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An examination of metamorphic conditions at Bjuröklubb, eastern Västerbotten county

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Introduction

About 60 km southeast of Skellefteå in Västerbotten, lies the peninsula of Bjuröklubb. The rocky shore that once was kept barren to allow it to be used a place to dry fish, still offers a generous area of exposed rock. Situated in the Bothnian Supergroup, with a safe distance to the Skellefte district and its dramatical geology and mineralizations. In recent years, however, Bjuröklubb has been center of attention for geologists, as it offers representations of several geological units and structures that are of significance to the understanding of the regional geological evolution. The controversy around the geological evolution models are still unresolved. My investigation attempts to shed light on the Bjuröklubb general geology, this ongoing discussion, and attempt to add a metamorphic perspective by extracting the local near peak pressure and temperature.

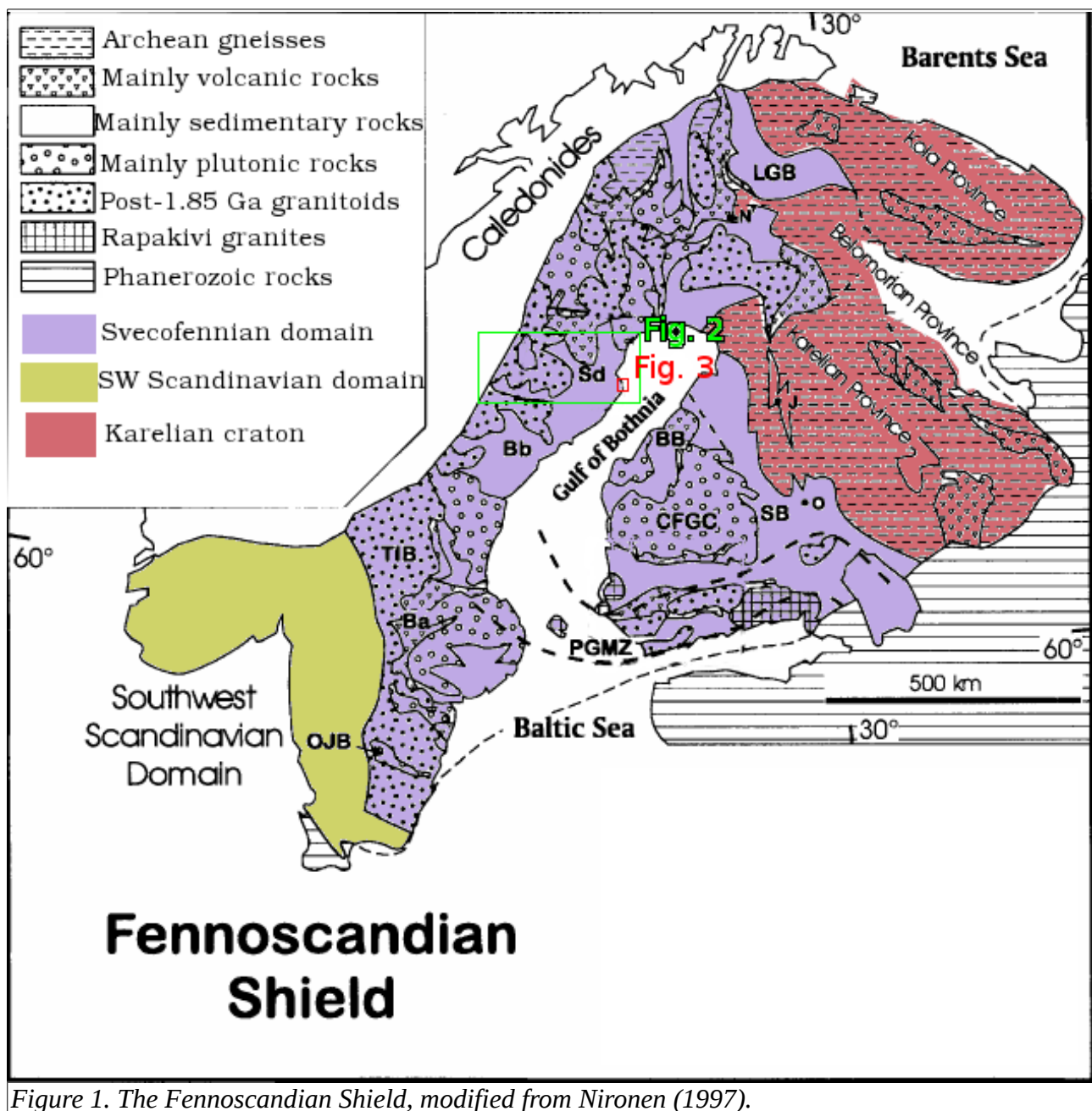


Figure 1. The Fennoscandian Shield, modified from Nironen (1997).

Geological background

The general geological context

The Svecofennian domain

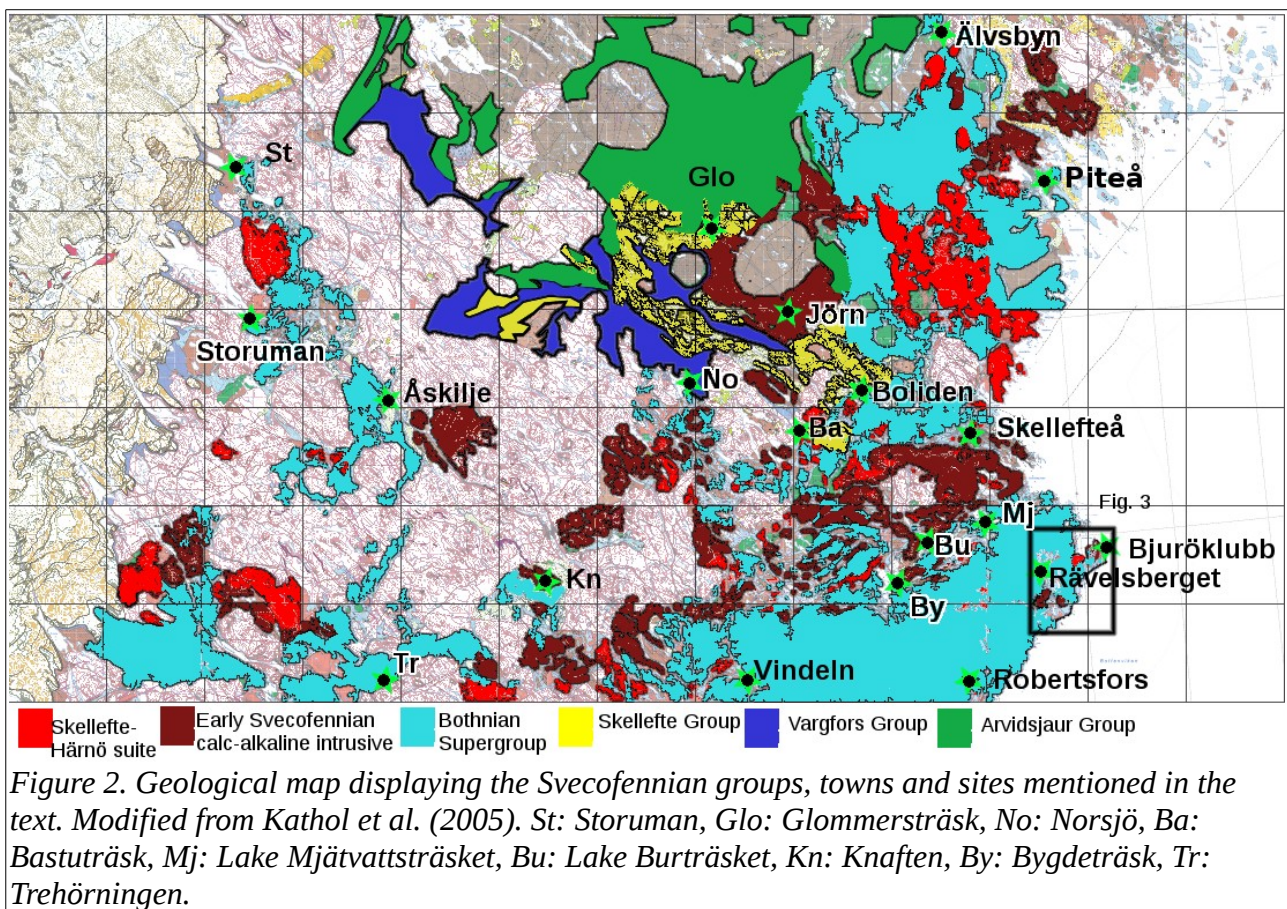
The Svecofennian domain is a part of the Fennoscandian (Baltic) Shield, that consists of the Karelian craton in the northeastern Finland and northwesternmost Russia, the Svecofennian domain and the southwest Scandinavian domain (Fig. 1)

The Svecofennian domain is characterized by its series of terranes accreted toward the Karelian craton from the west and southwest. These terranes are several arcs (both island and more mature) together with their related environments sediments volcanics and plutons (Korja and Heikinen, 2005).

Figure 4 shows the general stratigraphy of Svecofennian rocks of north-central Sweden. They are divided into the Bothnian Supergroup, the Skellefte Group, Vargfors and Arvidsjaur Groups and intrusive rocks.

Svecofennian supracrustal rocks: Bothnian Supergroup

1. The southeastern area (see fig. 2) between Skellefteå, Vindeln and Robertsfors, including Bjuröklubb, mainly consists of metagreywackes and metaargillites, that



originally were deposited by turbidity currents in a marine basin environment. These rocks were metamorphosed and deformed during the Svecokarelian deformation to paragneisses and veined gneisses. The veined gneisses have alternating dark, biotite-rich layers, and light quartz-feldspar dominated layers in mm to cm scale.

2. The second area is north of Skellefteå and Boliden, confined by the Jörn granitoid complex and Arvidsjaur volcanic rocks in the west, and Älvsbyn and Piteå in the north, and the coastline in the east. It has metagreywackes with varying degrees of deformation and metamorphism.
3. The northwest – southeast striking zone south of Norsjö and Bastuträsk, has turbiditic, generally argillitic greywackes.
4. The Knaften area, south of Lycksele, has > 1.95 Ga supracrustal and intrusive rocks.
5. Between Åskilje, Storuman and to the lake Storjuktan, there are turbiditic metagreywackes, muddy turbidites, coarse clastic rocks and intercalations of felsic

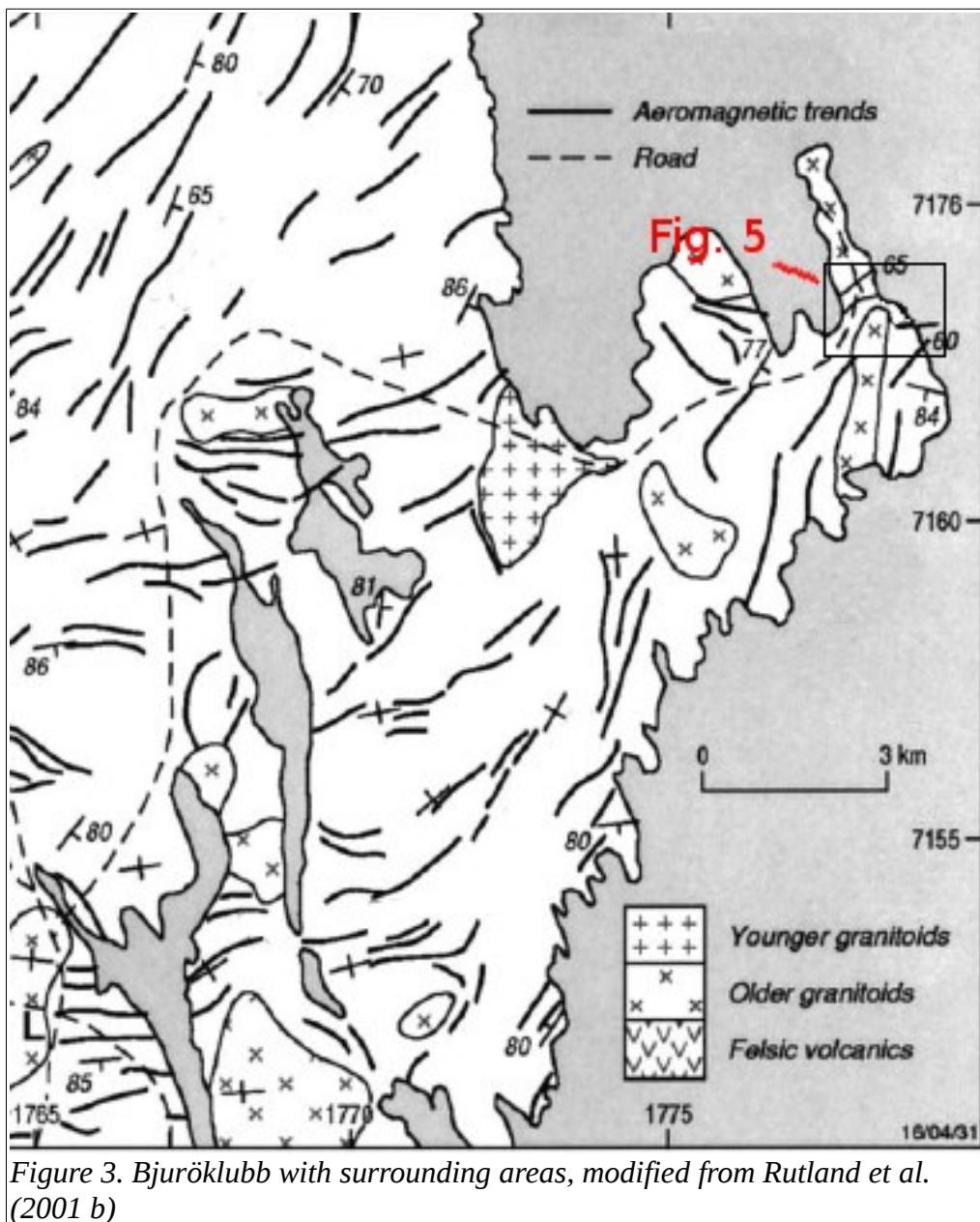


Figure 3. Bjuröklubb with surrounding areas, modified from Rutland et al. (2001 b)

and mafic volcanic rocks.

- Between Knaften and the Caledonian front lies subarea six, which has turbiditic metagreywackes with intercalated horizons of graphite and sulphide bearing shales.

Svecofennian supracrustal rocks: Skellefte Group

The Skellefte Group (fig. 4) are metavolcanic rocks mainly constrained within Jörn, Boliden, Norsjö and Glommersträsk. Generally subaqueously deposited lavas, lava- or cryptodomes of rhyolitic to basaltic composition, and derived sediments of these, and pyroclastic mass-flow deposits. Possibly excluding the western part of it, a signifying feature is the frequent interbedding of metavolcanics and metasediments. This often indicates a

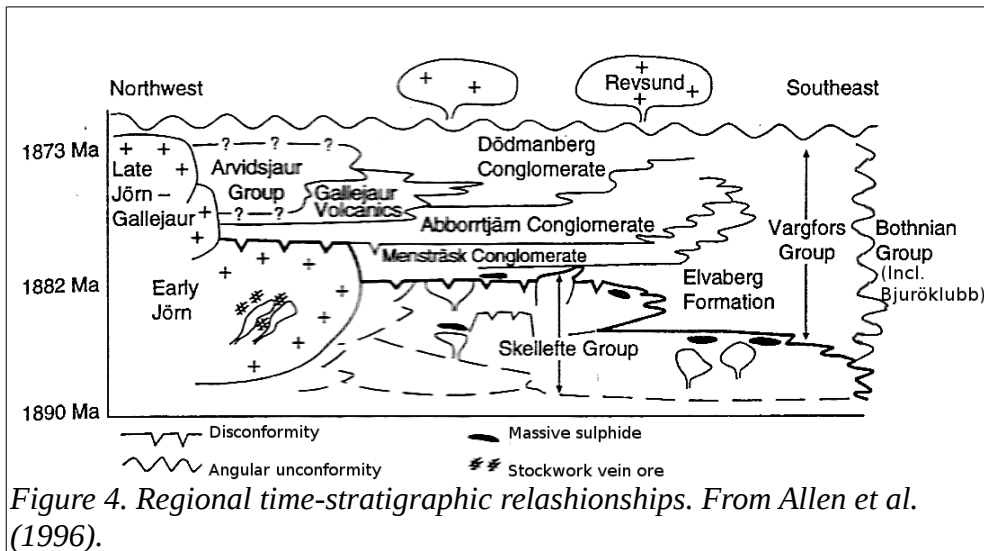


Figure 4. Regional time-stratigraphic relationships. From Allen et al. (1996).

below wave base deposition-environment. However, the mass flow deposits have abundant pumice fragments, indicating a shallow water, or subaerial environment of eruption.

Svecofennian supracrustal rocks: Vargfors Group

The Vargfors Group includes the Mensträsk conglomerate, argillites and greywackes of the Elvaberg formation, the Abbotjärn and Dödmanberg conglomerates and the Gallejaur volcanic rocks with its dykes and sills (fig. 4). This group occurs in and to the south of the Central Skellefte District. Vargfors sedimentary rocks are cut by a volcanic rock, constraining it to being 10 Ma younger than the Skellefte Group. It is also judged to be coeval with the Arvidsjaur Group and that part of it is the marine continuation of Arvidsjaur subaerial volcanic rocks.

Svecofennian supracrustal rocks: Arvidsjaur Group

North of the Skellefte and Vargfors group areas lies the Arvidsjaur Group, but Arvidsjaur Group units also occurs at a few other locations. It is almost exclusively of volcanic origin. It overlies the Skellefte Group and occurs as clasts in Vargfors conglomerates, meaning that it is older than the temporal end of Vargfors, and younger than the Skellefte Group (fig. 4).

Intrusive rocks

Jörn GII is an early Svecokarelian calc-alkaline rock of tonalitic composition and 1900-1860 Ma old. Jörn GI has positive ϵ_{Nd} values (Kathol and Weihed (2005)) indicating a primitive source, which then presumably is also true for GII. These rock mainly occur further

northwest in the Skellefte district (fig. 4), but also occur sporadically in this area, were they are metamorphosed to gneisses.

The Skellefte-Härnö suite is a late to post Svecokarelian intrusive rocks that are often situated in or adjacent to the Bothnian Supergroup. According to Kathol and Weihed (2005), they are probably the result of regional metamorphism. These come in two varieties. The first is more heterogenous or migmatitic, and the second homogenous and more intrusive, sometimes porphyritic.

Temporal and spatial constraints on metamorphism and deformation

According to Kathol and Weihed (2005), there is a poorly understood and contested deformational and metamorphic event occurred at not later than 1.88 Ga. A couple of points supporting this includes that 1.88 Ga plutons crosscuts deformed metasedimentary rocks of the Bothnian Supergroup. Also, a conglomerate of the Vargfors Group contains Jörn metagranodiorite clasts. The fabric of these clasts have differing strike and dip, suggesting that the clasts were deformed before the formation of the conglomerate.

Deformation and metamorphism generally have ages of between 1.86 and 1.78 Ga in the area, but it is debated whether it is a question of separate events, one multistage event, or one prolonged, spatially diachronous event (Kathol and Weihed (2005)).

Rutland et al. (2001 a), distinguishes two deformational phases. D1 with a D1.1 and a D1.2 part, and D2. An intrusion 'with weak fabric' in a metasedimentary host is dated to $1895 \pm 14/12$ Ma is taken to be the minimum age of D1 and maximum age of D2. D1.1 is a horizontal tectonic event, where the migmatites have a low angle schistosity, that D1.2 has been imposed upon. The Bygdeträsk subzone is a major ductile shear zone, with signs of transportation, it is essentially dip-slip with south-side up. This is where D2 occurs, and it clearly cuts D1. The authors rule out great crustal thickening and large horizontal movements across the strike, which if evident, would have supported the proposition of an accretion of juvenile volcanic arcs (previously suggested by other authors), due to the style of the D2 deformation. Instead they interpret it as deformation that affected already consolidated crust. The crustal thickness is taken to be developed earlier, perhaps during D1, because the D2 structures are highly localized. Weihed et al. (2002) , however, finds evidence for a pre 1.88 Ga deformational event (suggested by Rutland et al. (2001 a, b), supposedly their D1) insufficient, due to the weak relationship between the dating and the structures.

Plate tectonic concepts - A timeline modified from Kathol and Weihed (2005) with elaborations

- 1975: It is proposed that subduction to the northeast leads to accretion of island arcs onto the Karelian craton.
- 1980s: Geochemistry confirms the volcanic arc affinity of metavolcanics of the Skellefte Group.
- 1987: It is argued, with support from chemistry and Sm-Nd isotopes, that Jörn granitoid intrusions were emplaced in a convergent margin setting. Calc-alkaline intrusions are subduction-related.
- 1990: Ultramafic rocks of the Nickel zone, located between Lake Bjurträsket and Lake Mjätvattsträsket suggested to be related to an earlier southwest ward subduction that changed polarity.
- 1992: It is suggested that the metallogeny has implications for the tectonic model: The Skellefte District is an island arc and back-arc basins exists to the east and

west.

1987, 1990, 1993, 2002:

Electrical conductivity and seismic profiles unravel a north-dipping conductive and reflective slab just to the south of the Skellefte District, and is interpreted as a remnant ocean plate.

1996:

Allen et al. (1996) claim that the common understanding of the Skellefte district as an island arc, is inconsistent with well studied volcanic arc on oceanic crust. Even if they are subjected to periods of extension, they are invariably dominated by basalt and andesite. The overall felsic dominant composition of the Skellefte Group, as well as the composition of individual domains, rather points to it being arcs accreted on continental or mature arc crust. While the Skellefte Group is a mixture of shallow and moderately deep water settings, and is over 3 km thick, it must have continually subsided these 3 km while being deposited, while roughly the same setting prevailed. And while these kinds of submerged mainly felsic arc environments are uncommon, they are typical among arcs with major massive sulphide districts. These findings, and some structural expressions such as synvolcanic normal faults, indicate a strong extensional environment.

2001:

A new model is proposed by Rutland et al. (2001 a, b). They suggest a closure of a back arc basin model, supported by deformational structures in the Bygdeträsk shear zone (their D2 deformation). The style of D2 is said to rule out great crustal thickening and large horizontal movement across the strike. Its upright nature is also taken to mean that D1 is older than the deposition of the Skellefte Group and that the Robertsfors Group is the basement of the former. They lack direct stratigraphic evidence. D2 is supposed to have affected already consolidated crust. The crustal thickness is taken to be developed earlier, perhaps during D1, because the D2 structures are highly localized. The back arc basin closure could still have involved subduction, which could explain the cryptic D1.1 phase, and collision associated with the D1.2 phase. But D1 cannot have been related to subduction that was simultaneous to the deposition of the Skellefte Group or post Skellefte Group collision. If it is subduction related at all, it occurred earlier. The Skellefte volcanics are taken as a supracrustal sequence, deposited on a pre 1.9 Ga basement in the time between D1 and D2 on a far distance to the active continental margin of the time. Rutland et al. (2001 b) dates D2 to ~1860 Ma. Structural relationships suggests that a granitic phase in a D2-shear zone at Bjuröklubb is of the same ages. The granite was dated to 1860 Ma. They also dated two felsic intrusions from Rävålsberget, distinct from the Björklubb granite, that represents D2, to around 1860 Ma. At Trehörningen, they found dikes similar to those at Rävålsberget, but they are interpreted as originating between D1 and D2, since they themselves are folded (by D2), and contacts and xenoliths points to the host schist being deformed priorly also. Their age on these are 1874.5 ± 3.2 Ma, which they take to be a minimum age for D1.

2002:

Allen et al. (2002) adapts the tectonic model of arcs related to strong extension of continental or mature arc crust, such that it was located in an intra-arc region.

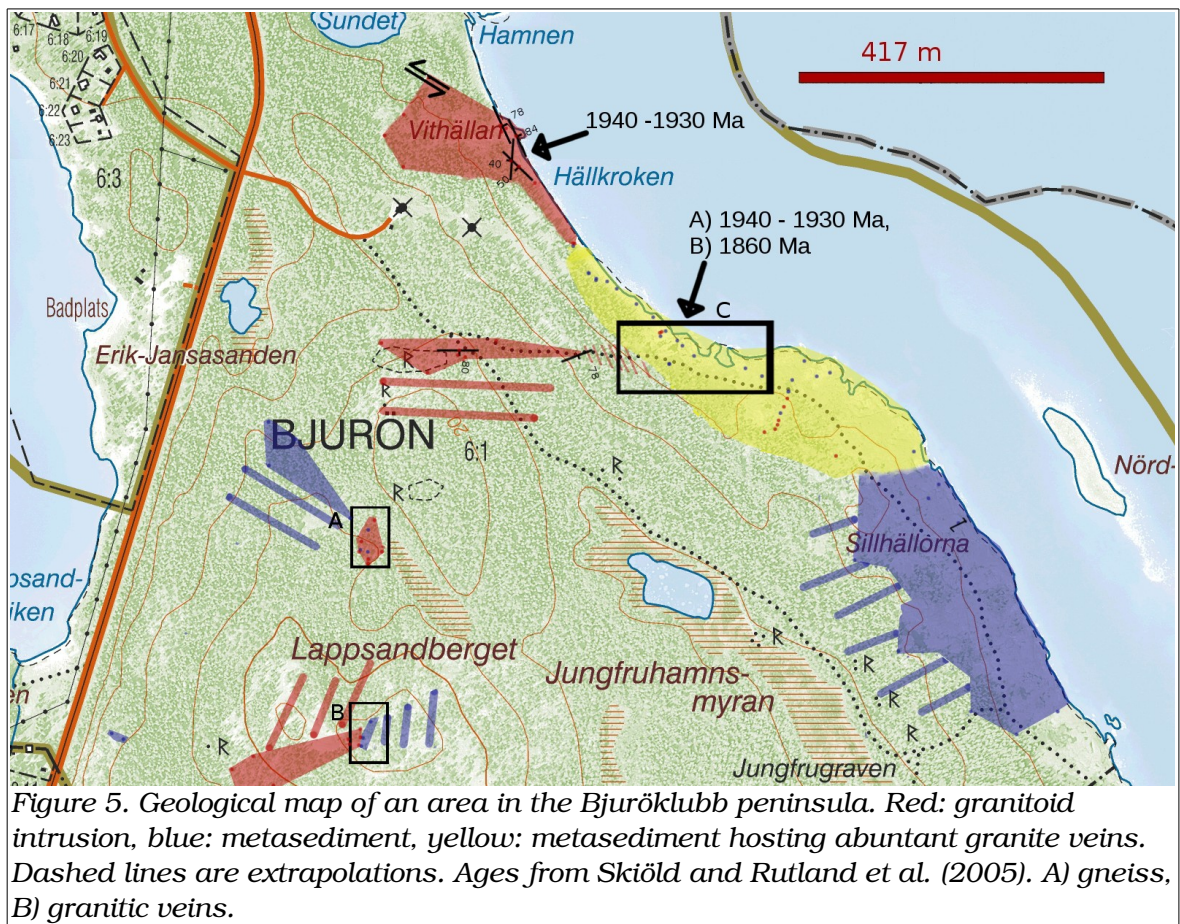
Weihed et al. (2002) rejects Rutland et al. (2001 a, b). They point out that their view relies on interpretations of relationships between intrusions in deformation structures. But since you can expect a high competency contrast between calc-alkaline intrusions and greywackes (the deformation could affect only the greywacke even if the intrusion is present), these relationships are not conclusive. On the contrary, in Bjuröklubb in the Burträsk Shear Zone, there is

an example of how a pegmatitic neosome (1860 Ma) cuts a middle to upper amphibolite facies rock, but is itself partly deformed. Since the intrusion is deformed itself, it seems like the early deformation of Rutland et al. (2001 a, b), D1, is actually an early phase of the deformation at 1860 Ma.

Another model is suggested by Juhlin et al. (2002). After the rifting of the Archean craton, southwest-directed subduction produced the Arvidsjaur-Kiruna continental arc. Simultaneously, northeast-ward subduction located further to the southwest, resulted in the Skellefte island arc. At ca 1.87 Ga, the Skellefte arc is still active, and the Arvidsjaur-Kiruna arc is attached to the Archean craton. Shortly after this, another arc or micro-continent collides with both the Skellefte and Arvidsjaur-Kiruna arc, thrusting the latter over the Karelian craton.

2005:

Skiöld & Rutland (2005) attempted to confirm the back-arc basin hypothesis suggested by Rutland et al. (2001 a, b). The Robertsfors metasediment is found to have archean and proterozoic sources. The 'total proterozoic population' of grains are dated to 1980 ± 6 Ma. Some of the younger proterozoic grains have dates that seems implausibly young, and are zoned and appears they have been overgrown. Therefore it is concluded that the maximum age of the deposition of the sedimentary protolith is ~ 1950 Ma, but possibly up to ~ 1980 Ma. This correlates well with ages obtained from the Vammala Migmatite Belt in Finland. Overgrowths determining a metamorphic event were dated to 1916 ± 5 Ma. That none of these were euhedrally zoned, is taken to prove the post-depositional nature of this event. A garnetiferous gneiss and a homogeneous foliated granitoid from Bjuröklubb were also dated using U-Pb isotopes, both to 1940-1930 Ma by isotope dilution thermal ionization mass spectrometry (ID-TIMS) and 1944 ± 4 Ma (the gneiss) and 1944 ± 5 Ma (the granitoid) respectively by secondary ion mass spectrometry (SIMS). They are therefore interpreted as different expressions of the same magmatic event. The crustal thickening between ~ 1.92 -191 Ma took place in large portions of the Svecofennian Province, and was the greatest in the Vammala Migmatite Belt. The authors claim that this episode of deformation and metamorphism is probably the most important in the Svecokarelian orogen, and can be correlated with the Lapland-Kola Orogen. D2, which may be superimposed on D1 occurred at ca 1.86 Ga. It is proposed that, it together with similar E-W trending belts for instance in Tampere would be distinguished as a second Svecokarelian episode, namely the Middle Svecokarelian (1.88-1.85 Ga). The back-arc basin model therefore seems confirmed. At a minimum, the old arc-accretion crustal growth model is ruled out.



Methods

To produce the map (fig. 5), a week was spent in the field, to map the shown areas and find suitable samples. About ten samples were selected for thin section analyses. These were described and examined for suitable sites for further investigation. The general composition of crystals representative of the minerals were determined by initial Scanning Electron Microscopy (SEM). This was followed by a Electron Microprobe (EMP) analysis for precise data. The EMP data is required to make accurate P-T calculations. SEM and EMP work in a similar way, that is firing electrons on the sample which then emits X-rays characteristic of a certain element. The EMP used 10 nA beam current, 15 kV accelerating voltage, and counting time for all elements was 10s on peak and 5s on \pm background. The composition data is used as input in the AX application to yield chemical activities. AX calculates composition input



together with datasets from laboratory experiments. It requires an initial rough estimation of the pressure and temperature, so I used 650 °C and 4.5 kbar for BK-10 and 700 °C and 8 kbar for BK-7. The activities are subsequently run in THERMOCALC, that calculates pressure and temperature from the thermodynamics of the relevant mineral reactions (in this case, five reactions). This assuming that the reactions are in equilibrium. Although completely absent from the rocks, the activity of muscovite was set to 1, to allow THERMOCALC to include more reactions, since it plausibly was present but consumed by the reactions. However, the difference from not including muscovite was minor.

The bedrock of Bjuröklubb

Figure 5 is the result of my mapping of a part of Bjuröklubb, which bedrock is a part of the Bothnian Supergroup. Since the contacts between rock types are unsharp and does not follow structures well, and due to its being located in a shear zone, the boundaries are inexact and extrapolation requires caution. The boundaries around Box C, are arbitrary. Some boundaries just roughly follow exposed rock rather than examined sites. The structural data are very much in wont, but they still allow the recognition of shearing and two distinct general foliation/ lamination strikes, roughly east-west and north-south. The metasediment becomes more sandy and is cut by granite veins, and occurs as xenoliths in granitic veins towards the north.

The granitoid area mainly consists of a foliated granitoid with quartz > feldspar > biotite > garnet. The crystals are about 1 mm in diameter. In the Vithällan area, the granitoid is cut by pegmatite veins, that carry granitoid xenoliths. The veins contain more feldspar than quartz, and some biotite and garnet. Crystal size vary from 1 mm to 3 cm. In turn, the pegmatite (and the granitoid) is cut by quartz veins.

The metasediment map unit are metasediments consisting of quartz, feldspar, biotite, garnet, cordierite and some graphite and iron sulphides (fig. 8, 9). Zones with abundant granitic intrusions are marked as a separate unit.



Figure 6. Granitic veins in the partially melted gneiss. Sample BK-7 is just like the "floating" gneiss chunk and taken within one meter to the left of it.

Box A

An area with a confusing dispersion of the metasedimentary rocks, I interpret these as xenoliths or rafts, since magmatic intrusion has clearly taken up adjacent material elsewhere in the area. The metasediments here can be rather crystalline, and are hard to interpret. In any case, this area is part of the granitoid intrusion.

Box B

Contact between the metasediment and the intrusion. It is the only seemingly sharp contact I found, but it is not straight enough to allow extrapolation.

Box C

The metasediment is abundantly intruded by granitic veins and partially melted. The contact with the granitoid to the west is gradational, with abundance of granitic veins decreasing towards it. Around the east and southeast side of the box, there is an increase in sulphides.

Description of the investigated rocks

Metasediment – BK-10

BK-10 (fig. 8) consists of quartz, cordierite and plagioclase in roughly the same

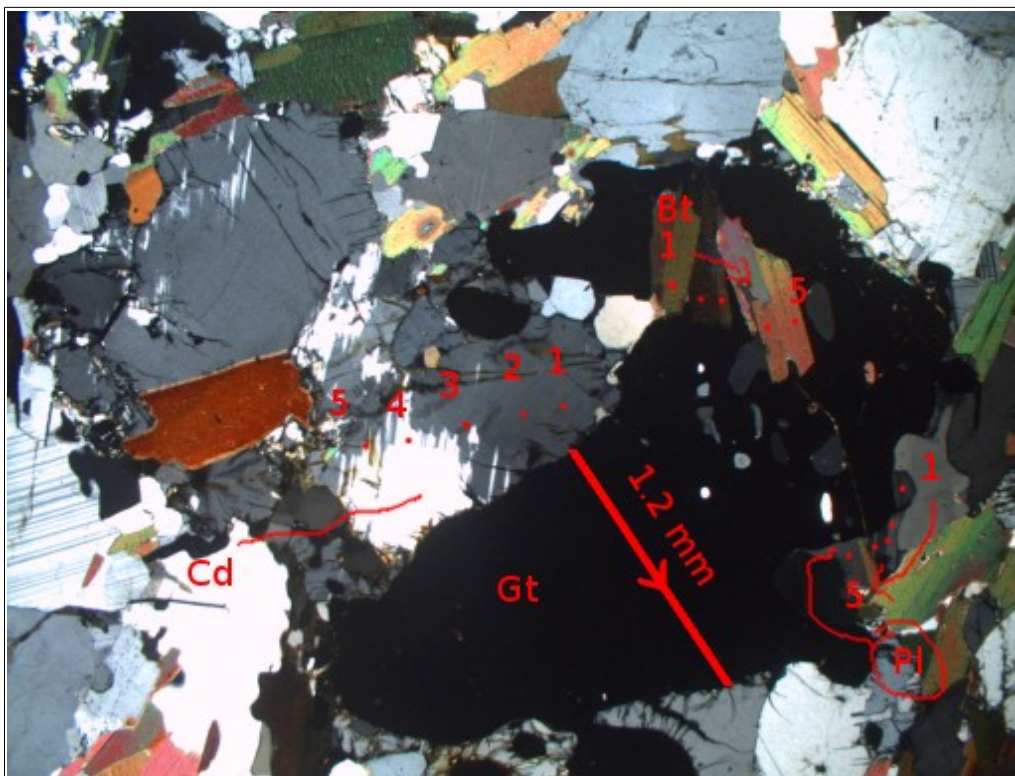


Figure 8. BK-10 in thin section with cross polarized light and marked sample points.

abundance. It has more biotite than garnet and some opaque minerals (including at least sulphides and graphite). In thin-section, the crystals have quite varying sizes, but the garnets are slightly bigger, but are not properly called porphyroblasts. It is hard to see the foliation on the microscopic level. Garnet crystals are often broken up and retreating in favour of

biotite. Biotite seems to be growing in general, due to its sharp edges and general shape, that it occurs

Figure 11 shows some element profiles in a BK-10 garnet. Note its homogeneity, its slight

Gneiss – BK-7

In BK-7 (see fig. 5) quartz and plagioclase are more abundant than, biotite and garnet and the sample also contains a little opaques and apatite. It is more strongly foliated than BK-10 and the thickness of the layers varies. Under microscope, the foliation is visible as bands of aligned biotite. It is mostly equigranular apart from biotite and the opaques. The garnets are subhedral, but occasionally approaching euhedral, and biotite is often aggregated around them. The biotite also looks slightly healthier than in BK-10, with sharp edges and typical biotite-shape. Therefore garnet and biotite appear to be in equilibrium, but if not, that biotite is growing.

Garnet in BK-7 shows the same chemical profile trend as the garnet in BK-10 (figure 9, 10).

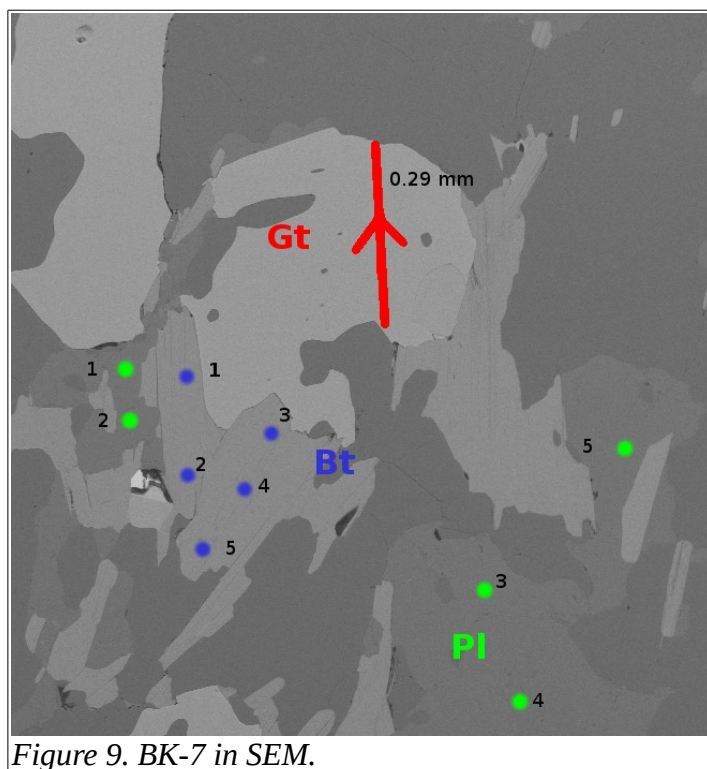


Figure 9. BK-7 in SEM.

Granitic veins

As seen in Figure 6, granitic veins cut the gneiss. The vein granite seems essentially the same as the granitoid (see fig. 5 and the following section), but is slightly finer grained and may have slightly less biotite.

Granitoid – BK-2, 3

The granitoid (see fig. 5) is tonalitic and has feldspar, quartz and biotite, and some garnets seemingly completely replaced by biotite (there are garnet-shaped biotite). The foliation consists of up to 2 cm long biotite aggregates. In thin section, it appears massive, and there are some crystals (feldspar and biotite) filling up most of or the entire view. On this level, garnet appears to have been replaced by quartz, since some quartz have garnet shapes. BK-3 has more anhedral to subhedral crystals, and BK-2 has some near euhedral crystals.

Pegmatite – BK-4

Cutting the granitoid, it has more feldspar than quartz, which is in turn more abundant than biotite. It has a pegmatitic structure with several centimeters large feldspars and biotite flakes. In thin-section you find regressing garnets, often completely replaced by biotite or quartz. The remaining garnet is very fragmented. However, the thin section is of low quality, since it is difficult to get good thin sections from this kind of pegmatites.

Pressure and temperature – results

Using the data from the electron microprobe, the pressure and temperature yielded with THERMOCALC is presented in Table 1. Since the garnet is homogenized apart from the rims, the center of it is probably closer to the peak metamorphism composition. But since it is hard at best to find the correct corresponding crystal part that the core was in equilibrium with, the rim, that most lately saw chemical exchange, albeit this probably includes later fluids, appears to be the best option. Both the start and the end of the garnet profiles are adjacent to cordierite, so they have a similar immediate environment. The upper left side in figure 8 appears to be the side that differs the most from the core. Therefore the upper left side seems to be the rim most plausibly in chemical contact with its surroundings, and that this garnet was subjected to at least 607 ± 74 °C and 4.8 ± 1.0 kbar, which is the average of the pressure and temperature resulting from the first three points on the upper left side of the garnet profile. The BK-7 garnet appears stable and the lower side of the profile is on the biotite side. Therefore 737 ± 269 °C and 7.7 ± 3.3 kbar is the most plausible result for BK-7.

Sample	Temperature [°C]	Pressure [kbar]	sd T [°C]	sd P [kbar]
BK-10-I	606,67	4,75	74,167	0,9834
BK-10-II	640,5	5,134	78,167	1
BK-10-Center	665	5.4	81	1
BK-7-I	737	7,65	269	3,3

Table 1. BK-10-I is based on the average output of the three first points in the garnet section (Table 4), BK-10-II on the last three and BK-7 on the first two of that garnet profile (Table 5).

Discussion

It has been considered whether the gneiss and similar adjacent rocks are in fact a highly deformed orthogneiss as suggested by Skiöld and Rutland (2005) and Nilsson and Kero (1998). The latter argues that the width of the layers and the texture (Fig. 6) support it being a paragneiss, but concludes the opposite due to a lack of zircon grains older than ~ 1960 Ma (since adjacent true sediment do). This is taken by Nilsson and Kero (1998) to be an expression of the early Jörn GI events. Skiöld and Rutland (2005) takes this gneiss to be an expression of the same event as the granitic veins due to their similar ages yielded by SIMS data, 1944 ± 5 Ma for the granitoid and 1944 ± 4 Ma for the gneiss. But Skiöld and Rutland (2005) do not positively rule out a sedimentary origin.

The metamorphism in the metasediment I judge to be have occurred due to the appearance of the granitic veins at ~1860 Ma. The metamorphism is similar to that in the gneiss (my sample is a xenolith in a vein) and the high temperatures would have overprinted metamorphic traces of the earlier granitoid. However, it is plausible that some deformation

structures are older. There is also a high temperature difference between the samples, even though it is within the margin of error. This could at least partially be explained by retrograde garnet to biotite metamorphism.

The low to intermediate pressures weigh against an island arc accretion model, but this model seems to be increasingly abandoned. The high temperatures do not necessarily add anything to the tectonic discussion.

Conclusions

Bjuröklubb is to be understood in the tectonic context of either a strongly extensional intra-arc basin on mature arc or continental arc crust, or the closing of a back-arc basin. The peninsula is dominated by metasediments that are intruded by tonalitic granitoids. These granitoids are themselves cut by pegmatite and granitic veins. It is noteworthy that there are still some question marks remaining about the origin of some of the rocks, i. e. whether the gneiss is an ortho- or paragneiss.

The deformation, intrusion and metamorphism occurred around 1860 Ma. The garnet element profiles of the two samples are chemically homogenous, which is characteristic of their high temperature environment. The intrusion was subject to temperatures around 737 °C and 7.65 kbar pressures, and the metasediment a few hundred meters away at least 607 °C and 4.75 kbar. The high temperature difference present in the metasediment, is probably partially due to retrograde metamorphism.

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Appendix

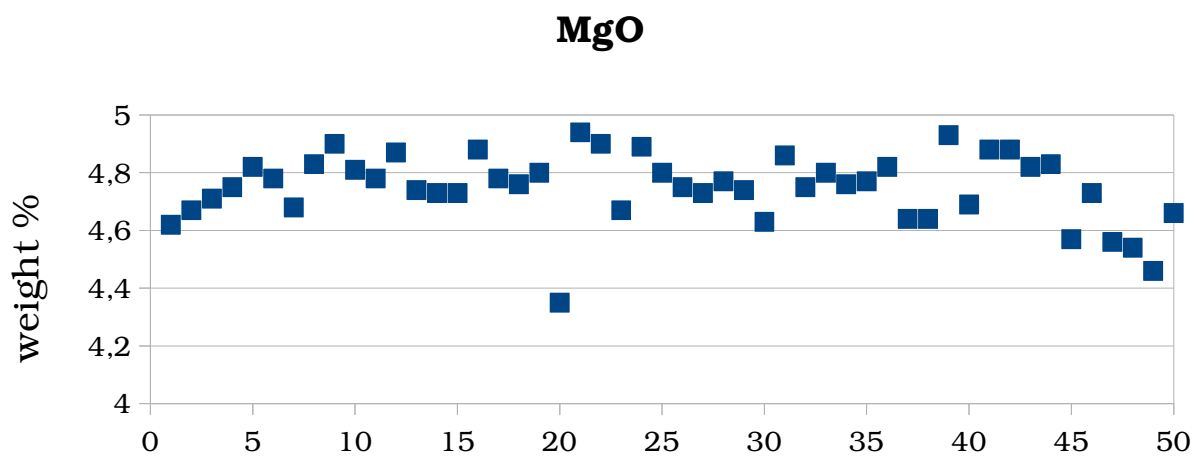
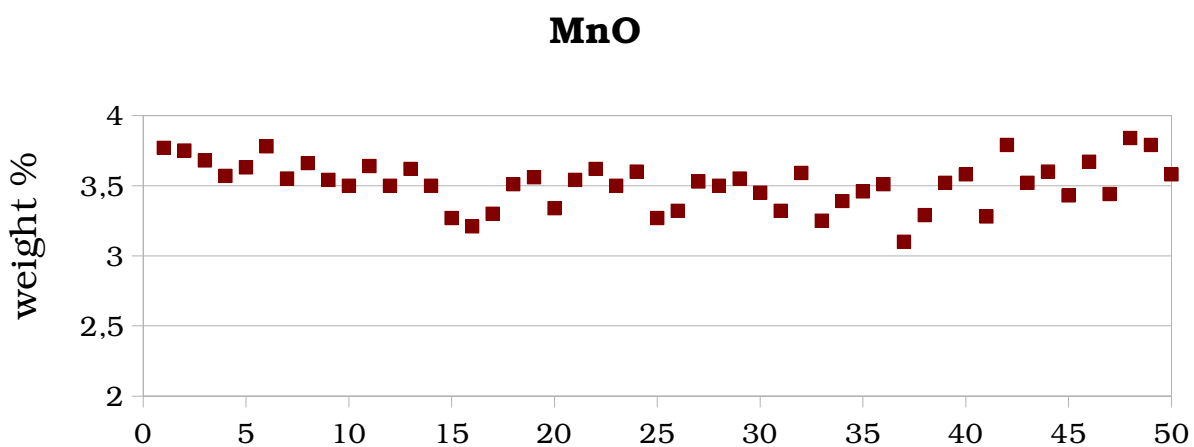
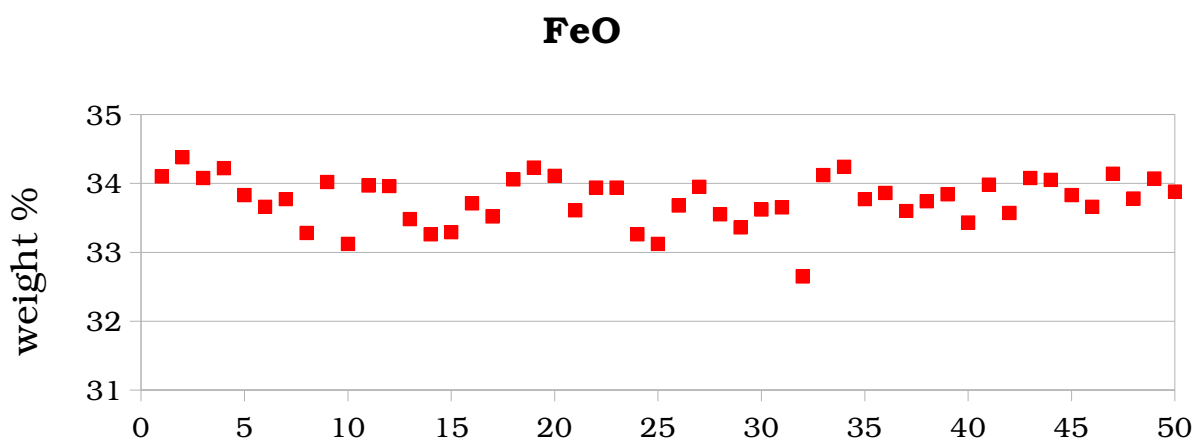


Figure 10. Magnesium in BK-7 garnet profile.



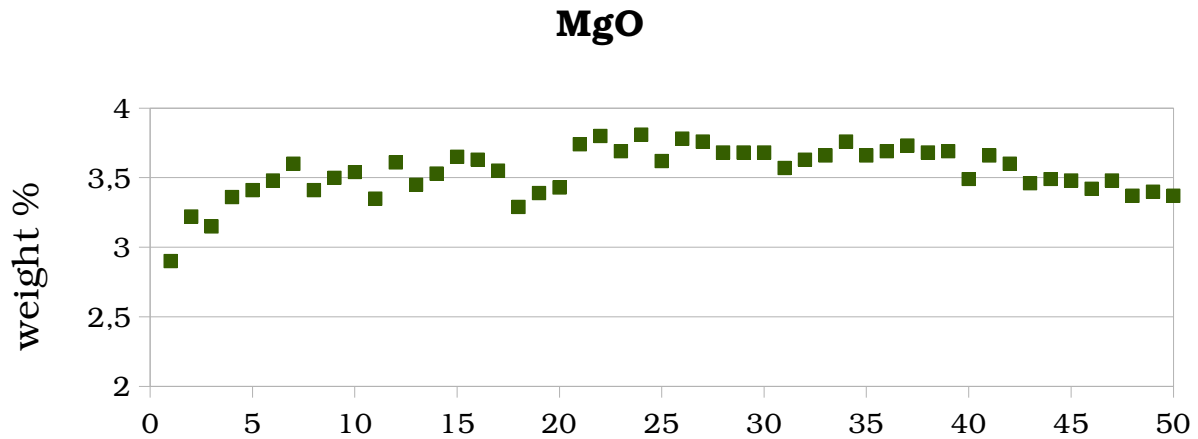


Figure 11. Iron, manganese and magnesium profiles in BK-10 garnet profile.

BK-10											
Datapoint	Al ₂ O ₃	SiO ₂	Na ₂ O	MgO	MnO	K ₂ O	CaO	TiO ₂	Cr ₂ O ₃	FeO	Total
Bt 1	19,74	36,35	0,21	9,31	0,09	9,02	0,04	2,01	0,13	18,82	95,71
Bt 2	19,76	36,33	0,24	9,07	0,02	9,15	0,02	2,00	0,06	19,38	96,02
Bt 3	19,87	35,95	0,17	9,01	0,08	8,80	0,00	2,05	0,05	19,72	95,70
Bt 4	19,89	36,56	0,19	9,26	0,00	8,57	0,03	1,88	0,09	18,74	95,21
Bt 5	19,43	35,96	0,20	9,05	0,00	8,92	0,00	2,35	0,12	19,74	95,77
Cd 1	32,52	49,43	0,14	7,85	0,23	0,03	0,03	0,00	0,00	8,82	99,05
Cd 2	32,00	49,71	0,14	7,94	0,11	0,01	0,00	0,02	0,01	9,25	99,19
Cd 3	32,29	49,55	0,10	7,83	0,37	0,00	0,00	0,00	0,00	8,87	99,01
Cd 4	32,44	49,29	0,11	7,61	0,27	0,00	0,05	0,03	0,00	9,09	98,89
Cd 5	32,51	49,29	0,11	7,95	0,30	0,00	0,00	0,00	0,00	9,21	99,37
Pl 1	24,40	62,45	7,25	0,00	0,01	0,17	6,31	0,00	0,00	0,11	100,71
Pl 2	24,50	62,34	6,90	0,01	0,00	0,10	6,20	0,00	0,00	0,14	100,20
Pl 3	24,62	61,71	6,79	0,00	0,00	0,28	6,42	0,00	0,00	0,11	99,93
Pl 4	24,24	62,46	6,83	0,01	0,19	0,17	6,10	0,03	0,00	0,26	100,28
Pl 5	24,69	62,13	7,04	0,00	0,11	0,14	6,38	0,01	0,01	0,14	100,64

Table 2. Chemical compositions in percent, of various points in BK-10 minerals, see Fig. 10.

BK-7											
Datapoint	Al ₂ O ₃	SiO ₂	Na ₂ O	MgO	MnO	K ₂ O	CaO	TiO ₂	Cr ₂ O ₃	FeO	Total
Biotite 1	16,93	37,01	0,15	11,5	0,09	8,92	0,03	3,44	0	18,15	96,264
Biotite 2	16,71	37,09	0,16	11,2	0,05	8,97	0,09	3,49	0,0087	18,21	95,938
Biotite 3	16,88	36,64	0,19	11,5	0,03	8,45	0	3,72	0,0354	18,1	95,564
Biotite 4	16,7	36,78	0,17	11,3	0	9,07	0,02	3,88	0,0346	17,82	95,788
Biotite 5	16,83	36,94	0,23	11,3	0,13	9,05	0,02	3,67	0	17,71	95,83
Plag 1	26,6	58,59	5,53	0	0	0,09	8,97	0	0	0,184	99,964
Plag 2	26,57	58,59	6	0	0,19	0,1	8,77	0	0,0394	0,185	100,44
Plag 3	26,31	58,96	5,91	0,01	0,02	0,12	8,59	0	0,0405	0,005	99,967
Plag 4	26,16	59,61	6,02	0	0	0,13	8,39	0	0	0,045	100,36
Plag 5	25,56	59,96	6,38	0,01	0,01	0,18	7,39	0	0,0027	0,067	99,555

Table 3. Chemical compositions in percent, of various points in BK-7-minerals, see Fig. 7.

BK-10 garnet profile line											
Datapoint	Al ₂ O ₃	SiO ₂	Na ₂ O	MgO	MnO	K ₂ O	CaO	TiO ₂	Cr ₂ O ₃	FeO	Total
1	20,53	37,92	0,03	2,9	3,77	0	1,13	0,08	0,0096	34,1	100,46
2	20,46	37,31	0,04	3,22	3,75	0	1,04	0	0,0685	34,38	100,27
3	20,49	37,55	0,04	3,15	3,68	0	0,98	0,02	0	34,08	100
4	20,76	37,2	0	3,36	3,57	0	1,03	0,05	0	34,22	100,2
5	20,57	37,85	0	3,41	3,63	0	1,03	0	0	33,83	100,32
6	21	37,84	0,03	3,48	3,78	0	1,08	0,01	0,0477	33,66	100,92
7	20,97	37,27	0,04	3,6	3,55	0,02	1,08	0,01	0,0115	33,77	100,32
8	20,43	37,26	0,03	3,41	3,66	0	1,08	0	0,0093	33,28	99,163
9	20,63	37,37	0,03	3,5	3,54	0,01	1,06	0	0,0471	34,02	100,21
10	20,81	37,71	0	3,54	3,5	0	1,11	0	0,0615	33,12	99,857
11	21,01	37,34	0,05	3,35	3,64	0,01	1,1	0,05	0,0271	33,97	100,54
12	20,95	37,74	0,04	3,61	3,5	0	1,06	0,02	0,01	33,96	100,9
13	21,05	37,83	0,05	3,45	3,62	0	1,05	0,02	0,034	33,48	100,59
14	20,85	37,3	0	3,53	3,5	0	1,08	0,04	0	33,26	99,559
15	20,8	37,71	0,06	3,65	3,27	0,02	1,13	0,03	0,0203	33,29	99,987
16	20,83	37,67	0,01	3,63	3,21	0	1,04	0	0	33,71	100,11
17	21,21	37,24	0,05	3,55	3,3	0	1,09	0,03	0	33,52	99,981
18	20,38	37,83	0,05	3,29	3,51	0	1	0,07	0,0292	34,06	100,22
19	20,85	37,59	0,03	3,39	3,56	0,02	1,1	0,12	0,0179	34,23	100,91
20	20,66	37,74	0,05	3,43	3,34	0	1,09	0	0,003	34,11	100,42
21	20,82	37,82	0,08	3,74	3,54	0	1	0	0,0388	33,61	100,64
22	21,04	38,11	0	3,8	3,62	0,03	1,13	0	0,0025	33,94	101,67
23	20,95	37,77	0,04	3,69	3,5	0,02	1,04	0,03	0,0894	33,94	101,07
24	21,36	38,16	0,03	3,81	3,6	0	1,13	0,03	0,0152	33,26	101,4
25	21	37,6	0,04	3,62	3,27	0	1,05	0,03	0,0108	33,12	99,751
26	21,05	37,72	0,03	3,78	3,32	0	1,09	0	0,0022	33,68	100,67
27	20,82	37,76	0	3,76	3,53	0	1,06	0,04	0,0427	33,95	100,96
28	21,12	37,66	0,06	3,68	3,5	0,02	0,97	0,01	0,0157	33,55	100,59
29	21,14	37,48	0,01	3,68	3,55	0	1,04	0,02	0,0229	33,36	100,31
30	20,97	37,36	0,05	3,68	3,45	0	1,06	0,02	0,0474	33,62	100,26
31	21	37,61	0,05	3,57	3,32	0,02	1,12	0	0,0309	33,65	100,37
32	20,85	37,64	0,04	3,63	3,59	0	1,12	0,06	0	32,65	99,574
33	21,16	37,88	0,05	3,66	3,25	0,02	1,08	0	0,0055	34,12	101,24
34	20,93	37,87	0,04	3,76	3,39	0,01	0,99	0	0	34,24	101,23
35	20,76	37,76	0,03	3,66	3,46	0,03	1,03	0,01	0,0227	33,77	100,53
36	20,85	38,17	0,05	3,69	3,51	0	1,15	0,05	0	33,86	101,34
37	20,94	37,92	0,04	3,73	3,1	0,01	1,08	0,01	0	33,6	100,43
38	20,97	37,94	0,03	3,68	3,29	0,04	1,05	0,04	0,0055	33,74	100,78
39	21,01	38,22	0,02	3,69	3,52	0	1,09	0,03	0,0513	33,84	101,48
40	20,85	37,72	0,04	3,49	3,58	0,02	1,09	0,04	0,0098	33,43	100,27
41	20,96	37,57	0,01	3,66	3,28	0	0,92	0	0,0167	33,98	100,4
42	21,07	37,87	0,07	3,6	3,79	0	1,07	0,05	0,0334	33,57	101,13
43	20,72	37,66	0	3,46	3,52	0	1,07	0,02	0,0204	34,08	100,56
44	21,03	37,53	0,02	3,49	3,6	0,02	1,05	0,01	0,012	34,05	100,81
45	20,97	37,7	0	3,48	3,43	0	1,11	0,03	0,0404	33,83	100,59
46	21,3	37,85	0,03	3,42	3,67	0,03	1,1	0	0,0008	33,66	101,06
47	21,07	37,75	0,01	3,48	3,44	0	1,1	0,02	0,0165	34,14	101,03
48	20,94	37,37	0,07	3,37	3,84	0,01	1,1	0,01	0,0162	33,78	100,5
49	21,15	38,19	0,02	3,4	3,79	0	1,02	0,01	0,0106	34,07	101,66
50	21,2	37,8	0,09	3,37	3,58	0	1,01	0	0	33,88	100,93

Table 4. BK-10 garnet profile chemical compositions in percent (see Fig. 10).

BK-7 garnet profile line											
Datapoint	Al ₂ O ₃	SiO ₂	Na ₂ O	MgO	MnO	K ₂ O	CaO	TiO ₂	Cr ₂ O ₃	FeO	Total
1	21,37	38,21	0,06	4,62	1,18	0,01	2,15	0	0	33,75	101,35
2	21,02	38,77	0,03	4,67	1,24	0,01	2,13	0,07	0,016	33,67	101,63
3	20,42	38,45	0,07	4,71	1,29	0,04	2,04	0	0,002	33,86	100,88
4	21,1	38,71	0,04	4,75	1,2	0,01	2	0	0,0193	33,1	100,92
5	21,28	38,55	0	4,82	1,19	0,01	2,05	0,01	0,0154	33,35	101,28
6	21,38	38,33	0,07	4,78	1,27	0,02	2,01	0,03	0,002	33,17	101,06
7	21,19	38,64	0,01	4,68	1,18	0	1,92	0	0,0565	33,29	100,96
8	20,98	38,07	0,02	4,83	1,26	0,01	2,03	0,01	0,0022	33,48	100,69
9	21,31	38,06	0,01	4,9	0,89	0	2,05	0,01	0	33,29	100,52
10	21,18	38,61	0,03	4,81	1,03	0,01	2	0,02	0,0124	33,67	101,38
11	21	38,08	0,02	4,78	1,13	0,01	2,09	0	0,04	33,97	101,12
12	21,09	38,6	0	4,87	1,21	0	2,1	0,1	0	33,38	101,34
13	21,42	38,71	0,02	4,74	1,05	0,01	2,06	0	0	32,92	100,93
14	21,29	38,73	0,04	4,73	1,02	0,02	2,09	0,02	0,0415	33,34	101,32
15	21,52	38,31	0,03	4,73	1,23	0,01	2,04	0,06	0,0041	33,13	101,07
16	21,31	38,42	0	4,88	1,25	0	1,96	0,02	0,0598	33,62	101,52
17	21,3	38,37	0,03	4,78	1,15	0	2,19	0	0	33,69	101,51
18	21,08	38,35	0,01	4,76	1,25	0,01	2,14	0	0	33,27	100,87
19	21,37	38,48	0,03	4,8	1,11	0,01	2,13	0,09	0,0108	33,54	101,57
20	21,34	38,45	0,01	4,35	0,91	0	2	0,01	0	33,56	100,63
21	21,09	38,46	0,04	4,94	1,27	0,01	2,13	0,02	0,0279	33,68	101,66
22	21,12	37,7	0	4,9	1,13	0,02	2,05	0,03	0	33,7	100,66
23	21,41	38,24	0,02	4,67	0,93	0	2,13	0,02	0	33,59	101,01
24	21,46	38,34	0,05	4,89	1,06	0,01	2,02	0	0	33,44	101,26
25	21,17	38,47	0,04	4,8	1,05	0	2,08	0,03	0,0163	33,45	101,11
26	21,24	38,62	0,03	4,75	1,25	0,02	2	0,01	0	33,44	101,36
27	21,1	38,31	0,02	4,73	1,27	0,01	2,1	0	0,0119	33,96	101,5
28	21,17	38,4	0,02	4,77	1,18	0,01	1,73	0,05	0	33,56	100,9
29	21,14	38,78	0	4,74	1,11	0	2,18	0	0	32,97	100,92
30	21,26	38,39	0,08	4,63	1,23	0	2,01	0,09	0,0342	33,76	101,49
31	21,24	37,97	0,02	4,86	1,21	0,01	2,15	0,02	0,0749	33,2	100,74
32	21,46	38,5	0,02	4,75	1,16	0	2,07	0	0,0019	33,44	101,4
33	21,4	38,47	0,01	4,8	1,12	0	1,94	0	0,0017	33,29	101,04
34	21,3	38,25	0	4,76	1,07	0,02	2	0,06	0,013	33,73	101,2
35	21,37	38,69	0,01	4,77	1,06	0,03	1,99	0	0,008	33,61	101,53
36	21,36	38,41	0,04	4,82	0,88	0,01	1,98	0,02	0	33,73	101,26
37	21,08	38,18	0	4,64	1	0	2,09	0	0,0071	33,83	100,83
38	21,11	38,43	0,03	4,64	1,1	0	2,08	0,05	0	33,97	101,41
39	21,29	38,45	0,03	4,93	1,26	0	2,05	0,01	0	33,86	101,88
40	21,25	38,45	0	4,69	0,99	0	2,22	0,01	0,0323	34,16	101,81
41	21,14	38,5	0,02	4,88	0,96	0,01	2,09	0,03	0,0033	33,67	101,3
42	21,39	38,21	0,01	4,88	0,99	0	1,99	0,05	0,0267	33,63	101,18
43	21,04	38,74	0,02	4,82	1,11	0,02	1,97	0,05	0	34,09	101,86
44	21,61	38,14	0,01	4,83	1,07	0,02	1,98	0	0,0144	33,74	101,42
45	21,36	38,44	0	4,57	1,29	0	2,05	0,02	0,0492	34,19	101,97
46	21,35	38,71	0,04	4,73	1,22	0,01	2,01	0,02	0,0047	33,65	101,74
47	21,32	38,2	0,04	4,56	1,2	0,02	2,01	0	0,0132	33,75	101,11
48	21,04	38,35	0	4,54	0,96	0	1,95	0	0,0168	33,82	100,68
49	20,95	38,19	0,03	4,46	1,09	0,03	2,1	0,02	0,0019	33,56	100,42
50	20,98	38,31	0,03	4,66	1,17	0,01	1,95	0	0	33,37	100,48

Table 5. BK-7 garnet profile chemical compositions in percent (see Fig. 7).

THERMOCALC output texts

See Fig. 8, 9 for datapoint locations.

calcs use:

BK-10. Garnet #1, biotite #1, cordierite #1, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00200	5.00e-5	0.410	0.0420	0.0450	0.0410	0.390	
sd(a)/a	0.68750	0.83491	0.15000	0.37927	0.37362	0.38162	0.11163	
	fcrd	an	mu	q	H2O			
a	0.160	0.470	1.00	1.00	1.00			
sd(a)/a	0.21600	0.08427	0	0				

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + phl + 6an = 2gr + east + 2crd
- 5) gr + alm + mu = ann + 3an

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	2.7	1.98	-37.31	0.51	-0.01345	3.417	5.297	0.880	
2	4.4	1.59	-88.82	1.07	-0.03938	10.388	10.396	2.143	
3	5.4	0.60	99.13	2.27	-0.12941	15.186	-8.134	1.157	
4	3.9	3.97	-69.20	1.39	0.18244	-3.811	-10.970	1.964	
5	5.2	1.01	34.76	1.15	-0.12444	7.391	5.429	0.961	

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 >0.45, 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	4.6	1.0	595	73	0.850	0.79	
	P	sd(P)	T	sd(T)	cor	fit	e* hat
py	4.72	1.47	601	109	0.934	0.79	-0.05 0.74

gr	4.67	0.96	595	73	0.843	0.78	-0.22	0.06
alm	4.63	0.97	597	76	0.766	0.79	0.05	0.23
phl	4.70	0.96	593	73	0.846	0.57	0.84	0.02
ann	4.44	1.06	590	74	0.826	0.75	-0.37	0.30
east	4.73	0.96	605	74	0.851	0.61	-0.93	0.03
crd	4.60	1.01	591	80	0.868	0.79	-0.09	0.07
fcrd	4.60	0.97	581	87	0.790	0.77	0.22	0.46
an	4.65	0.96	595	73	0.848	0.79	0.07	0.01
mu	4.65	0.95	595	73	0.850	0.79	0	0
q	4.65	0.95	595	73	0.850	0.79	0	0

T = 595;C, sd = 73,

P = 4.6 kbars, sd = 1.0, cor = 0.850, sigfit = 0.79

=====

calcs use:

BK-10. Garnet #1, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00200	5.00e-5	0.410	0.0370	0.0520	0.0380	0.390	
sd(a)/a	0.68750	0.83491	0.15000	0.39138	0.35353	0.38888	0.11163	
	fcrd	an	mu	q	H2O			
a	0.160	0.470	1.00	1.00	1.00			
sd(a)/a	0.21600	0.08427		0	0			

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	3.7	1.75	-35.74	0.51	-0.01571	3.486	5.246	0.889
2	4.9	1.41	-85.40	1.07	-0.04379	10.457	10.194	2.147
3	4.0	0.53	105.17	2.27	-0.13719	15.311	-7.844	1.131
4	2.9	1.60	-2.52	1.59	-0.21332	10.746	21.411	2.501
5	4.0	0.89	36.61	1.15	-0.12665	7.403	5.574	0.953

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 >0.45, 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	4.5	0.9	589	72	0.848	0.71		
	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.33	1.42	576	107	0.933	0.71	0.12	0.74
gr	4.52	0.93	589	72	0.842	0.71	-0.17	0.06
alm	4.51	0.95	589	74	0.761	0.71	0.00	0.24
phl	4.54	0.93	587	72	0.845	0.59	0.63	0.02
ann	4.45	1.03	587	73	0.823	0.71	-0.10	0.30
east	4.60	0.93	600	73	0.850	0.45	-1.02	0.03
crd	4.51	0.99	589	78	0.867	0.71	-0.00	0.07
fcrd	4.49	0.94	583	85	0.790	0.71	0.08	0.46
an	4.51	0.93	589	72	0.847	0.71	0.05	0.01
mu	4.51	0.93	589	72	0.848	0.71	0	0
q	4.51	0.93	589	72	0.848	0.71	0	0

T = 589;C, sd = 72,
 P = 4.5 kbars, sd = 0.9, cor = 0.848, sigfit = 0.71

calcs use:

BK-10. Garnet #2, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd		
a	0.00260	3.40e-5	0.400	0.0420	0.0450	0.0410	0.390		
sd(a)/a	0.66950	0.92604	0.15000	0.37927	0.37362	0.38162	0.11163		
	fcrd	an	mu	q	H2O				
a	0.160	0.470	1.00	1.00	1.00				
sd(a)/a	0.21600	0.08427	0	0	0				

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	4.1	1.71	-35.74	0.51	-0.01571	3.486	5.035	0.866	

2	5.3	1.37	-85.40	1.07	-0.04379	10.457	9.609	2.091
3	4.1	0.54	105.17	2.27	-0.13719	15.311	-8.035	1.157
4	2.5	1.66	-2.52	1.59	-0.21332	10.746	22.073	2.596
5	3.7	0.97	36.61	1.15	-0.12665	7.403	5.839	1.041

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 >0.45, 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	4.9	1.0	621	76	0.848	0.85		
	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.83	1.52	615	114	0.934	0.85	0.05	0.75
gr	4.96	0.99	620	76	0.842	0.79	-0.57	0.05
alm	4.89	1.00	623	79	0.762	0.85	0.08	0.23
phl	4.97	0.98	619	76	0.844	0.67	0.81	0.02
ann	4.75	1.09	617	77	0.823	0.82	-0.29	0.30
east	5.00	0.99	632	77	0.849	0.65	-1.01	0.03
crd	4.87	1.04	617	83	0.867	0.85	-0.07	0.07
fcrd	4.90	0.99	615	91	0.785	0.85	0.09	0.47
an	4.92	0.98	621	76	0.846	0.84	0.16	0.00
mu	4.91	0.98	621	76	0.848	0.85	0	0
q	4.91	0.98	621	76	0.848	0.85	0	0

T = 621°C, sd = 76,

P = 4.9 kbars, sd = 1.0, cor = 0.848, sigfit = 0.85

calcs use:

BK-10. Garnet #2, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd		
a	0.00260	3.40e-5	0.400	0.0370	0.0520	0.0380	0.390		
sd(a)/a	0.66950	0.92604	0.15000	0.39138	0.35353	0.38888	0.11163		
	fcrd	an	mu	q	H2O				
a	0.160	0.470	1.00	1.00	1.00				
sd(a)/a	0.21600	0.08427	0	0	0				

Independent set of reactions

- 1) $py + east + 3q = phl + crd$
- 2) $3py + 2mu = phl + east + 2crd$
- 3) $4alm + 2mu + 3q = 2ann + 3fcrd$
- 4) $py + 2gr + 3east + 6q = 3phl + 6an$
- 5) $gr + alm + mu = ann + 3an$

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	4.2	1.72	-35.74	0.51	-0.01571	3.486	4.984	0.875	
2	5.5	1.37	-85.40	1.07	-0.04379	10.457	9.407	2.095	
3	4.0	0.53	105.17	2.27	-0.13719	15.311	-7.746	1.131	
4	2.6	1.68	-2.52	1.59	-0.21332	10.746	21.920	2.622	
5	3.6	0.97	36.61	1.15	-0.12665	7.403	5.984	1.034	

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 >0.45, 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	4.8	1.0	615	75	0.846	0.80			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	4.42	1.47	589	112	0.933	0.78	0.23	0.74	
gr	4.81	0.96	614	75	0.841	0.75	-0.52	0.05	
alm	4.76	0.97	616	78	0.756	0.80	0.03	0.24	
phl	4.80	0.96	613	75	0.843	0.71	0.59	0.02	
ann	4.76	1.06	614	76	0.819	0.80	-0.03	0.30	
east	4.87	0.96	627	76	0.847	0.54	-1.10	0.03	
crd	4.78	1.02	615	82	0.866	0.80	0.01	0.07	
fcrd	4.78	0.97	618	89	0.786	0.80	-0.04	0.46	
an	4.78	0.96	614	75	0.845	0.79	0.14	0.00	
mu	4.77	0.96	615	75	0.846	0.80	0	0	
q	4.77	0.96	615	75	0.846	0.80	0	0	

T = 615°C, sd = 75,

P = 4.8 kbars, sd = 1.0, cor = 0.846, sigfit = 0.80

calcs use:

BK-10. Garnet #3, biotite #1, cordierite #1, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00250	3.50e-5	0.420	0.0420	0.0450	0.0410	0.390	
sd(a)/a	0.67228	0.91713	0.15000	0.37927	0.37362	0.38162	0.11163	

	fcrd	an	mu	q	H2O
a	0.160	0.470	1.00	1.00	1.00
sd(a)/a	0.21600	0.08427	0	0	

Independent set of reactions

- 1) $py + east + 3q = phl + crd$
- 2) $3py + 2mu = phl + east + 2crd$
- 3) $4alm + 2mu + 3q = 2ann + 3fcrd$
- 4) $py + 2gr + 3east + 6q = 3phl + 6an$
- 5) $gr + alm + mu = ann + 3an$

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	1.71	-35.74	0.51	-0.01571	3.486	5.074	0.868
2	5.3	1.38	-85.40	1.07	-0.04379	10.457	9.727	2.099
3	4.2	0.54	105.17	2.27	-0.13719	15.311	-8.230	1.157
4	2.5	1.65	-2.52	1.59	-0.21332	10.746	22.054	2.584
5	3.8	0.97	36.61	1.15	-0.12665	7.403	5.762	1.033

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 >0.45, 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	4.9	1.0	613	75	0.849	0.85

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.85	1.51	610	113	0.934	0.85	0.03	0.75
gr	4.95	0.98	613	75	0.843	0.80	-0.58	0.05
alm	4.88	0.99	616	78	0.764	0.85	0.08	0.23
phl	4.96	0.98	612	75	0.846	0.66	0.83	0.02
ann	4.72	1.08	609	76	0.824	0.82	-0.33	0.30
east	4.99	0.98	624	76	0.850	0.67	-0.99	0.03
crd	4.85	1.04	609	82	0.868	0.85	-0.08	0.07
fcrd	4.88	0.99	606	89	0.787	0.85	0.10	0.47
an	4.91	0.98	613	75	0.848	0.84	0.16	0.00
mu	4.90	0.98	613	75	0.849	0.85	0	0
q	4.90	0.98	613	75	0.849	0.85	0	0

T = 613;C, sd = 75,
P = 4.9 kbars, sd = 1.0, cor = 0.849, sigfit = 0.85

calcs use:

BK-10. Garnet #3, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00250	3.50e-5	0.420	0.0370	0.0520	0.0380	0.390	
sd(a)/a	0.67228	0.91713	0.15000	0.39138	0.35353	0.38888	0.11163	

	ferd	an	mu	q	H2O
a	0.160	0.470	1.00	1.00	1.00
sd(a)/a	0.21600	0.08427	0	0	0

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3ferd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	4.1	1.73	-35.74	0.51	-0.01571	3.486	5.023	0.877
2	5.4	1.38	-85.40	1.07	-0.04379	10.457	9.524	2.103
3	4.1	0.53	105.17	2.27	-0.13719	15.311	-7.941	1.131
4	2.6	1.67	-2.52	1.59	-0.21332	10.746	21.902	2.610
5	3.7	0.96	36.61	1.15	-0.12665	7.403	5.906	1.026

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 >0.45, 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	4.8	1.0	607	74	0.848	0.80

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.45	1.46	584	111	0.933	0.78	0.20	0.74
gr	4.80	0.96	606	74	0.842	0.74	-0.53	0.05

alm	4.75	0.97	608	77	0.758	0.79	0.04	0.24
phl	4.79	0.95	606	74	0.845	0.69	0.61	0.02
ann	4.73	1.06	606	75	0.821	0.79	-0.06	0.30
east	4.86	0.96	619	75	0.849	0.54	-1.08	0.03
crd	4.76	1.01	607	81	0.867	0.80	-0.00	0.07
fcrd	4.77	0.96	609	88	0.788	0.80	-0.03	0.46
an	4.77	0.95	607	74	0.846	0.78	0.15	0.00
mu	4.76	0.95	607	74	0.848	0.80	0	0
q	4.76	0.95	607	74	0.848	0.80	0	0

T = 607°C, sd = 74,

P = 4.8 kbars, sd = 1.0, cor = 0.848, sigfit = 0.80

calcs use:

BK-10. Garnet #48, biotite #1, cordierite #1, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00330	4.60e-5	0.380	0.0420	0.0450	0.0410	0.390	
sd(a)/a	0.65196	0.83666	0.15000	0.37927	0.37362	0.38162	0.11163	
	fcrd	an	mu	q	H2O			
a	0.160	0.470	1.00	1.00	1.00			
sd(a)/a	0.21600	0.08427	0	0	0			

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	1.68	-35.74	0.51	-0.01571	3.486	4.796	0.853
2	5.8	1.34	-85.40	1.07	-0.04379	10.457	8.894	2.041
3	4.0	0.54	105.17	2.27	-0.13719	15.311	-7.830	1.157
4	3.1	1.58	-2.52	1.59	-0.21332	10.746	21.230	2.467
5	4.0	0.90	36.61	1.15	-0.12665	7.403	5.588	0.962

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 >0.45, 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	5.2	1.0	647	80	0.849	0.80		
	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.03	1.57	634	119	0.935	0.80	0.11	0.75
gr	5.24	1.01	647	80	0.842	0.79	-0.30	0.06
alm	5.21	1.02	648	82	0.765	0.80	0.03	0.23
phl	5.27	1.01	646	80	0.846	0.65	0.73	0.02
ann	5.12	1.11	645	80	0.823	0.79	-0.17	0.30
east	5.31	1.01	660	80	0.850	0.54	-1.11	0.03
crd	5.20	1.07	646	87	0.868	0.80	-0.03	0.07
fcrd	5.19	1.02	641	94	0.791	0.80	0.09	0.46
an	5.22	1.01	647	80	0.847	0.80	0.09	0.01
mu	5.21	1.01	647	80	0.849	0.80	0	0
q	5.21	1.01	647	80	0.849	0.80	0	0

T = 647;C, sd = 80,
 P = 5.2 kbars, sd = 1.0, cor = 0.849, sigfit = 0.80

calcs use:

BK-10. Garnet #48, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd		
a	0.00330	4.60e-5	0.380	0.0370	0.0520	0.0380	0.390		
sd(a)/a	0.65196	0.83666	0.15000	0.39138	0.35353	0.38888	0.11163		
	fcrd	an	mu	q	H2O				
a	0.160	0.470	1.00	1.00	1.00				
sd(a)/a	0.21600	0.08427	0	0	0				

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	4.7	1.70	-35.74	0.51	-0.01571	3.486	4.746	0.861	
2	5.9	1.34	-85.40	1.07	-0.04379	10.457	8.691	2.044	
3	3.9	0.53	105.17	2.27	-0.13719	15.311	-7.540	1.131	

4	3.2	1.60	-2.52	1.59	-0.21332	10.746	21.077	2.494
5	3.8	0.90	36.61	1.15	-0.12665	7.403	5.733	0.955

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 >0.45, 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	5.1	1.0	641	78	0.848	0.79		
	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.62	1.52	607	117	0.934	0.76	0.28	0.74
gr	5.09	0.99	641	78	0.841	0.78	-0.25	0.06
alm	5.07	1.00	640	81	0.760	0.79	-0.02	0.24
phl	5.10	0.98	640	78	0.845	0.72	0.50	0.02
ann	5.12	1.09	642	79	0.820	0.79	0.09	0.30
east	5.17	0.99	654	79	0.849	0.46	-1.20	0.03
crd	5.10	1.05	644	85	0.868	0.79	0.06	0.07
fcrd	5.08	1.00	644	93	0.791	0.79	-0.04	0.46
an	5.07	0.98	641	78	0.846	0.79	0.07	0.01
mu	5.07	0.98	641	78	0.848	0.79	0	0
q	5.07	0.98	641	78	0.848	0.79	0	0

T = 641;C, sd = 78,

P = 5.1 kbars, sd = 1.0, cor = 0.848, sigfit = 0.79

calcs use:

BK-10. Garnet #49, biotite #1, cordierite #1, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd		
a	0.00320	3.90e-5	0.400	0.0420	0.0450	0.0410	0.390		
sd(a)/a	0.65429	0.83999	0.15000	0.37927	0.37362	0.38162	0.11163		
	fcrd	an	mu	q	H2O				
a	0.160	0.470	1.00	1.00	1.00				
sd(a)/a	0.21600	0.08427		0	0				

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd

- 3) $4alm + 2mu + 3q = 2ann + 3fcrd$
- 4) $py + 2gr + 3east + 6q = 3phl + 6an$
- 5) $gr + alm + mu = ann + 3an$

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	4.5	1.68	-35.74	0.51	-0.01571	3.486	4.827	0.854	
2	5.7	1.34	-85.40	1.07	-0.04379	10.457	8.986	2.047	
3	4.1	0.54	105.17	2.27	-0.13719	15.311	-8.035	1.157	
4	2.8	1.58	-2.52	1.59	-0.21332	10.746	21.591	2.472	
5	3.9	0.91	36.61	1.15	-0.12665	7.403	5.702	0.965	

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 >0.45, 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	5.2	1.0	641	79	0.850	0.84			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	5.01	1.56	628	118	0.935	0.83	0.11	0.75	
gr	5.23	1.01	640	79	0.843	0.79	-0.50	0.06	
alm	5.17	1.02	643	81	0.766	0.84	0.06	0.23	
phl	5.25	1.01	639	79	0.846	0.68	0.76	0.02	
ann	5.07	1.11	638	79	0.824	0.82	-0.22	0.30	
east	5.28	1.01	652	80	0.851	0.60	-1.08	0.03	
crd	5.16	1.07	638	86	0.869	0.84	-0.05	0.07	
fcrd	5.18	1.02	636	93	0.792	0.84	0.06	0.46	
an	5.20	1.01	640	79	0.848	0.83	0.15	0.01	
mu	5.19	1.00	641	79	0.850	0.84	0	0	
q	5.19	1.00	641	79	0.850	0.84	0	0	

T = 641;C, sd = 79,

P = 5.2 kbars, sd = 1.0, cor = 0.850, sigfit = 0.84

calcs use:

BK-10. Garnet #49, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00320	3.90e-5	0.400	0.0370	0.0520	0.0380	0.390	
sd(a)/a	0.65429	0.83999	0.15000	0.39138	0.35353	0.38888	0.11163	

	fcrd	an	mu	q	H2O
a	0.160	0.470	1.00	1.00	1.00
sd(a)/a	0.21600	0.08427	0	0	

Independent set of reactions

- 1) $py + east + 3q = phl + crd$
- 2) $3py + 2mu = phl + east + 2crd$
- 3) $4alm + 2mu + 3q = 2ann + 3fcrd$
- 4) $py + 2gr + 3east + 6q = 3phl + 6an$
- 5) $gr + alm + mu = ann + 3an$

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	4.6	1.70	-35.74	0.51	-0.01571	3.486	4.776	0.863	
2	5.9	1.35	-85.40	1.07	-0.04379	10.457	8.784	2.051	
3	4.0	0.53	105.17	2.27	-0.13719	15.311	-7.746	1.131	
4	2.9	1.60	-2.52	1.59	-0.21332	10.746	21.438	2.499	
5	3.7	0.90	36.61	1.15	-0.12665	7.403	5.847	0.958	

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 >0.45, 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	5.0	1.0	634	77	0.848	0.81

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.60	1.51	601	116	0.934	0.78	0.28	0.74
gr	5.08	0.98	633	77	0.842	0.78	-0.45	0.06
alm	5.04	0.99	635	80	0.761	0.81	0.01	0.24
phl	5.07	0.98	633	77	0.846	0.74	0.54	0.02
ann	5.07	1.08	635	78	0.821	0.81	0.05	0.30
east	5.15	0.98	647	78	0.849	0.51	-1.17	0.03
crd	5.07	1.04	636	84	0.868	0.81	0.04	0.07
fcrd	5.06	0.99	640	92	0.792	0.81	-0.08	0.46
an	5.05	0.98	634	77	0.847	0.80	0.13	0.01
mu	5.04	0.98	634	77	0.848	0.81	0	0
q	5.04	0.98	634	77	0.848	0.81	0	0

T = 634;C, sd = 77,

P = 5.0 kbars, sd = 1.0, cor = 0.848, sigfit = 0.81

calcs use:

BK-10. Garnet #50, biotite #1, cordierite #1, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00320	3.90e-5	0.410	0.0420	0.0450	0.0410	0.390	
sd(a)/a	0.65429	0.83999	0.15000	0.37927	0.37362	0.38162	0.11163	

	fcrd	an	mu	q	H2O
a	0.160	0.470	1.00	1.00	1.00
sd(a)/a	0.21600	0.08427	0	0	0

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	4.5	1.68	-35.74	0.51	-0.01571	3.486	4.827	0.854
2	5.7	1.34	-85.40	1.07	-0.04379	10.457	8.986	2.047
3	4.2	0.54	105.17	2.27	-0.13719	15.311	-8.134	1.157
4	2.8	1.58	-2.52	1.59	-0.21332	10.746	21.591	2.472
5	3.9	0.91	36.61	1.15	-0.12665	7.403	5.677	0.965

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 >0.45, 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	5.2	1.0	639	78	0.850	0.84

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.04	1.56	626	117	0.935	0.84	0.10	0.75
gr	5.25	1.01	638	78	0.844	0.79	-0.52	0.06
alm	5.19	1.02	641	81	0.767	0.84	0.07	0.23
phl	5.26	1.01	637	78	0.847	0.68	0.77	0.02

ann	5.08	1.11	635	79	0.825	0.83	-0.23	0.30
east	5.30	1.01	650	79	0.851	0.61	-1.07	0.03
crd	5.17	1.07	636	85	0.869	0.84	-0.05	0.07
fcrd	5.19	1.02	635	93	0.793	0.84	0.06	0.46
an	5.22	1.01	638	78	0.849	0.83	0.16	0.01
mu	5.21	1.00	639	78	0.850	0.84	0	0
q	5.21	1.00	639	78	0.850	0.84	0	0

T = 639;C, sd = 78,
P = 5.2 kbars, sd = 1.0, cor = 0.850, sigfit = 0.84

calcs use:

BK-10. Garnet #50, biotite #1, cordierite #5, feldspar #1. Assumed P/T in AX: 650 C, 4.5 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	crd	
a	0.00320	3.90e-5	0.410	0.0370	0.0520	0.0380	0.390	
sd(a)/a	0.65429	0.83999	0.15000	0.39138	0.35353	0.38888	0.11163	
	fcrd	an	mu	q	H2O			
a	0.160	0.470	1.00	1.00	1.00			
sd(a)/a	0.21600	0.08427	0	0	0			

Independent set of reactions

- 1) py + east + 3q = phl + crd
- 2) 3py + 2mu = phl + east + 2crd
- 3) 4alm + 2mu + 3q = 2ann + 3fcrd
- 4) py + 2gr + 3east + 6q = 3phl + 6an
- 5) gr + alm + mu = ann + 3an

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	1.70	-35.74	0.51	-0.01571	3.486	4.776	0.863
2	5.9	1.35	-85.40	1.07	-0.04379	10.457	8.784	2.051
3	4.0	0.53	105.17	2.27	-0.13719	15.311	-7.844	1.131
4	2.9	1.60	-2.52	1.59	-0.21332	10.746	21.438	2.499
5	3.8	0.90	36.61	1.15	-0.12665	7.403	5.822	0.958

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 >0.45, 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	5.1	1.0	632	77	0.849	0.81			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	4.63	1.51	600	115	0.934	0.79	0.27	0.74	
gr	5.10	0.98	631	77	0.842	0.78	-0.47	0.06	
alm	5.06	0.99	633	80	0.762	0.81	0.02	0.24	
phl	5.09	0.98	631	77	0.846	0.74	0.54	0.02	
ann	5.08	1.08	633	78	0.822	0.81	0.04	0.30	
east	5.16	0.98	645	78	0.850	0.52	-1.16	0.03	
crd	5.08	1.04	634	84	0.869	0.81	0.03	0.07	
fcrd	5.08	0.99	638	92	0.794	0.81	-0.08	0.46	
an	5.07	0.98	632	77	0.847	0.80	0.14	0.01	
mu	5.06	0.98	632	77	0.849	0.81	0	0	
q	5.06	0.98	632	77	0.849	0.81	0	0	

T = 632;C, sd = 77,
P = 5.1 kbars, sd = 1.0, cor = 0.849, sigfit = 0.81

calcs use:

BK-7. Garnet #1, biotite #1, feldspar #1. Assumed P/T in AX: 700 C, 8 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an		
a	0.00840	0.000370	0.360	0.0590	0.0410	0.0380	0.650		
sd(a)/a	0.57129	0.77542	0.15000	0.34392	0.38633	0.38888	0.05000		
	mu	q	H2O						
a	1.00	1.00	1.00						
sd(a)/a	0	0							

Independent set of reactions

- 1) py + gr + mu = phl + 3an
- 2) py + 2gr + 3east + 6q = 3phl + 6an
- 3) gr + alm + mu = ann + 3an

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	6.6	1.13	-9.22	0.70	-0.11124	7.058	8.559	1.034	
2	4.7	1.66	-3.25	1.59	-0.21160	10.635	19.319	2.291	
3	6.2	0.94	35.30	1.15	-0.12470	7.349	4.437	0.892	

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	7.7	3.3	741	272	0.857	1.77			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	6.86	5.37	673	433	0.946	1.73	0.20	0.62	
gr	8.70	3.61	740	244	0.709	1.59	-0.50	0.71	
alm	7.73	3.38	744	285	0.854	1.77	0.04	0.05	
phl	8.61	2.95	826	247	0.883	1.42	0.75	0.14	
ann	7.84	3.57	763	348	0.849	1.76	-0.10	0.34	
east	7.09	1.94	713	155	0.857	1.00	-1.49	0.07	
an	7.75	3.36	741	270	0.848	1.76	0.10	0.03	
mu	7.71	3.34	741	272	0.857	1.77	0	0	
q	7.71	3.34	741	272	0.857	1.77	0	0	

T = 741;C, sd = 272,
 P = 7.7 kbars, sd = 3.3, cor = 0.857, sigfit = 1.77
 =====

calcs use:
 BK-7. Garnet #1, biotite #3, feldspar #1. Assumed P/T in AX: 700 C, 8 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an	
a	0.00840	0.000370	0.360	0.0560	0.0390	0.0380	0.650	
sd(a)/a	0.57129	0.77542	0.15000	0.34963	0.39308	0.38888	0.05000	
	mu	q	H2O					
a	1.00	1.00	1.00					
sd(a)/a	0	0						

- Independent set of reactions
- 1) py + gr + mu = phl + 3an
 - 2) py + 2gr + 3east + 6q = 3phl + 6an
 - 3) gr + alm + mu = ann + 3an

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	6.6	1.13	-9.22	0.70	-0.11124	7.058	8.507	1.036	
2	4.8	1.67	-3.25	1.59	-0.21160	10.635	19.162	2.298	

3 6.3 0.95 35.30 1.15 -0.12470 7.349 4.387 0.895

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	7.8	3.2	742	264	0.859	1.71			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	6.95	5.22	677	420	0.947	1.67	1.67	0.20	0.62
gr	8.72	3.50	741	237	0.711	1.53	-0.48	0.71	
alm	7.78	3.28	745	277	0.855	1.70	0.04	0.05	
phl	8.65	2.86	826	239	0.884	1.37	0.74	0.14	
ann	7.90	3.48	764	340	0.851	1.70	-0.10	0.35	
east	7.15	1.95	714	156	0.859	0.97	-1.43	0.07	
an	7.81	3.27	742	263	0.850	1.70	0.09	0.03	
mu	7.76	3.25	742	264	0.859	1.71	0	0	
q	7.76	3.25	742	264	0.859	1.71	0	0	

T = 742;C, sd = 264,

P = 7.8 kbars, sd = 3.2, cor = 0.859, sigfit = 1.71

calcs use:

BK-7. Garnet #2, biotite #1, feldspar #1. Assumed P/T in AX: 700 C, 8 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an			
a	0.00810	0.000380	0.360	0.0590	0.0410	0.0380	0.650			
sd(a)/a	0.57481	0.77434	0.15000	0.34392	0.38633	0.38888	0.05000			
	mu	q	H2O							
a	1.00	1.00	1.00							
sd(a)/a	0	0								

Independent set of reactions

- 1) py + gr + mu = phl + 3an
- 2) py + 2gr + 3east + 6q = 3phl + 6an
- 3) gr + alm + mu = ann + 3an

Calculations for the independent set of reactions

(for $x(\text{H}_2\text{O}) = 1.0$)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)	
1	6.5	1.13	-9.22	0.70	-0.11124	7.058	8.569	1.035	
2	4.7	1.66	-3.25	1.59	-0.21160	10.635	19.302	2.290	
3	6.3	0.94	35.30	1.15	-0.12470	7.349	4.410	0.891	

Average PT (for $x(\text{H}_2\text{O}) = 1.0$)

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	7.6	3.3	733	266	0.857	1.75			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	6.81	5.28	666	424	0.947	1.72	0.20	0.62	
gr	8.61	3.55	733	239	0.709	1.57	-0.50	0.71	
alm	7.66	3.32	737	278	0.853	1.75	0.04	0.05	
phl	8.52	2.90	816	242	0.883	1.41	0.75	0.14	
ann	7.77	3.50	755	340	0.849	1.74	-0.10	0.34	
east	7.04	1.92	706	153	0.857	0.99	-1.47	0.07	
an	7.69	3.30	733	265	0.848	1.74	0.10	0.03	
mu	7.64	3.28	733	266	0.857	1.75	0	0	
q	7.64	3.28	733	266	0.857	1.75	0	0	

T = 733;C, sd = 266,

P = 7.6 kbars, sd = 3.3, cor = 0.857, sigfit = 1.75

calcs use: BK-7. Garnet #2, biotite #3, feldspar #1. Assumed P/T in AX: 700 C, 8 kbar.

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an		
a	0.00810	0.000380	0.360	0.0560	0.0390	0.0380	0.650		
sd(a)/a	0.57481	0.77434	0.15000	0.34963	0.39308	0.38888	0.05000		
	mu	q	H2O						
a	1.00	1.00	1.00						
sd(a)/a	0	0							

Independent set of reactions

1) 3east + 6q = py + phl + 2mu

2) py + gr + mu = phl + 3an

3) $gr + alm + mu = ann + 3an$

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	12.0	2.99	15.19	1.23	0.01088	-3.482	2.112	1.347	
2	6.6	1.13	-9.22	0.70	-0.11124	7.058	8.516	1.037	
3	6.3	0.95	35.30	1.15	-0.12470	7.349	4.360	0.894	

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	7.7	3.2	734	259	0.859	1.69			
	P	sd(P)	T	sd(T)	cor	fit	e*	hat	
py	6.89	5.12	670	412	0.947	1.66	0.19	0.62	
gr	8.63	3.44	734	232	0.711	1.52	-0.48	0.71	
alm	7.72	3.22	738	271	0.855	1.69	0.04	0.05	
phl	8.56	2.80	816	234	0.884	1.35	0.73	0.14	
ann	7.83	3.41	756	332	0.850	1.68	-0.10	0.34	
east	7.10	1.94	707	154	0.859	0.96	-1.42	0.07	
an	7.74	3.21	734	258	0.850	1.68	0.09	0.03	
mu	7.70	3.19	734	259	0.859	1.69	0	0	
q	7.70	3.19	734	259	0.859	1.69	0	0	

T = 734;C, sd = 259,

P = 7.7 kbars, sd = 3.2, cor = 0.859, sigfit = 1.69

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