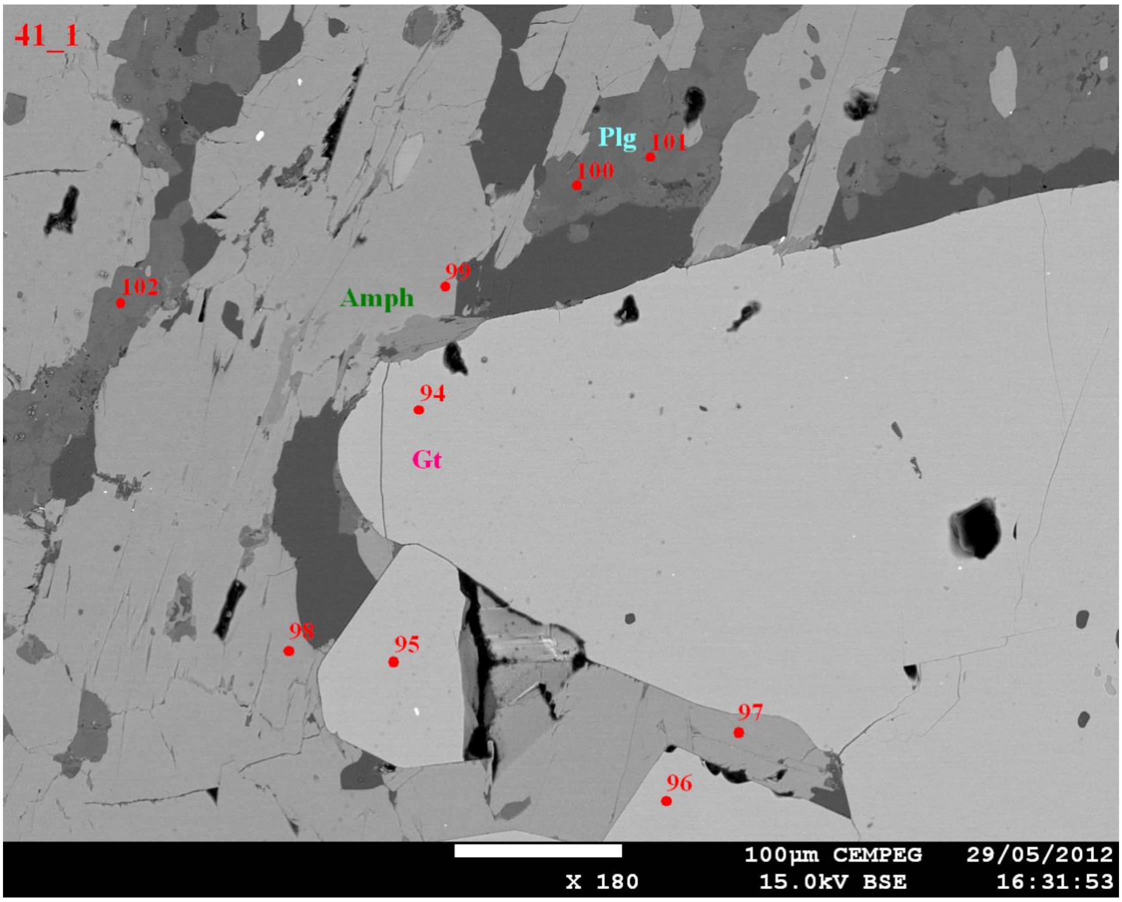

Figure 11. EPMA image of sample OUF 4, sample site 41_1

41_11			
Mineral	**Point**	**T**	**P**
Garnet	95	389°C	3.0 kbars
Amphibole	99	sd = 40	sd = 0.9
Plagioclase	100		

41_12			
Mineral	**Point**	**T**	**P**
Garnet	96	389°C	3.0 kbars
Amphibole	97	sd = 40	sd = 0.9
Plagioclase	102		

Table 3. Sample chemistry and calculated results sample site 41_1. OUF 2.

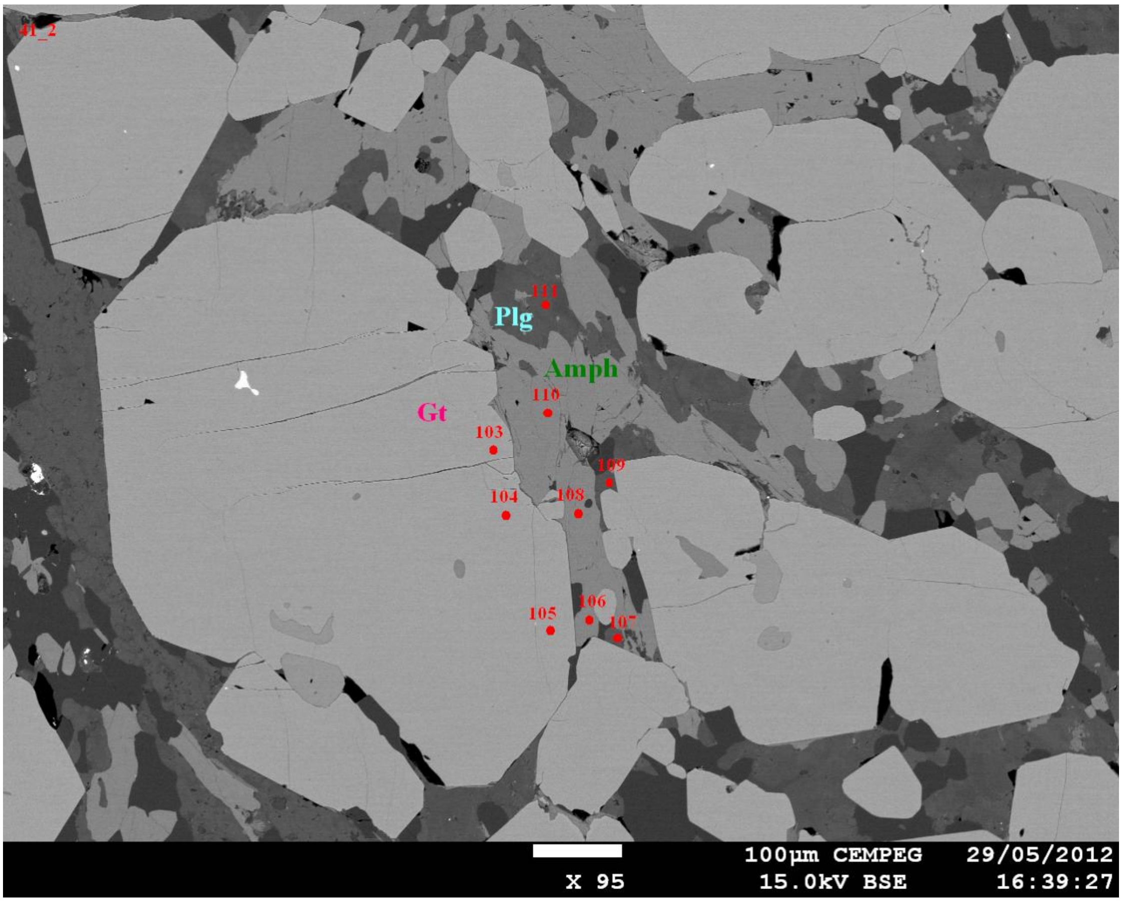

Figure 12. EPMA image of sample OUF 4, sample site 41_2.

41_21			
Mineral	**Point**	**T**	**P**
Garnet	103	386°C	2.9 kbars
Amphibole	110	sd = 49	sd = 1.1
Plagioclase	111		

41_22			
Mineral	**Point**	**T**	**P**
Garnet	104	391°C	2.9 kbars
Amphibole	108	sd = 48	sd = 1.1
Plagioclase	109		

41_23			
Mineral	**Point**	**T**	**P**
Garnet	105	396°C	3.0 kbars
Amphibole	106	sd = 65	sd = 1.4
Plagioclase	107		

Table 4. Sample chemistry and calculated results sample site 41_1. OUF 2

3.7.3 Average T & P

Calculated average T & P for OUF2 and OUF4 Thermocalc 3.33 modelling.

Avarage P & T				
Sample	Avarage T (° C)	Avarage Tsd	Avarage P (kbar)	Avarage Psd
21_51	490	83	4.1	1
21_52	419	115	3.5	1.4
21_53	508	92	4.1	1.1
21_6	519	98	4.9	1.1
	484	**97**	**4.15**	**1.15**

Table 3. Sample chemistry and calculated results site 21_5-21_6. OUF 2

Avarage T & P				
Sample	Avarage T (° C)	Avarage Tsd	Avarage P (kbar)	Avarage Psd
41_11	389	40	3	0.9
41_12	385	48	2.9	1.1
41_21	386	49	2.9	1.1
41_22	391	48	2.9	1.1
41_23	396	65	3	1.4
	389.4	**50**	**2.94**	**1.12**

Table 4. Sample chemistry and calculated results 41_. OUF 4

4.0 Discussion

The P & T calculations made from sample OUF2 corresponds well with the tectonic setting described by Talbot (2008). Andalusite to kyanite zone greenschist to amphibolite facies level of metamorphism fits well with the idea of reworked sediments in an accretionary prism metamorphosed during orogeny, in this case two orogenic events. Probable prograde andalusite on Utö is likely coherent with prograde andalusite found in greywackes all around Bergslagen, representing Svecokarelian regional metamorphism.

Data from sample OUF4 gave lower T/P results that doesn't correspond well with the geologic history according to Talbot (2008) or results in line with the bulk composition. Coexistence of amphibole and andalusite indicates higher T conditions than the results are showing. Probable reasons for the low T is an inaccurate EPMA analysis of the amphibole composition due to its complicated chemistry and the fact that the grains analysed were too altered and not in equilibrium. The petrographic- and the EPMA analysis clearly shows that the OUF4 sample is more altered then the OUF2 sample, which indicates that the data retrieved from OUF4 is less reliable.
It is however possible to argue for an alternate explanation, OUF4 T and P results might reflect a part of a retrograde path. OUF4 T and P result fits well as part of a retrograde path in a P-T-t path relative to the assumed prograde OUF2 T and P results.

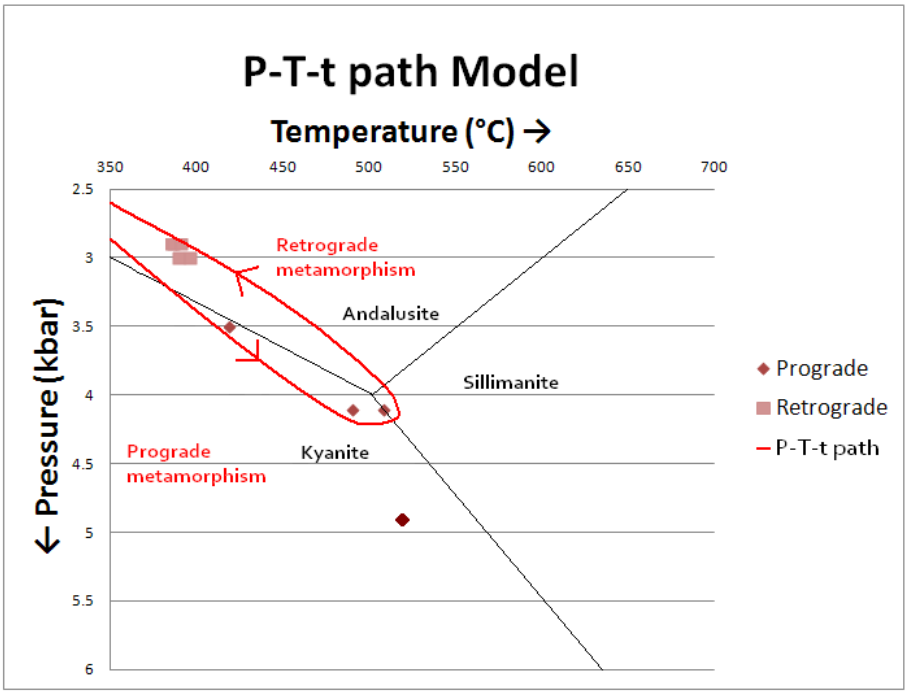

Figure 13. *PTt model. Modelled from Thermocalc 3.21 P and T results*.

OUF2 data points plot in the kyanite field in the PTt model. Earlier published material does not support the existence of kyanite on Utö, neither do I. The stability field of andalusite can vary with the chemistry, variations in magnesium and iron ratios can affect the stability field. A shift in the stability field might be a probable explanation, all but one data point plot close to the andalusite field boundary.

Macroscopic zoning in the porphyroblasts of garnet is visible in sample OUF2 which corresponds well with the two assumed metamorphic phases. Thermocalc model made on site 21_52 from points 35, 38 and 40 gave slightly lower values for T and P, likely because point 35 is significantly closer to the garnet core then all other points, it might simply indicate disequilibrium since it is isolated from surrounding minerals. It is hard to explain why site 21_6 gives slightly higher values for T and P, except that the mineral grains show a higher degree of alteration and probable disequilibrium.

The garnets present in sample OUF2 and OUF4 appear very different, in hand specimen OUF4 shows a lighter pink colour and a more sugary like surface due to the specific breakdown of the garnet. Sample OUF2 shows a cleaner fuller colour and the breakdown looks more representative for garnets in general. This difference is most likely related to difference in the rocks bulk composition.

4.1 Sources of error

The most evident source of error is the subjectivity that to some extend influence all observations, especially mapping and petrographic analysis. The errors are minimized by second opinions from senior geologist in the field, by the microscope and by the EPMA and during data processing.

In order to attain usable activity composition data in the a-X output file some assumptions had to be made.

1. Andalusite was set as a stable phase. The presence of andalusite had to be alleged even though it was not present in the thin section (OUF 2 & 4), but within 5-20 meters from the sample site in the same rock formation.
2. Muscovite was set as a stable phase and indefinite presence. Muscovite is present in the thin section OUF 2 & 4 but no EPMA data was retrieved.

A macroscopic zoning is clearly visible in the garnet porphyroblasts but no zoning profile was performed with the EPMA on OUF 2 to confirm the observation.

The data sampling and processing performed in the EPMA, AX_2 and THERMOCALC 3.21 yields a standard deviation based on the individual standard deviation for every element analysed, an uncertainty hard to control. A compositionally heterogeneous mineral makes the geothermobarometric calculation vary with the composition, to avoid that several points close to each other have been sampled so that a mean value could be calculated.

Thermocalc 3.21 calculations could have been done iteratively, which means that the first P and T calculated is re-run in AX_2 and Thermocalc 3.21 giving new values for P and T which are then re-run and so on till there is no change in calculated results. Instead AX_2 was executed ones with conditions fixed to T: 550°C and P: 5.0 kbar. Repeated calculations in this manner might have yielded more accurate results. Data set 21_5 executed with this method starting at T: 550°C and P: 5.0 kbar gave results of T: 533°C and P: 5.0 kbar. Since andalusite is present in the rock it is reasonable to argue that T should not be higher than 500°C and P not higher than 4.0 kbar. Starting with these values gives the result T: 490°C P: 4.1 kbar, which happens to be the results yielded from the initial calculation. The starting value put in to AX_2 is a possible source of error.

5.0 Conclusion

The oldest parts of the rock suite at Utö is represented by the greywacke at Fårskärsudd which sample OUF2 is extracted from. A dark clay rich sediment layer deposited on the shelf by turbidity currents in a calm deep water environment and later reworked and metamorphosed twice in an accreassionary prism built up by the subducting oceanic plate and the shelf.

Relaying on the accuracy of the EPMA analysis and the AX_2 and thermocalc modelling I conclude that the andalusite and garnet bearing greywacke at Fårskärsudd represented by sample OUF2 formed in the transition between greenshist and amphibolite facies conditions at a temperature of approximately **484°C** and a pressure of approximately **4.15 kbar**.
The amphibole bearing greywacke NE of Fårskärsudd is likely to record part of a retrograde path, formed at an average temperature of **389.4 °C** and pressure of **2.94 kbar.** T and P values fits well in a P-T-t path model.

Acknowledgements

This bachelor thesis is not solely built on my own efforts, my supervisors Alasdair Skelton and Joakim Mansfeld supported me with knowledge and unfailing patience the whole way. Secondly I want to thank Magnus Ripa at the Geological survey of Sweden (SGU) for letting me take part in a very important project. The help of Jarek Maika at Uppsala University was crucial for the quality of my data, thank you. Lastly, I thank Adam Engström and Linnea Lundin for inspiring discussions and good company at Utö.

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Software

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Appendices

Thermocalc 3.21 and AX_2 modelling results and output files

21_51

Thermocalc output file

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THERMOCALC 3.21 running at

11.52 on Tue 27 Nov,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.000370	0.00210	0.450	0.0172	0.130	0.0170	0.900
sd(a)/a	0.77542	0.68425	0.15000	0.49533	0.24533	0.49667	0.10000

	and	q	H2O	mu
a	1.00	1.00	1.00	1.00
sd(a)/a	0	0		0

Independent set of reactions

1) gr + 2and + q = 3an

2) 5py + 3east + 4mu = 7phl + 12and

3) py + phl + 2mu = 3east + 6q

4) alm + mu = ann + 2and + q

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	4.6	0.97	33.73	0.59	-0.12206	4.993	5.850	0.747

2	3.8	3.70	-234.51	2.17	0.06368	9.416	23.294	5.411
3	7.3	3.24	-13.35	1.24	-0.01324	3.490	-0.259	1.751
4	3.6	0.86	3.64	1.01	-0.00560	2.438	-1.242	0.288

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 >0.40, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.73

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	4.1	1.0	490	83	0.767	0.89

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	3.39	1.34	429	120	0.884	0.74	0.51	0.59
gr	4.03	0.96	511	94	0.646	0.83	0.39	0.52
alm	4.24	1.03	494	84	0.745	0.83	-0.31	0.11
phl	4.20	1.08	504	97	0.820	0.87	0.21	0.21
ann	4.40	1.09	497	84	0.730	0.77	0.50	0.30
east	3.99	0.96	489	83	0.765	0.70	-0.81	0.02
an	4.05	0.96	497	87	0.725	0.87	-0.17	0.10
and	4.06	0.96	490	83	0.767	0.89	0	0
q	4.06	0.96	490	83	0.767	0.89	0	0
mu	4.06	0.96	490	83	0.767	0.89	0	0

T = 490°C, sd = 83,

P = 4.1 kbars, sd = 1.0, cor = 0.767, sigfit = 0.89

21_51	Compound %											
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	34	36.8	0	20.19	0	0	34.1	1.8	1.363	4.08	0.042	0.059	98.474
Biotite	36	34	1.68	16.08	0.0246	0	25.3	0.039	6.95	0.041	0.191	8.76	93.056
Plagioclase	39	46.3	0.03	31.57	0	0	0.48	0.028	0	17.95	1.216	0.076	97.633
T=490°C, sd = 83													
P=4.1 kbars, sd = 1.0													

21_52

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THERMOCALC 3.21 running at

11.57 on Tue 27 Nov,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

```
          py     gr     alm    phl    ann   east    an
a       0.000290 0.00520  0.330  0.0163  0.130  0.0150  0.910
sd(a)/a   0.78480 0.61517 0.15152 0.50147 0.24533 0.51082 0.10000

         and     q    H2O    mu
a        1.00   1.00   1.00   1.00
sd(a)/a     0      0          0
```

Independent set of reactions

1) gr + 2and + q = 3an

2) 5py + 3east + 4mu = 7phl + 12and

3) py + phl + 2mu = 3east + 6q

4) alm + mu = ann + 2and + q

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	5.7	0.89	33.73	0.59	-0.12206	4.993	4.976	0.684
2	3.0	3.75	-234.51	2.17	0.06368	9.416	24.511	5.483
3	7.4	3.32	-13.35	1.24	-0.01324	3.490	-0.337	1.793
4	2.7	0.87	3.64	1.01	-0.00560	2.438	-0.932	0.288

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 >0.40, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.73

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	3.5	1.4	419	115	0.776	1.67

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	2.37	1.62	320	133	0.888	1.34	1.00	0.59
gr	3.44	1.21	466	108	0.639	1.39	0.99	0.54
alm	3.91	1.36	428	102	0.761	1.48	-0.72	0.10
phl	3.51	1.61	416	134	0.827	1.67	-0.07	0.21
ann	4.23	1.25	436	89	0.752	1.28	1.17	0.26

east 3.49 1.35 418 107 0.774 1.56 -0.87 0.01

an 3.51 1.36 436 114 0.722 1.58 -0.48 0.13

and 3.55 1.44 419 115 0.776 1.67 0 0

q 3.55 1.44 419 115 0.776 1.67 0 0

mu 3.55 1.44 419 115 0.776 1.67 0 0

T = 419°C, sd = 115,

P = 3.5 kbars, sd = 1.4, cor = 0.776, sigfit = 1.67

21_52	Compund %											
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	35	37.07	0.0499	20.33	0.0021	0	31.5	3.31	1.1957	5.76	0.0287	0.018	99.2145
Biotite	38	34.33	1.76	15.91	0.0469	0	25.6	0.0638	6.92	0.025	0.1261	8.74	93.5515
Plagioclase	40	46.03	0.0753	34.53	0	0	0.56	0	0.0099	18.25	1.0934	0.102	100.6539
T=419°C, sd = 115													
P=3.5 kbars, sd = 1.4													

21_53

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THERMOCALC 3.21 running at

11.08 on Tue 27 Nov,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.000520	0.00210	0.430	0.0188	0.140	0.0180	0.910
sd(a)/a	0.76107	0.68425	0.15116	0.48501	0.23500	0.49008	0.10000

	and	q	H2O	mu
a	1.00	1.00	1.00	1.00
sd(a)/a	0	0		0

Independent set of reactions

1) gr + 2and + q = 3an

2) 5py + 3east + 4mu = 7phl + 12and

3) py + phl + 2mu = 3east + 6q

4) alm + mu = ann + 2and + q

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	4.6	0.97	33.73	0.59	-0.12206	4.993	5.883	0.747
2	4.6	3.63	-234.51	2.17	0.06368	9.416	22.043	5.307
3	7.7	3.20	-13.35	1.24	-0.01324	3.490	-0.517	1.725
4	3.2	0.84	3.64	1.01	-0.00560	2.438	-1.122	0.279

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 >0.40, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.73

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	4.1	1.1	508	98	0.761	1.14

P	sd(P)	T	sd(T)	cor	fit	e*	hat

py 3.19 1.33 425 123 0.880 0.93 0.67 0.59

gr 4.02 0.97 541 99 0.641 1.02 0.58 0.52

alm 4.32 1.07 513 90 0.737 1.04 -0.43 0.12

phl 4.18 1.21 521 113 0.815 1.13 0.18 0.21

ann 4.53 1.09 518 86 0.722 0.95 0.67 0.29

east 3.99 0.96 507 86 0.759 0.95 -0.93 0.02

an 4.05 1.05 518 99 0.718 1.10 -0.25 0.10

and 4.06 1.09 508 98 0.761 1.14 0 0

q 4.06 1.09 508 98 0.761 1.14 0 0

mu 4.06 1.09 508 98 0.761 1.14 0 0

T = 508°C, sd = 98,

P = 4.1 kbars, sd = 1.1, cor = 0.761, sigfit = 1.14

21_53	Compound %												
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	37	37.4	0.022	20.3	0.004	0	34.88	1.78	1.284	4.26	0	0.0203	99.95
Biotite	41	34.7	1.72	16.7	0.015	0	25.43	0.02	7.01	0.021	0.158	9.34	95.124
Plagioclase	40	46	0.075	34.5	0	0	0.563	0	0.01	18.25	1.093	0.1022	100.65
T=508°C, sd = 98													
P=4.1 kbars, sd = 1.1													

21_6

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THERMOCALC 3.21 running at

12.00 on Tue 27 Nov,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

py gr alm phl ann east an

a 0.000260 0.00170 0.480 0.0127 0.0740 0.0210 0.910

sd(a)/a 0.78878 0.69799 0.15000 0.52903 0.31796 0.47190 0.10000

	and	q	H_2O	mu
a	1.00	1.00	1.00	1.00
sd(a)/a	0	0		0

Independent set of reactions

1) gr + 2and + q = 3an
2) py + 3east + 4q = 3phl + 4and
3) 5py + 3east + 4mu = 7phl + 12and
4) alm + mu = ann + 2and + q

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	4.3	0.99	33.73	0.59	-0.12206	4.993	6.094	0.760
2	3.3	18.00	-69.27	1.14	0.03006	0.812	6.746	2.268
3	4.5	3.82	-234.51	2.17	0.06368	9.416	22.301	5.592
4	5.2	1.01	3.64	1.01	-0.00560	2.438	-1.870	0.352

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 >0.40, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.73

however a larger value may be OK - look at the diagnostics!

avP sd avT sd cor fit

lsq 4.9 1.1 519 92 0.792 0.44

P sd(P) T sd(T) cor fit e* hat

py 5.26 1.64 547 134 0.901 0.39 -0.20 0.61

gr 4.96 1.14 499 104 0.664 0.32 -0.32 0.56

alm 4.83 1.19 517 92 0.778 0.39 0.17 0.07

phl 5.05 1.28 530 107 0.839 0.41 0.16 0.22

ann 4.68 1.27 514 93 0.760 0.31 -0.36 0.32

east 4.92 1.14 519 92 0.791 0.43 -0.03 0.02

an 4.94 1.14 514 96 0.750 0.41 0.14 0.10

and 4.93 1.13 519 92 0.792 0.44 0 0

q 4.93 1.13 519 92 0.792 0.44 0 0

mu 4.93 1.13 519 92 0.792 0.44 0 0

T = 519°C, sd = 92,

P = 4.9 kbars, sd = 1.1, cor = 0.792, sigfit = 0.44

21_6		Compound %											
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	42	37.5	0.03	21.2	0.0176	0	35.37	1.84	1.224	3.88	0.009	0.048	101.144
Biotite	43	33.2	1.69	17.11	0	0	26.51	0.082	7.27	0.08	0.151	7.86	93.9868
Plagioclase	44	45.3	0	34.54	0.0102	0	0.479	0.023	0	18.7	1.195	0.059	100.267
T=519°C, sd = 92													
P=4.9 kbars, sd = 1.1													

41_11

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THERMOCALC 3.21 running at

13.00 on Thu 29 Nov,2012 with thermodynamic dataset produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	cumm	grun	an	and
a	0.00240	0.000940	0.410	0.0280	0.0670	0.810	1.00
sd(a)/a	0.67514	0.73231	0.15000	0.43640	0.35000	0.35000	0

	q	H_2O
a	1.00	1.00
sd(a)/a	0	

Independent set of reactions

1) gr + 2and + q = 3an

2) 10gr + 3cumm + 27and = 7py + 30an + $3H_2O$

3) 10gr + 3grun + 27and = 7alm + 30an + $3H_2O$

Calculations for the independent set of reactions

(for x(H_2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.0	1.65	33.73	0.59	-0.12206	4.993	6.337	1.280
2	5.9	2.04	691.20	6.35	-1.49137	43.242	31.875	13.709
3	4.7	2.08	515.29	7.90	-1.45395	40.023	65.243	12.887

Average PT (for x(H_2O) = 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 >0.33, 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   3.0  0.9   389   40-0.467 0.89

       P  sd(P)    T  sd(T)   cor   fit    e*   hat
    py   2.90  0.90   406    47 -0.454  0.54  -0.66  0.37
    gr   3.20  1.12   380    48 -0.643  0.82  -0.21  0.27
   alm   2.79  1.00   384    42 -0.255  0.80   0.25  0.27
  cumm   2.96  0.89   392    41 -0.464  0.84   0.18  0.03
  grun   2.79  1.00   384    42 -0.255  0.80  -0.25  0.27
    an   3.38  1.27   373    53 -0.716  0.77   0.30  0.55
   and   2.97  0.89   389    40 -0.467  0.89     0    0
     q   2.97  0.89   389    40 -0.467  0.89     0    0
   H2O   2.97  0.89   389    40 -0.467  0.89     0    0
```

T = 389°C, sd = 40,

P = 3.0 kbars, sd = 0.9, cor = -0.467, sigfit = 0.89

41_11		Compound %											
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	95	38.13	0.0053	21.11	0.1274	0	34.17	1.81	2.73	3.01	0	0.0005	101.0932
Amphibole	99	53.68	0.0404	1.1423	0.0909	0	29.12	0.3235	14.07	0.2768	0.0506	0.0404	98.8349
Plagioclase	100	51.14	0	31.71	0.0499	0	0.306	0	0	15.1	3.2	0.0617	101.5678
T=389°C, sd = 40													
P=3.0 kbars, sd = 0.9													

41__12

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THERMOCALC 3.21 running at

13.29 on Tue 27 Nov,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	cumm	grun	an	and
a	0.00193	0.00116	0.400	0.0300	0.0620	0.910	1.00
sd(a)/a	0.68984	0.72081	0.15000	0.42759	0.35161	0.35000	0

	q	H2O
a	1.00	1.00
sd(a)/a	0	

Independent set of reactions

1) gr + 2and + q = 3an

2) 10gr + 3cumm + 27and = 7py + 30an + 3H2O

3) 10gr + 3grun + 27and = 7alm + 30an + 3H2O

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	3.8	1.64	33.73	0.59	-0.12206	4.993	6.476	1.274
2	6.0	2.04	691.20	6.35	-1.49137	43.242	31.532	13.681
3	4.5	2.07	515.29	7.90	-1.45395	40.023	66.692	12.823

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 >0.33, 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	2.9	1.1	385	48	-0.468	1.21

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	2.84	0.89	408	46	-0.456	0.74	-0.91	0.36
gr	3.23	1.25	374	53	-0.642	1.12	-0.28	0.27
alm	2.70	1.08	378	45	-0.254	1.09	0.34	0.27
cumm	2.91	1.02	389	47	-0.465	1.14	0.24	0.03
grun	2.69	1.08	378	45	-0.253	1.09	-0.34	0.28
an	3.49	1.34	364	55	-0.720	1.05	0.40	0.56
and	2.93	1.08	385	48	-0.468	1.21	0	0
q	2.93	1.08	385	48	-0.468	1.21	0	0
H2O	2.93	1.08	385	48	-0.468	1.21	0	0

T = 385°C, sd = 48,

P = 2.9 kbars, sd = 1.1, cor = -0.468, sigfit = 1.21

41_12		Compund %										
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	96	38.04	0	20.67	0.7613	0	34.52	1.74	2.59	3.32	0.0823	0	101.7236
Amphibole	97	53.52	0	1.0524	0.0038	0	28.57	0.305	14.09	0.2954	0.1224	0.0323	97.9917
Plagioclase	102	46.81	0.024	34.56	0	0	0.451	0.013	0	18.58	1.2088	0.0133	101.6598
T=386°C, sd = 49												
P=2.9 kbars, sd = 1.1												

41_21

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THERMOCALC 3.21 running at

16.14 on Wed 20 Jun,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	cumm	grun	an	and
a	0.00200	0.00104	0.390	0.0330	0.0590	0.900	1.00
sd(a)/a	0.68750	0.72687	0.15128	0.41524	0.35000	0.35000	0

	q	H_2O
a	1.00	1.00
sd(a)/a	0	

Independent set of reactions

1) gr + 2and + q = 3an

2) 10gr + 3cumm + 27and = 7py + 30an + $3H_2O$

3) 10gr + 3grun + 27and = 7alm + 30an + $3H_2O$

Calculations for the independent set of reactions

(for $x(H_2O) = 1.0$)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	3.7	1.65	33.73	0.59	-0.12206	4.993	6.552	1.277
2	5.9	2.04	691.20	6.35	-1.49137	43.242	32.256	13.704
3	4.4	2.07	515.29	7.90	-1.45395	40.023	67.424	12.857

Average PT (for $x(H_2O) = 1.0$)

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 >0.33, 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	2.9	1.1	386	49	-0.470	1.24

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	2.78	0.90	410	46	-0.458	0.75	-0.93	0.36
gr	3.19	1.29	374	54	-0.645	1.15	-0.29	0.27
alm	2.64	1.11	379	46	-0.256	1.11	0.35	0.28
cumm	2.87	1.05	390	48	-0.467	1.17	0.24	0.02
grun	2.64	1.11	379	46	-0.258	1.11	-0.35	0.27
an	3.45	1.37	365	56	-0.720	1.07	0.41	0.56
and	2.88	1.10	386	49	-0.470	1.24	0	0
q	2.88	1.10	386	49	-0.470	1.24	0	0
H2O	2.88	1.10	386	49	-0.470	1.24	0	0

T = 386°C, sd = 49,

P = 2.9 kbars, sd = 1.1, cor = -0.470, sigfit = 1.24

41_21		Compound %										
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	103	38.36	0.0304	20.86	0.4186	0	34.25	1.94	2.62	3.18	0.009	0	101.6679
Amphibole	110	54.34	0.0054	0.8514	0.0139	0	28.39	0.325	14.39	0.294	0.139	0.0046	98.7528
Plagioclase	111	47.52	0	33.12	0	0	0.409	0	0	18.15	1.38	0	100.5791
T=386°C, sd = 49													
P=2.9 kbars, sd = 1.1													

41_22

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THERMOCALC 3.21 running at

17.49 on Mon 25 Jun,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	cumm	grun	an	and
a	0.00210	0.000900	0.410	0.0300	0.0640	0.880	1.00
sd(a)/a	0.68425	0.73460	0.15122	0.42759	0.35156	0.35000	0

	q	H2O
a	1.00	1.00
sd(a)/a	0	

Independent set of reactions

1) gr + 2and + q = 3an

2) 10gr + 3cumm + 27and = 7py + 30an + 3H2O

3) 10gr + 3grun + 27and = 7alm + 30an + 3H2O

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	3.6	1.65	33.73	0.59	-0.12206	4.993	6.630	1.281
2	5.7	2.05	691.20	6.35	-1.49137	43.242	33.655	13.741
3	4.2	2.08	515.29	7.90	-1.45395	40.023	68.302	12.901

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 >0.33, 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	2.9	1.1	391	48	-0.468	1.19

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	2.76	0.91	415	48	-0.456	0.73	-0.89	0.37
gr	3.17	1.25	379	54	-0.644	1.10	-0.28	0.27
alm	2.62	1.08	384	46	-0.254	1.07	0.34	0.28
cumm	2.84	1.02	395	47	-0.464	1.13	0.24	0.03
grun	2.62	1.08	384	46	-0.255	1.07	-0.34	0.27
an	3.41	1.33	370	55	-0.716	1.03	0.40	0.55
and	2.86	1.07	391	48	-0.468	1.19	0	0
q	2.86	1.07	391	48	-0.468	1.19	0	0
H2O	2.86	1.07	391	48	-0.468	1.19	0	0

T = 391°C, sd = 48,

P = 2.9 kbars, sd = 1.1, cor = -0.468, sigfit = 1.19

41_22		Compound %										
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	104	38.26	0	21.12	0.0442	0	34.39	1.74	2.61	2.99	0	0.049	101.2035
Amphibole	108	53.74	0.028	0.9563	0	0	28.54	0.3131	14	0.246	0.078	0	97.9023
Plagioclase	109	47.57	0	33.36	0.059	0	0.829	0	0	17.26	1.67	0.008	100.7566
T=391°C, sd = 48													
P=2.9 kbars, sd = 1.1													

41_23

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THERMOCALC 3.21 running at

18.05 on Mon 25 Jun,2012 with thermodynamic dataset

produced at an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	cumm	grun	an	and
a	0.00210	0.000750	0.430	0.0390	0.0550	0.860	1.00
sd(a)/a	0.68425	0.74389	0.15000	0.39308	0.35273	0.35000	0

	q	H2O
a	1.00	1.00
sd(a)/a	0	

Independent set of reactions

1) gr + 2and + q = 3an

2) 10gr + 3cumm + 27and = 7py + 30an + 3H2O

3) 10gr + 3grun + 27and = 7alm + 30an + 3H2O

Calculations for the independent set of reactions (for $x(H_2O)$ = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	3.5	1.66	33.73	0.59	-0.12206	4.993	6.743	1.287
2	5.6	2.05	691.20	6.35	-1.49137	43.242	34.002	13.781
3	3.9	2.09	515.29	7.90	-1.45395	40.023	70.223	12.954

Average PT (for $x(H_2O)$ = 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 >0.33, 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	3.0	1.4	396	65	-0.460	1.57

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	2.91	0.90	428	49	-0.446	0.96	-1.17	0.38
gr	3.45	1.63	380	72	-0.639	1.45	-0.38	0.27
alm	2.72	1.42	387	61	-0.247	1.41	0.45	0.27
cumm	3.02	1.34	401	64	-0.456	1.49	0.29	0.02
grun	2.71	1.42	387	61	-0.245	1.40	-0.45	0.28
an	3.75	1.72	367	74	-0.709	1.35	0.53	0.55
and	3.04	1.41	396	65	-0.460	1.57	0	0
q	3.04	1.41	396	65	-0.460	1.57	0	0

H_2O 3.04 1.41 396 65 -0.460 1.57 0 0

T = 396°C, sd = 65,

P = 3.0 kbars, sd = 1.4, cor = -0.460, sigfit = 1.57

41_23		Compound %											
Mineral	point	SiO2	TiO2	Al2O3	Cr2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	105	38.19	0	21.16	0.0764	0	34.73	1.79	2.63	2.8	0	0.0125	101.3889
Amphibole	106	53.41	0	0.8223	0.0447	0	27.88	0.285	14.74	0.2	0.075	0.0467	97.5034
Plagioclase	107	48.46	0.0487	33.4	0	0	0.8264	0.047	0	16.98	1.95	0.0005	101.7126
T=396°C, sd = 65													
P=3.0 kbars, sd = 1.4													