

Phase Equilibria Modeling of Metapelitic Hornfelses Using Pseudosections; Implications for Contact Metamorphism

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Abstract

The Dorbeh contact aureole, located south of Urmia, NW Iran, comprises hornfelses, calc-silicate rocks, and calcite dolomite marbles. The metapelites consist of garnet + cordierite + sillimanite + biotite + chlorite + ilmenite ± andalusite ± chloritoid ± spinel ± quartz. Two significant mineral parageneses are recognized in the rocks. One of them is a low-grade paragenesis, which includes chlorite and chloritoid, without alumino-silicates or cordierite (P1). The second one is chloritoid- and chlorine-free and andalusite/sillimanite- and cordierite-bearing (P2). The most important feature of the Dorbeh contact aureole is the presence of characteristic reaction textures in the pelitic hornfelses, formed due to their especially low silica whole rock chemistry, along with the scarcity of staurolite, which is predicted by models. According to the pressure-temperature (P-T), pressure-chemical composition (P-X), and temperature-chemical composition (T-X) pseudosections on several metapelitic samples, including both spinel present (quartz absent), and quartz present (spinel absent) samples, a pressure of ~3.2 kbar and temperature of ~700 °C are estimated for the observed peak equilibria including garnet + cordierite + sillimanite ± spinel ± quartz. In addition, low-grade paragenesis was formed in low-grade zones at an estimated pressure of ~2.5 kbar and temperature of ~450 °C. Residual chlorite and chloritoid at the high temperature conditions, in addition to the lack of staurolite, are signatures of a high degree of overstepping during the prograde metamorphism. The rapid variations in metamorphic conditions caused the incomplete reactions and unstable presence of such low temperature phases in the peak conditions.

Keywords: Metapelitic Hornfelses; Microstructures; Phase Equilibria Modeling; Pseudosections; Dorbeh.

Introduction

The thermodynamic conditions of formation and textural relationships of spinel are studied due to its low abundance and its diagnostic presence in metamorphic terrains (1, 2). The occurrence of this mineral has been reported in a wide range of igneous and metamorphic rocks even in ultramafic rocks (3, 4). It is also relatively

common phase in low silica metapelites (5-7). Spinel is common mineral in metapelites (with or without quartz), and is well known from granulite-facies low silica metapelites under low-pressure/high-temperature conditions (8). Also, it may also occur in the upper amphibolite facies under appropriate bulk-composition or even in contact metamorphism (9). Numerous reactions based on field evidence and experimental

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studies have been proposed for the formation of spinel under progressive metamorphism, often involving sillimanite and a ferromagnesian reactant such as cordierite, garnet, or staurolite. For the occurrence of gahnite (zinc-rich spinel), the breakdown of sphalerite, or zinc-bearing staurolite has also been suggested. These reactions have been proposed in parageneses with or without muscovite + quartz (10). The presence of muscovite and quartz constrains the spinel-forming reactions and limits the stability of spinel in the paragenesis.

In this study, an effort has been made to closely examine the phase equilibria, along with potential compositional changes and reactions involved in the stability of spinel and/or quartz in parageneses of pelitic systems and their thermodynamic conditions, within a contact aureole where the pressure and composition of the protolith were almost constant, and the main variable was temperature. Phase relationships (11) such as phase stability field and reaction textures, determination of the protolith's sedimentary provenance (12), quantitative textural studies on the crystal size distribution (CSD) and spatial distribution pattern (SDP) of garnet porphyroblasts in this aureole and mineral chemistry (13) of these hornfelses have already been investigated.

Geological Setting

The contact aureole of Dorbeh in south of Urmia (Figure 1a), north of Oshnavieh, at a longitude of 45° 9' 10" and latitude of 37° 8' 9", is formed in the Sanandaj–Sirjan structural zone of Iran. It is formed around the dioritic-gabbroic stock of Dorbeh (Figure 1b). The diorite is one of the bodies known as the Urmia Plutonic Complex (UPC), which, along with granites and alkali syenite/granites, extends in the northwest end of the Sanandaj–Sirjan zone south of Urmia.

The exposed intrusions, such as Dorbeh (13, 14), Bonar Valley near Gysian Silvana (15), Zharabad granite/syenite, and Sosanabad alkali granite in Silvana, were most likely the result of partial mantle melting with significant crustal interaction in the northern Urmia-Dokhtar magmatic arc (16, 17). They formed during the Neo-Tethys subduction beneath Eurasia in the Late Cretaceous.

The ascent of these high-temperature dioritic-gabbroic plutons led to the formation of metamorphic aureoles in contact with the country rocks. These diorites are mostly intruded within the Dorud and Ruteh formations' shales and carbonates ranging in age from the Permian to the Triassic (Figure 1b). The intrusions caused contact aureoles, and produced hornfelses, and calc-silicates, occasionally forming skarns in the area (11), all were covered by Miocene units (18).

The important exposed units in the northwest of the area are ophiolitic units and a mélange resulting from the Neo-Tethyan subduction (19). These fragments in the Silvana to Oshnavieh can be compared to the ophiolites from the Iraqi Zagros in northeastern Iraq, and the southeastern Anatolia, which all of them formed along the main Neo-Tethyan suture developed in the Late Cretaceous (3). K-Ar age dating on amphibole minerals indicates an age of approximately 93 to 100 Ma for this intrusion (14), which confirms its relation to the Neo-Tethyan subduction in the Late Cretaceous. The Dorbeh stock, with an approximate length of 12 km and a width of 2 to 3 km, has a mineralogical composition similar to other gabbros and diorites in the region, such as Darreh-Bonar and Parvaneh (13, 17), and includes plagioclase, amphibole, diopside, alkali feldspar, and less quartz. In terms of petrological diversity, a small amount of quartz monzodiorite-gabbrodiorite is observed alongside a high volume of diorite in the area (Figure 1a), which intruded pelitic and carbonate rocks. It is necessary to estimate the metamorphic conditions in each contact aureole, such as Dorbeh, depending on local protolith diversity or heat distribution mechanisms.

Materials and Methods

P-T conditions for Dorbeh metamorphic stages were estimated from mineral compositions of four samples with different assemblages and more abundance using multi-equilibrium calculations and pseudosection modeling. Pseudosections were calculated with Geo-Pseudosection 3 v.3.6.3.972 (20) in the NCKFMASH+Mn system ($\text{Na}_2\text{O}-\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2-\text{K}_2\text{O}-\text{CaO}-\text{FeO}-\text{MnO}-\text{H}_2\text{O}$). The effective bulk composition used for the samples is reported on top of the P-T grids. In the modeling, H_2O was specified as a pure fluid component, meaning that the calculated stability fields correspond to fluid-saturated conditions imposed by this assumption. Solid-solution models follow the formulations of 21 for most phases, with amphibole and melt activity-composition relations are taken from 22. Four samples (D-2023-01 to -04; Table 1) were analyzed for microstructural features and employed in phase-equilibria modeling.

Results

Petrography and Microstructures

The studied metapelitic hornfelses are dark at mesoscopic scale with a notable presence of large garnet porphyroblasts (> 1 cm in diameter; ~20-50 modal %), which are clearly discernible in virtual slide scan images (whole slide imaging; WSI; Supplementary Figures 1, 2).

Table 1. Summary of petrographic observations in Dorbeh area.

Rock type	Sample No.	Amp	Pl	Cpx	Qz	Ttn	Ore M.					
Dorbeh intrusive body (Gabbro-Diorite)	E12	xxx	xxx	x	x	x	x					
	E61	xx	xx	xxx	x	o	x					
	E13	xxx	xxx	xx	o	x	x					
	E17	xx	xx	x	x	o	x					
	E12	xxx	xxx	xx	o	x	x					
		Cld	Chl	Pl	Bt	Grt	Spl	Qz	Ilm	Crd	And	Sil
Contact aureole metamorphic rocks (Hornfelse)	D-2023-04	x	x	x	x	xxx	x	o	x	o	xx	x
	D-2023-02	o	x	o	xxx	xxx	xx	x	xx	xx	o	o
	D-2023-03	x	xx	x	x	o	xx	x	xx	x	x	xxx
	E33	o	xx	o	o	xxx	xx	o	x	xx	o	xxx
	D-2023-01	x	x	o	x	xxx	xx	o	x	o	o	o
	E20	o	x	x	o	xx	o	x	x	xx	x	xxx
	E18	x	x	x	x	xx	o	xx	o	xx	o	o
	E14	x	o	x	x	xx	o	x	o	xx	o	o
	E11	x	o	x	o	xx	xx	o	x	xx	xx	xx

Symbols are: x: rare; xx: common; xxx: abundant, o: absent.

Mineral phase abbreviations are: Amp: amphibole; Pl: plagioclase; Cpx: clinopyroxene; Qz: quartz; Ttn: titanite; Ore M.: opaque minerals; Cld: chloritoid; Chl: chlorite; Bt: biotite; Grt: garnet; Spl: spinel; Ilm: ilmenite; Crd: cordierite; And: andalusite; Sil: sillimanite according to the Whitney and Evans (2010).

Additionally, these rocks contain cordierite, sillimanite, biotite, chlorite, andalusite, chloritoid, plagioclase, and minor amounts of spinel and/or quartz (Figure 2). Opaque minerals, mostly ilmenite and graphite, are also observed in smaller amounts in these rocks, too. They fall into two groups: spinel-present/quartz-absent, and quartz-present/spinel-absent. The modeling and all the investigation are based on the above category.

Two distinct parageneses were identified in the metapelites are including: a low-grade assemblage (P1) and a peak-grade assemblage (P2). P1 is composed of chlorite (Chl) $\pm$ muscovite (Ms) + biotite (Bt) + chloritoid (Cld) + garnet (Grt) + quartz (Qz) $\pm$ plagioclase (Pl). P2 consists of biotite + garnet + ilmenite (Ilm) + sillimanite (Sil)/andalusite (And) $\pm$ cordierite (Crd) $\pm$ spinel (Spl) $\pm$ quartz $\pm$ plagioclase. Overall, P1 represents the low-grade stage, in which chlorite and chloritoid are present, whereas P2 corresponds to the peak-grade stage, where these phases are consumed and replaced by aluminosilicates, cordierite, and spinel.

Some fine rectangular chloritoid crystals preserved as metastable phases, occur together with andalusite, and biotite in the rock matrix (Figure 2a, b). Ore minerals and spinel are abundant and can be seen either as inclusions in garnet, cordierite (Figure 2c-f), and aluminosilicates or as individual crystals within the rock matrix (Figure 2g, h). In some samples, quartz is present only in very minor amounts. Green spinels (hercynite) are not observed in contact with quartz. Porphyroblasts exhibit a high growth rate during progressive metamorphism; and enclosed spinel before its complete consumption and, like a shield, effectively isolating it from the surrounding matrix quartz.

Fibrous sillimanite crystals (fibrolites) are seen in association with cordierite, and andalusite crystals mostly around garnet crystals (Figure 2c, d). The observed paragenetic assemblages, along with the lack of staurolite, generate diagnostic reaction textures for interpreting the metamorphic processes.

A previous mineral chemistry study determined that chlorites in Dorbeh pelitic hornfelses are ripidolite and brunsvigite, chloritoids are Fe-rich, garnets are almandine, spinels are hercynite, and finally ore phase is mostly ilmenite, all of them are in association with a considerable number of aluminosilicates, including andalusite or sillimanite (13).

Petrographic and microscopic studies show no evidence of retrogressive reaction textures, such as symplectites or coronas, in these rocks. Multiple parageneses have been identified in this aureole, included (Table 1): Cld + Chl; Cld + And; Grt + Cld; And + Grt; Spl + Grt; And + Sil; Grt + And + Sil; Crd + Sil; Grt + And + Sil + Qz; Grt + Crd + Sil + Spl. Plagioclase, quartz, H₂O, and biotite and ilmenite are present as excess phases. The reactions responsible for the formation of these phases as well as the corresponding compatibility diagrams have been discussed in detail elsewhere (11). The peak paragenesis in the Dorbeh aureole consists of garnet (Grt) + biotite (Bt) + cordierite (Crd) + sillimanite (Sil) + ilmenite (Ilm) $\pm$ spinel (Spl) $\pm$ quartz (Qz), comparable to the assemblages reported from aluminous granulites, metapelites in western Brazil (23), and the Kandalur belt in southern India (24).

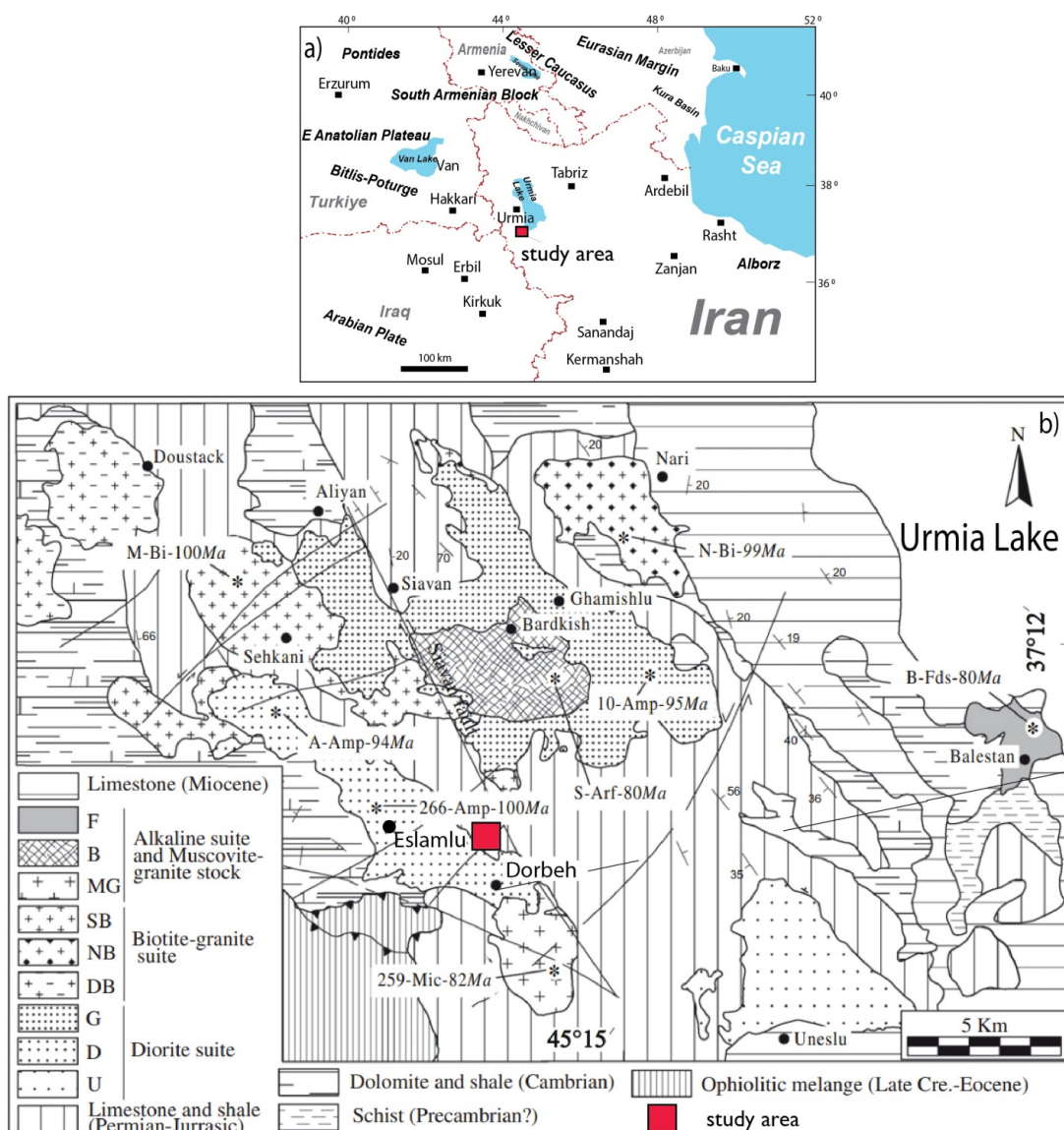


Figure 1. a) The study area is located at the Iran map. b) Simplified geological map of the NW corner of Iran, focusing on the Dorbeh area, modified after (18) A sample location is indicated using a red box.

Whole rock Geochemistry

The considerable effect of the whole-rock composition on garnet growth in metamorphic rocks has been previously examined (25). The whole rock analyses results indicated that they are rich in iron oxide (20-25 wt.%), aluminum oxide (23-35 wt.%), and Ti oxide (6-7.5 wt.%) but relatively poor in silica (30-35 wt.%). The sedimentary protolith corresponds to iron-rich shale and graywacke rock type, likely representing lateritic pelites (12).

Based on this bulk rock chemistry, the parageneses of the Dorbeh contact aureole can be evaluated within the classical KFLASH-T system. The high Ti content of the Dorbeh hornfelses, is accommodated in minerals such as ilmenite, spinel, and biotite. Although elements such as Ti may slightly change the stability field of garnet in the KFLASH system, the overall phase relationships remain largely unaffected considerably (26). The Fe-rich compositions of the mafic phases including biotite,

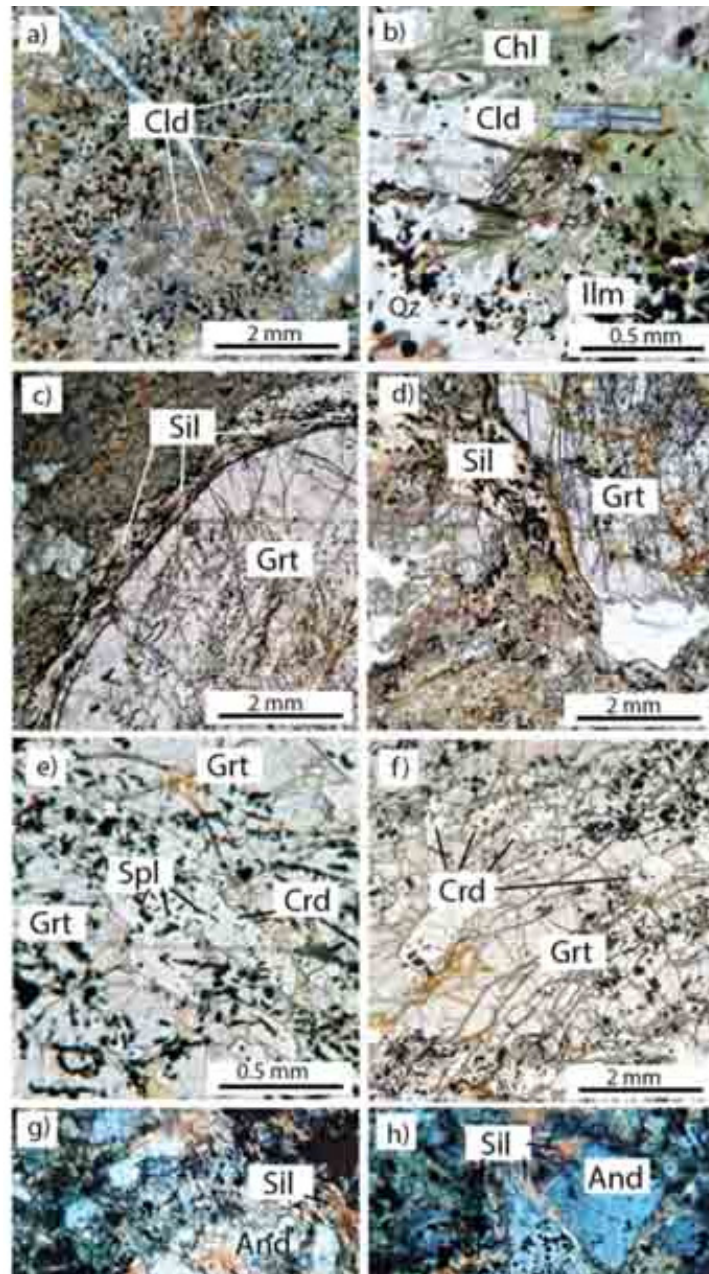


Figure 2. a-f) Plane-polarized-light photomicrographs of Dorbeh aureole samples showing coarse garnet porphyroblasts in an multi-phase matrix including chlorite, chloritoid, ilmenite (a-c), and sillimanite, spinel, and cordierite (c-f) . g-h) Cross-polarized photomicrographs for displaying aluminosilicates + cordierite + spinel paragenetic relationships. Mineral phase abbreviations are: Amp: amphibole; Pl: plagioclase; Cpx: clinopyroxene; Qz: quartz; Ttn: titanite; Ore M.: ore minerals; Cld: chloritoid; Chl: chlorite; Bt: biotite; Grt: garnet; Spl: spinel; Ilm: ilmenite; Crd: cordierite; And: andalusite; Sil: sillimanite according to the (38).

garnet, chloritoid, and chlorite are consistent with such Fe-rich chemistry of the protolith, too.

Discussion

P-X and T-X Diagrams

We provided a series of P-X (Figure 3), and T-X (Figure 4) pseudosections were constructed for different representative samples of the studied metamorphic hornfelses from the Dorbeh aureole, each showing various diagrams illustrates the stability of metamorphic phases and the reactions in the context of the corresponding bulk rock chemistry. The calculations were performed using GeoPS, an interactive visual computing tool for thermodynamic phase equilibria modeling (20).

In P-X and T-X diagrams the line graphs in the

diagrams represent mineral stability fields and phase boundaries as a function of pressure (P, in kbar) / temperature (T, in degree of centigrade) against compositional changes (X, typically in expressed as mole fraction).

The labeled mineral assemblages (e.g., "Grt Bt Ilm Pl Spl", "Grt H₂O Ilm Pl", etc.) represent different mineral phases that occur during metamorphism under varying the stable phases under specific pressure/temperature and compositional (P-T-X) conditions, where these phases are stable or unstable, referring to minerals that are present or absent under various conditions, often with additional notes on the reactions and mineral transformations occurring. Additional annotations such



Figure 3. P_X diagrams for predicted phases by GeoPS model on the four Dorbeh metapelites bulk rock composition. Yellow ellipses applied for showing early stage (P1), and peak stage (P1) position. Additionally, phases in/out pressure are determined and melt-in paragenesis is detected as maximum pressure estimation.



Figure 4. T-X diagrams for predicted phases by GeoPS model on the four Dorbeh metapelites bulk rock composition. Yellow ellipses applied for showing early stage (P1), and peak stage (P1) position. Additionally, phases in/out temperature are determined and melt-in paragenesis is detected as maximum temperature estimation.

as ‘Sil in–Spl in’, ‘Sil in–out’, or ‘fAth out’ indicate reaction boundaries marking the appearance or disappearance of phases. The modeling also distinguishes two principal rock types: spinel-bearing and quartz-bearing compositions. Samples D-2023-01 and D-2023-03 are spinel-bearing and lack quartz at peak conditions, whereas samples D-2023-02 and D-2023-04 contain quartz but lack spinel.

The yellow-highlighted areas mark the "Peak stage paragenesis" indicating the peak metamorphic conditions. This refers to the highest-pressure and temperature conditions experienced by the rocks during their metamorphic evolution. These areas show the parageneses of minerals that are present during the peak stage. Additionally, "Early stage paragenesis" display the low degree conditions and the stable paragenesis which

is common in the aureole.

Sample D-2023-01: This sample shows an increasing temperature trend with peak stage paragenesis occurring at the range of 600-700 °C. Mineral assemblages such as “Grt Bt Ilm” are stable across a wide compositional range change. A “melt-in” starts near 700 °C, indicating that temperatures above this threshold will lead to partial melting of the assemblage which is not observed in the Dorbeh sample.

Sample D-2023-02: Peak metamorphism occurs at slightly higher temperatures (~700–750 °C). The “melt-in” line boundary and other mineral assemblages phase stability fields follow similar trends to D-2023-01, with the system becoming unstable at higher temperatures.

Sample D-2023-03: This sample shows lower peak temperatures ($\sim 600^\circ\text{C}$). Phase transitions toward melt

occur more rapidly, with several “in” and “out” reactions appearing at comparatively lower temperatures.

Sample D-2023-04: Peak metamorphism for this sample occurs around 700-750 °C, similar to D-2023-02. The “melt in” zones begin at higher temperatures.

All samples follow the general pattern of increasing temperature during metamorphism, but the exact conditions at which different reactions occur vary between the samples, slightly. The stability fields of garnet, biotite, and ilmenite are important in understanding the metamorphic history, showing different compositions and reactions across the temperature-composition spectrum.

Melting begins in the higher temperature ranges (around 700 °C), which is a critical point in understanding the conditions under which partial melting of the rock occurs.

The P-X diagrams for all of the samples show a pressure of about 3.2-3.4 kbar for the peak stage in Dorbeh aureole (Figure 3).

The phase diagrams highlight two contrasting scenarios: (1) spinel-bearing, quartz-absent compositions, and (2) quartz-bearing, spinel-absent compositions. These contrasting chemistries exert a strong control on the predicted reaction pathways and stable parageneses.

P-T Pseudosection Modeling and Parageneses Proportions

The P-T modeling shows how temperature and pressure affect the stability of the various minerals and mineral assemblages in a distinct chemical bulk-rock composition. The colored fields on the P-T diagrams (Figure 5) indicate different mineral stability ranges that are stable under specific conditions of pressure and temperature. For example, the pink field corresponds to the assemblage “Bt Grt H₂O Ilm Pl Sil Spl” is stable. The solid lines typically represent the phase boundaries between different mineral assemblages. The red dashed lines in the diagrams indicate specific phase changes, such as melt-in (where melting begins).

Left side diagrams (spinel present, quartz absent): In these samples diagrams show the stability of the spinel phase under certain across a well-defined P-T condition. The spinel is stable interval, particularly within the pink region, which representing the “Bt Grt H₂O Ilm Pl Sil Spl” assemblage. As temperature increases, the assemblage begins to melt, transitioning into the “melt-in” boundary region.

Right side diagrams (spinel absent, quartz present): In this version of these diagrams, quartz is stable in the system, indicated by the yellow region. The reaction boundary lines indicate how specific mineral phases, like

“Grt Sil Crd ...” react with quartz in the melt free part of the system. The melt-in boundary indicates the temperature at which the system begins to melt which is the end of the progression in heating. For the diagrams, this typically occurs between 650 °C and 700 °C, representing the upper thermal unit of the Dorbeh aureole.

The pink field shows the stable “Bt Grt H₂O Ilm Pl Sil Spl” assemblage. At higher temperatures (around 650-700 °C), the system enters the melt-in region, signaling the start of partial melting. The system is stable in the range of about 3.3 to 3.4 kbar pressure.

For all the samples temperature ranges until melting beginning (i.e., “melt-in”) is around 650 °C to 700 °C, and the pressure range is around 3.2 to 3.4 kbar. This suggests that the metamorphic conditions are consistent in the area, with these temperatures and pressures being critical for the initiation of partial melting event as the possibly uppermost condition for the aureole. The presence or absence of spinel and quartz significantly influences the stability of the mineral assemblages. In the quartz-bearing samples the melt-in temperature might shift slightly higher, indicating that the presence of quartz may slightly delay the melting process in some of these rocks, and quartz pushing the melt-in region to higher temperatures. These diagrams help in understanding the metamorphic history of the Dorbeh rocks by showing which mineral assemblages are stable at various P-T conditions and when melting occurs.

Moreover, the predicted phase proportions in the special P-T range confirmed the observed assemblages in the Dorbeh aureole (Figure 6; Supplementary Figures 3-6). At the right-hand side diagrams Crd and Qz appeared at the estimated conditions, and Spl formed at the post-peak P-T (after melt formation) which is not reached in the studied aureole. Although, in the left-hand side diagrams Spl appeared in the lower part of the diagrams, before melt formation together with Sil, after Qz consumption and Ilm formation, and Crd is not predicted in these samples at all (Figure 5). Cordierite appears only in samples with slightly higher SiO₂ and lower FeO contents (D-2023-02 and D-2023-04). In contrast, the more Fe-rich and Si-poor samples (D-2023-01 and D-2023-03) fall outside the Crd stability field in the NCKFMASH+Mn model. Also, cordierite may persist metastably due to reaction overstepping during rapid heating in the aureole.

Chl and Cld are stable in the first lower half of the P-T profile, means that they should remove and react before the peak stage conditions, while we observed them in the samples together with the peak phases such as Grt, Sil, Crd, and Spl (Figure 5). It showed that the Chl and Cld are remained as unstable phases until the high

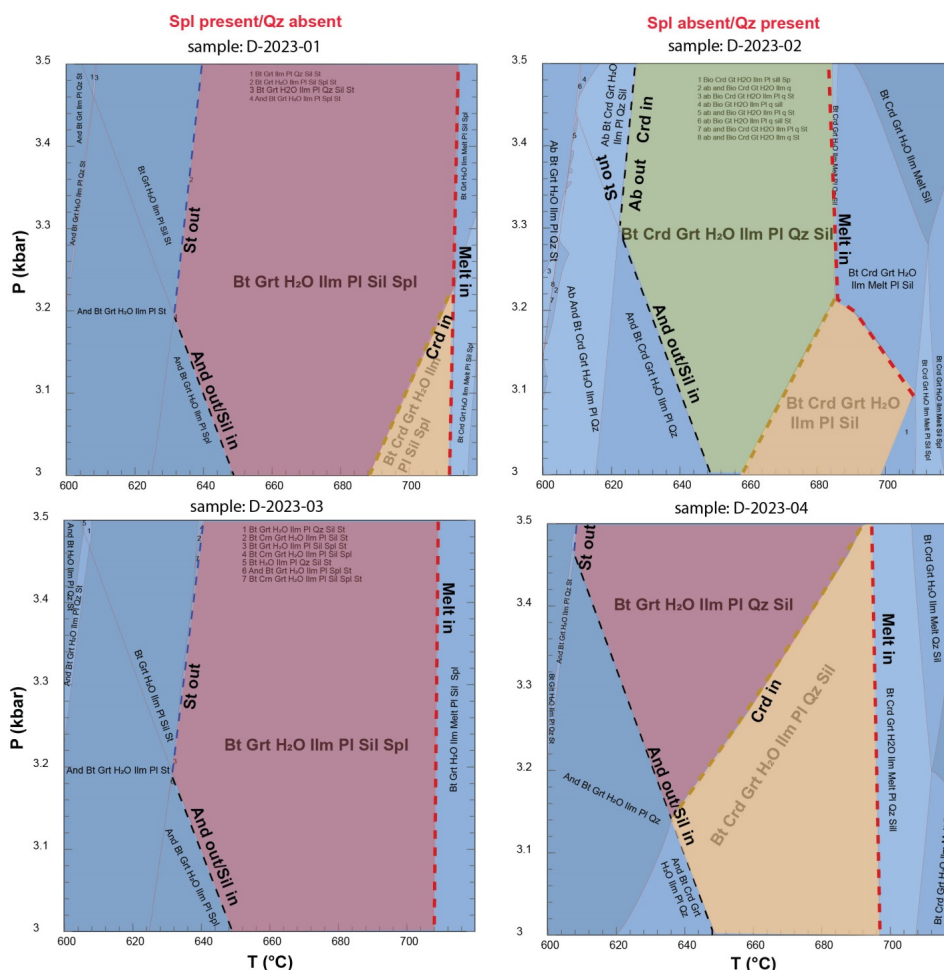


Figure 5. P-T pseudosections calculated for Dorbeh aureole metapelites in peak-stage (spinel-bearing and spinel-free assemblages) together with phases in/out P-T field evaluation by colour dashed areas. Melt-in reactions line is showing by red dashed lines. The left hand side grids for Spl-bearing/Qz-free paragenesis and the right hand side for Qz-bearing/Spl-free paragenesis.

temperature phases crystallized because of their high initial modal proportion. They were not finished during reactions running.

Grt appeared in all of the samples, although its proportion is less in the one them. It is confirmed by some rare samples with not Grt in their assemblage list (Table 1). There is no any Ky or St in the studied samples whereas they are predicted by models (Figure 6). It occurred because of high speed of the metamorphism process during heat flow from the intrusion into the contact aureole. It is equal to high degree of overstepping under cooling conditions which is routine in the contact metamorphism (13).

Thermodynamic Conditions for Spinel Formation

The characteristics and thermodynamic conditions for the formation of the spinel are of special importance for metamorphic geologists, as this mineral is one of the most important geo-thermobarometers used in high-grade metamorphic rocks (27, 28; 29). It is mainly observed in rocks of pelitic composition in the KFMASH system (30, 31) with its Fe-rich endmember, hercynite. The zinc component present in the spinel structure (gahnite endmember) can increase its stability in the garnet field to higher pressures (32). Additionally, high oxygen fugacity and Al-Fe-rich environments increase the stability field of spinel-bearing assemblages (33).

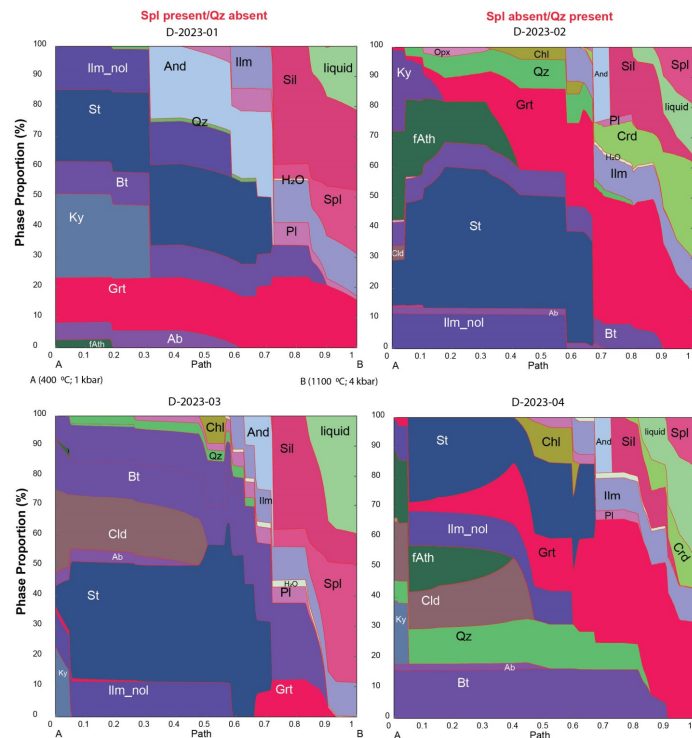


Figure 6. Suggested phase proportions in the Dorbeh metapelites using GeoPS. In two samples including D-2023-03, and -04, chloritoid is appeared in low P-T half of the graph.

In low-grade metamorphic rocks, spinel is the product of the breakdown of sphalerite or staurolite (7, 34). Additionally, the formation of spinel from the breakdown of zinc-rich biotites also occurs during decompression processes (35). In general, spinel appears in low silica rocks or at least in low silica parts of rocks (36, 37). In high-silica rocks, this mineral is enclosed by porphyroblasts such as garnet and andalusite, because under metamorphic conditions lower than the granulite facies, the two minerals spinel and quartz strongly react with each other to form mafic minerals. Of course, the $Qz + Spl$ paragenesis (abbreviations from 38) has been reported in high-grade Al- and Mg-rich granulites in orogenic belts, which can be explained in relation to the high concentration of ZnO (23).

It should be noted that staurolite has not been observed in the Dorbeh metapelites, which is a reactant phase responsible for spinel formation in metamorphic rocks. This may be due to the complete consumption of this mineral during prograde metamorphism or its not forming because of progressive metamorphism rate and heat charge into the aureole. Additionally, considering the silica-poor nature of the Dorbeh rocks (~25% lower than the average composition of the metapelites; 39), the

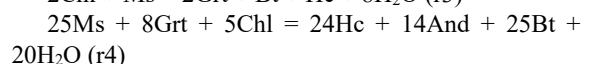
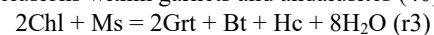
formation of spinel from such a protolith is expected. The suggested reaction by 7 is:



If r1 is responsible for the formation of spinel in the aureole, the significant association of spinel and aluminosilicates, including sillimanite and andalusite, would also be explained. Also, for Fe- and Al-rich systems such as the Dorbeh hornfelses, the following reaction has been proposed: $Fe-St = Sil + Hc + Ilm + H_2O$ (r2)

Considering the high Ti content of the protolith and the large amount of ilmenite in the rocks, r2 seems to be an appropriate reaction than r1. Additionally, based on mineral chemistry (Fe-rich chloritoid, Fe-rich garnet, abundant ilmenite, and absence of muscovite), reaction r2 is the most plausible mechanism for spinel formation.

The following two reactions involving muscovite could have been responsible for the formation of spinel inclusions within garnets and andalusites (40):



Although muscovite is not observed in the Dorbeh hornfelses, it may be consumed during the event. As the absence of staurolite in the reported assemblages, the r3

and r4 are more acceptable for occurrence in the Dorbeh aureole during the process of spinel formation.

In the hornfels of the contact aureole in the Eastern Alps in Italy, evidence of the breakdown of iron-rich staurolite in quartz-free parts of the rocks within coarse-grained sillimanites has been observed. The produced spinel, seen as fine grains scattered within other porphyroblasts, too (7). Similar assemblages, also, have been reported in the Archaean block of Western Australia metamorphic rocks, consisting of chloritoid + aluminosilicates + garnet + Fe-spinel (34).

The metapelites of the Dorbeh contact aureole formed around a dioritic-gabbroic intrusive stock. The mafic bodies are mostly water-poor, which causes an a_{H_2O} gradient between the intrusion and the country rocks. This gradient leads to the dehydration of the metapelites

in the wall rock, providing an appropriate explanation for the absence of partial melting occurrences in such rocks.

The Interpretation of the Peak Paragenesis Using Isoleths Intersections

A detailed examination of the phase relationships in metamorphic rocks can serve as a suitable method alongside approaches based on quantitative data to assess how progressive metamorphism occur.

According to the literature, the formation of the Grt + Crd + Sil paragenesis at temperatures around 575–650 °C and at water activity <0.2 is possible (40). The Grt + Crd + Sil + Hc paragenesis can also form at contact metamorphism pressures (between 2 and 3 kbar) at temperatures below 800 °C (40). The experience of such temperatures in the Dorbeh aureole can be confirmed by the P-T modeling (4.1 and 4.2 subsections).

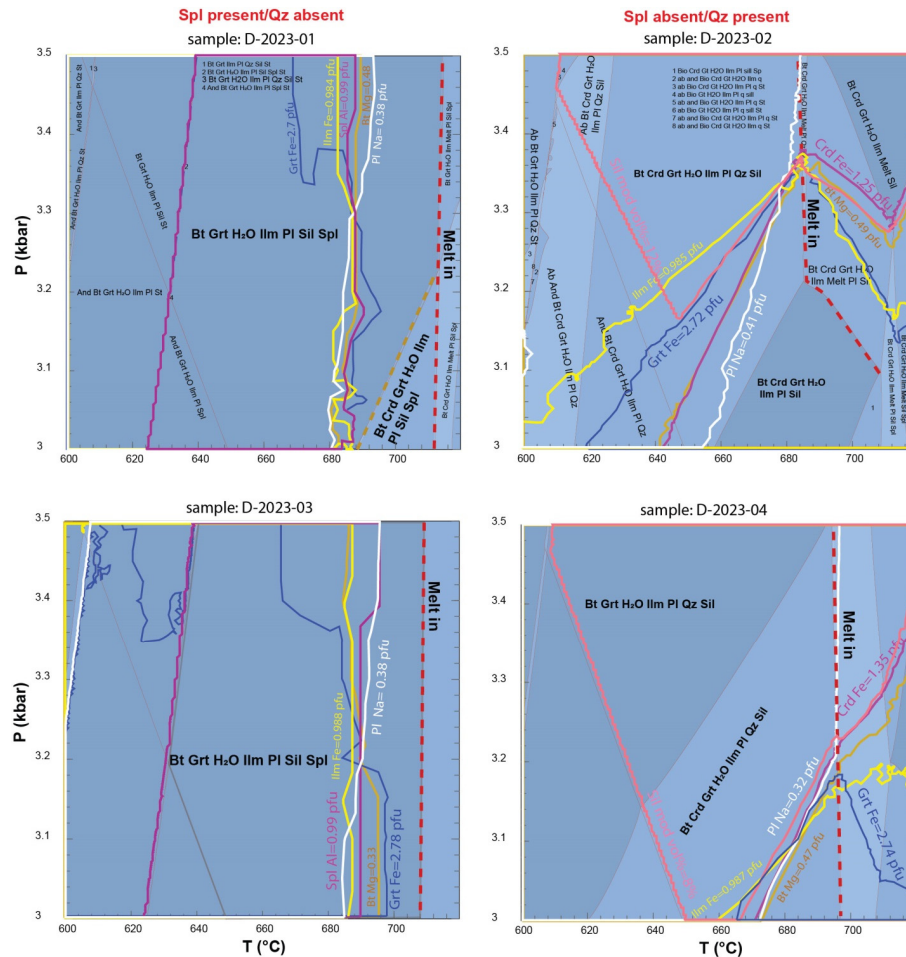


Figure 7. P-T evaluation of the Dorbeh metapelites superimposed on the four pseudosection, showing stability domains of calculated parageneses based on the effective bulk-rock composition by GeoPS. The isopleths intersections between the essential phases used for P-T estimation.

Additionally, we used a method is based on the direct observation of reaction textures and is more objective in estimating metamorphic conditions through the method of cross-cutting equilibrated predicted and observed phases isopleths in a P-T range (Figure 7). For all of the four modeled samples, the intersection of isopleths including Fe in Grt; Fe in Ilm; Mg in Bt; Na in Pl; Al in Spl (in left-hand side samples; Spl present - Qz and Crd absent); Fe in Crd (in right-hand side samples; Spl absent- Qz and Crd present), indicates pressure of 3.2-3.4 kbar at the temperature of >680-690 °C. All of them with crossing melt-in isopleth or occurs before its P-T domain (Figure 7). The estimated P-T are fully consistent with the former results evaluated based on P-X; T-X and P-T pseudosections output results (Supplementary Figure 7).

Conclusions

- The Dorbeh contact aureole generated around a dioritic-gabbroic stock in the Sanandaj-Sirjan structural zone of Iran, contains Fe- and Al-rich metapelitic hornfelses derived from iron-rich shale and graywacke protoliths. This study confirms the bulk-composition controls on mineral assemblages considerably and highlights the utility of phase-equilibria applications on modeling for the geo-thermobarometry without direct use on the mineral compositions.

- The absence of green spinel in contact with quartz, suggesting its defense by porphyroblasts, petrographic observations analysis identifies important minerals like garnet, cordierite, sillimanite, and spinel. Although no sign of staurolite was observed in the samples, evidence suggests that spinel in the aureole may have resulted from the breakdown of staurolite.

- Thermodynamic modeling and microstructural observations indicate that peak metamorphic conditions of ~700 °C at pressures ~3.2 kbar for the P2 paragenesis including "Grt Crd Sil Hc" assemblage. Additionally, early stage conditions evaluated using P1 which in it chlorite and chloritoid are stable present phases are temperature of 450 °C at pressure of 2.5 kbar.

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Data availability

Data table was used for the research described as the Table 1.

Declarations Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships

that could have appeared to influence the work reported in this paper.

Author contributions statement

Author 1: Conceptualization, Investigation, Resources, Data Curation, Software, Data Interpretation, Writing - Original Draft, Visualization, Supervision, Project Administration, and Funding Acquisition; *Author 2:* Review, Validation, and Data Interpretation.

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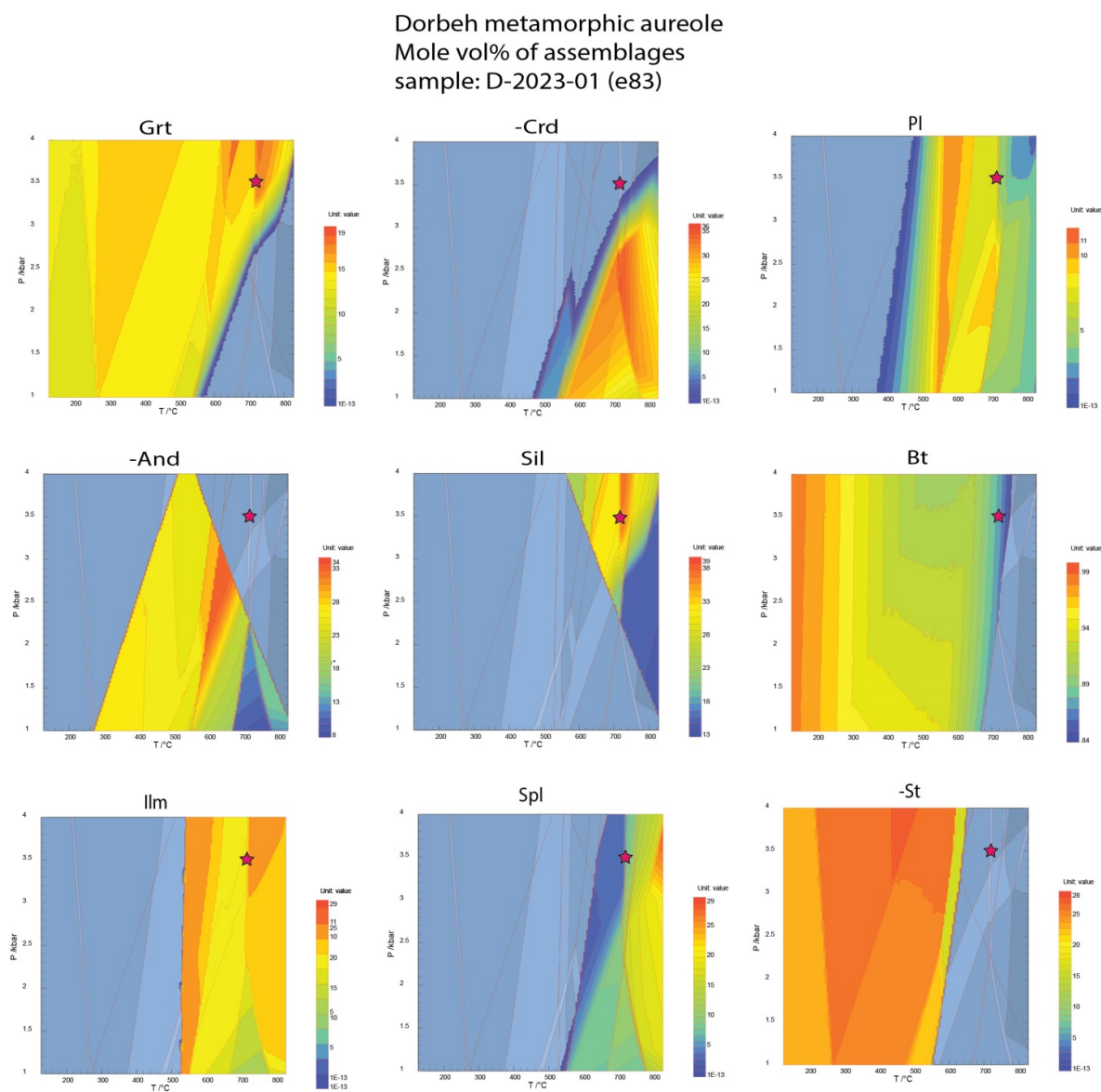
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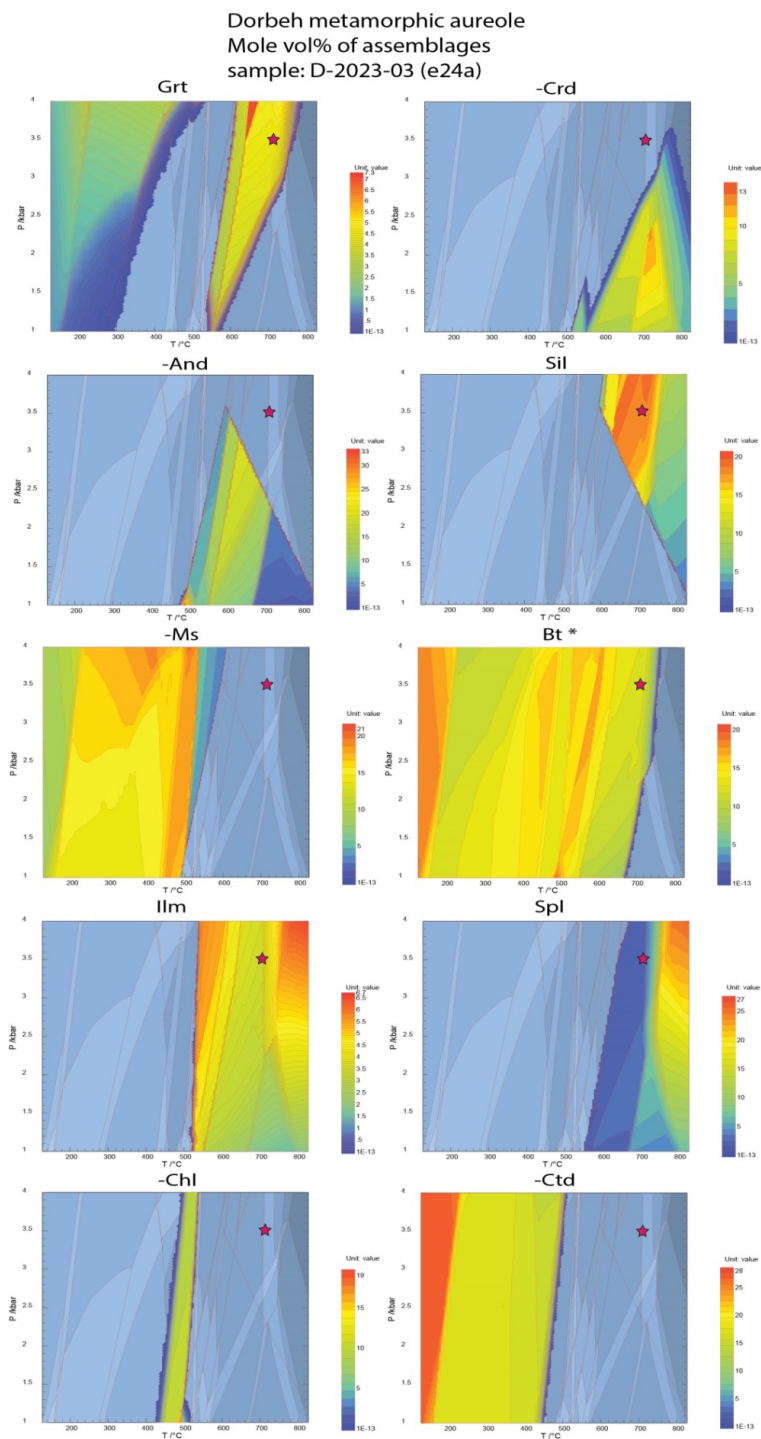
Suppl. Figure 1. Whole-slide image (WSI), of representative Dorbeh aureole metapelitic sample, showing grano-blastic microstructure, and garnet abundance.



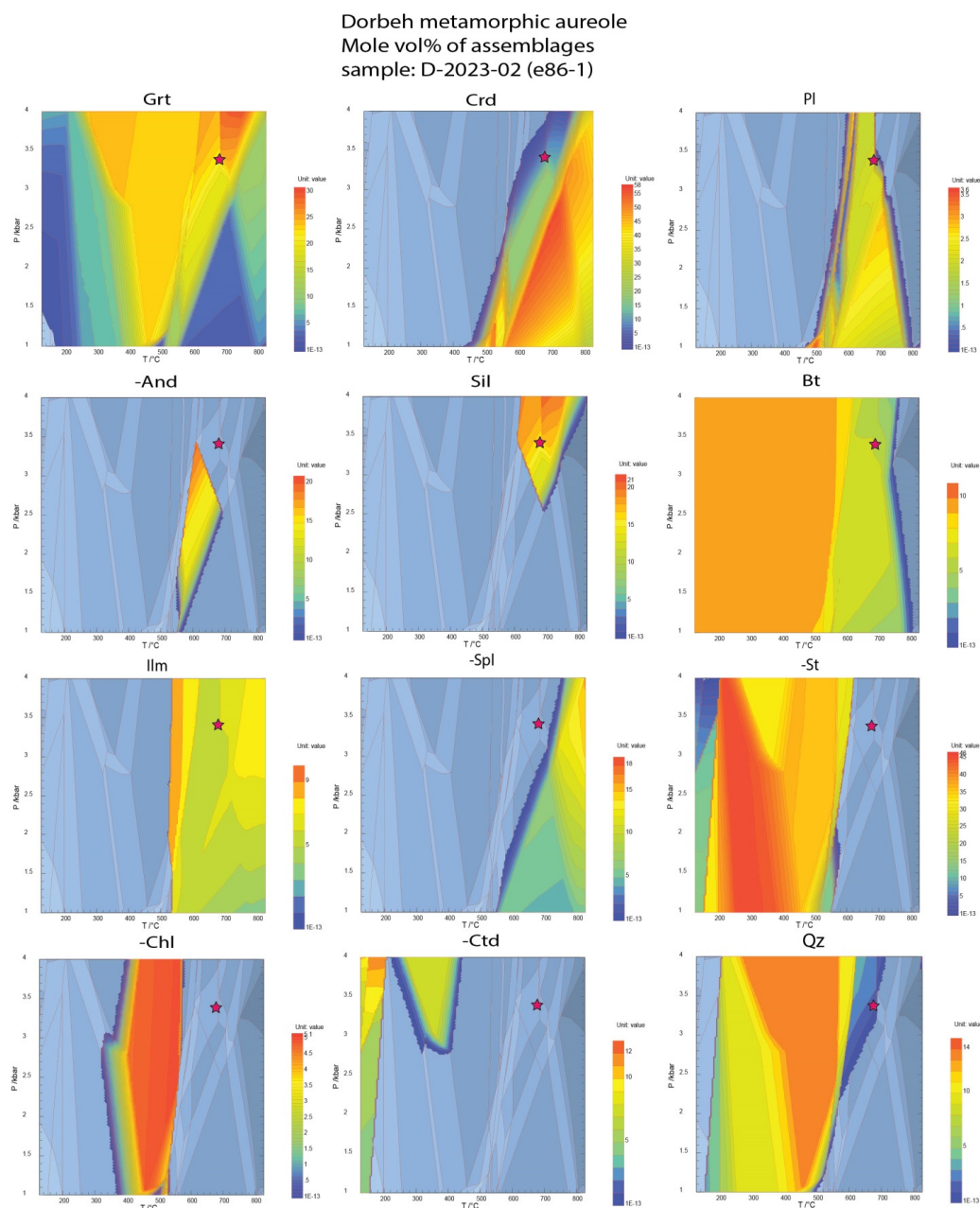
Suppl. Figure 2. Another whole-slide image (WSI), of representative Dorbeh aureole metapelitic sample showing idioblastic garnet porphyroblast within fine grained matrix.



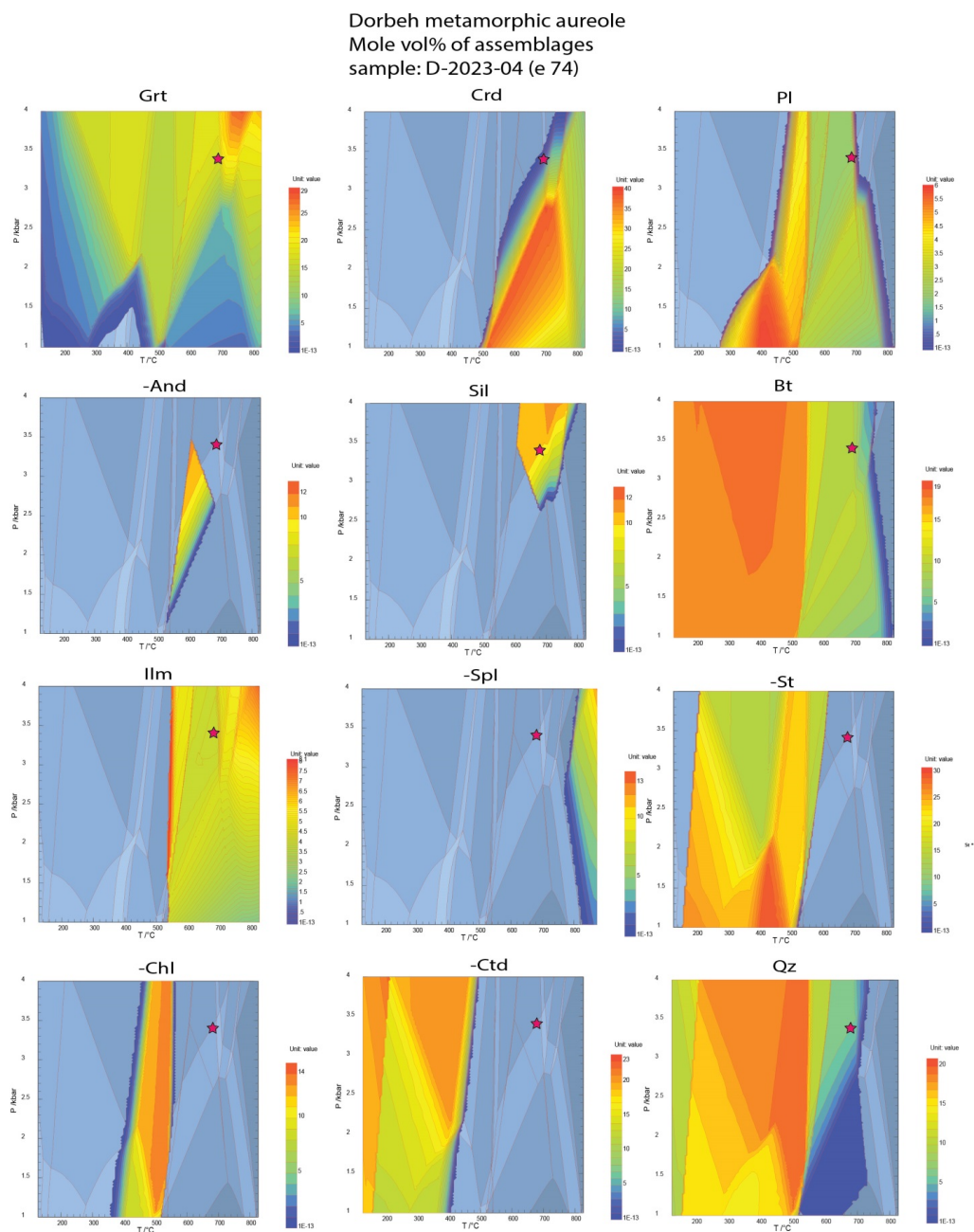
Suppl. Figure 3 Predicted phase-proportion volume percentages for the sample D-2023-01.



Suppl. Figure 4 Predicted phase-proportion volume percentages for the sample D-2023-03.



Suppl. Figure 5 Predicted phase-proportion volume percentages for the sample D-2023-02.



Suppl. Figure 6 Predicted phase-proportion volume percentages for the sample D-2023-04.