The Early Jurassic metamorphic history of the Yukon-Tanana terrane of
northwestern British Columbia: Insights from a new inverse garnet
fractionation modelling technique

by

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Abstract

A metamorphic study was conducted on metapelites of the Boundary Ranges and Florence Range metamorphic suites in the Yukon-Tanana terrane of north-western British Columbia. A new inverse garnet fractionation modelling technique was developed as the software program G_FRAC. Through the combined application of G_FRAC and THERIAK-DOMINO, and its integration with Lu-Hf garnet-whole rock age dating of select samples, prograde and retrograde P-T points were estimated for Early Jurassic metamorphism of these two suites. The Boundary Ranges Suite experienced two garnet growth events in this period at 201.7 ± 2.8 Ma and 192.4 ± 0.4 Ma with the younger event reaching peak conditions of $\sim 550^\circ\text{C}$ and 700 to 800 MPa. The Florence Range suite experienced a synchronous garnet growth event between 190.9 ± 3.3 Ma and 185.3 ± 1.1 Ma reaching a peak pressure of ~ 1000 MPa at $\sim 620^\circ\text{C}$ and a peak temperature of 690 to 730°C at 600 to 750 MPa before cooling to $\sim 610^\circ\text{C}$ and ~ 670 MPa. The results of two of these models were verified with the forward garnet growth modelling program THERIA_G.

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1. Introduction

Throughout its protracted history, the Canadian Cordillera has undergone several rifting and collision episodes resulting in a complex mosaic of different tectonic terranes (Nelson et al., 2013). Amongst these terranes, the Yukon-Tanana terrane (YTT) is the largest, and records several metamorphic events that provide insight into tectonic activity spanning from the Early Mississippian to Early Cretaceous (Currie, 1994; Creaser et al., 1997; Erdmer et al., 1998; Philippot et al., 2001; Berman et al., 2007; Knight et al., 2013; Staples et al., 2013, 2014; Kellett et al., 2018; Gaidies et al., 2020). Understanding the conditions and timing of these metamorphic events is crucial to our understanding of the tectonism and formation of the Canadian Cordillera.

Determining the conditions of metamorphism has been challenging and imprecise in the poly-metamorphosed rocks of the YTT (Berman et al., 2007). Garnet is a common mineral in metapelites that can aid in unravelling the tectonometamorphic history of the YTT. The utility of garnet in determining conditions of metamorphism is well documented (e.g. Blackburn and Navarro, 1977; Chakraborty and Ganguly, 1991; Florence and Spear, 1991; Evans, 2004; Caddick et al., 2010; Gaidies et al., 2015). These previous studies have focused on major element composition of garnet but an increasing number of studies have also

been investigating mineral reactions and garnet growth mechanics through the trace element composition of garnet (e.g. Skora et al., 2006; Konrad-Schmolke et al., 2008b; George et al., 2018; Rubatto et al., 2020; Gaidies et al., 2020). With the application of high resolution X-ray micro-computed tomography, laser ablation ICPMS mapping, and electron probe microanalysis, we can gain great insight into the P-T history of a rock. These data can be used for effective garnet growth modelling with tools like THERIA_G (Gaidies et al., 2008) and CZGM (Faryad and Ježek, 2019). These tools are forward garnet growth models that apply thermodynamic and kinetic principles to predict garnet growth zoning and diffusion.

Not every rock is suitable for garnet growth modelling. Many metamorphic processes can affect the composition of garnet such that models are unable to accurately predict observed compositional zoning (e.g. Pattison and Tinkham, 2009; Pattison et al., 2011; Spear and Wolfe, 2019; McCarron et al., 2019). In this study we sidestep possible issues such as metamorphic overstepping, open system behavior, inaccurate thermodynamic databases, and chemical sequestration by other phases by taking an inverse modelling approach. We have developed a program called G_FRAC which uses measured garnet chemical composition and volume to model garnet fractionation. This approach has allowed us to determine consistent and realistic P-T points along both prograde and retrograde metamorphic P-T paths for samples that could not be otherwise modelled with THERIA_G.

With G_FRAC, THERIAK-DOMINO (de Capitani and Petrakakis, 2010), and THERIA_G (Gaidies et al., 2008), we unravel the P-T history of garnet-bearing metapelites of the YTT in the Atlin Lake area in northwest BC, where recent petrochronological work (Soucy La Roche et al., in review) provides a general tectonometamorphic framework to understand these polymetamorphic rocks. This study expands on this work by providing

metamorphic P-T paths that have eluded previous studies in the region.

2. Geological Setting

The North American Cordillera comprises a complex collage of terranes and is the birthplace of the suspect terrane concept (Coney et al., 1980). Whereas many aspects of these terranes and their boundaries are poorly constrained, it is generally accepted that each terrane represents distinct but not necessarily isolated tectonic units (Nelson et al., 2013). The northern Cordilleran terranes are grouped into Ancestral North America, Intermontane, Arctic, Insular, West Alaska, and Outboard superterranes on the basis of their provenance and timing of accretion (Colpron and Nelson, 2020; Nelson et al., 2013; Colpron et al., 2007). The study area is located within the Intermontane Belt of the northern Cordillera (Fig. 2.1).

The Intermontane Belt consists of the Slide Mountain, Yukon-Tanana, Quesnellia, Stikinia, and Cache Creek terranes (Colpron and Nelson, 2020; Nelson et al., 2013; Colpron et al., 2007). These terranes initiated outboard of the Laurentian margin and preserve a protracted history spanning from the initiation of subduction on the western margin of Laurentia in the Devonian to the final accretion of these terranes by the Middle Jurassic (Nelson et al., 2013). During their Paleozoic to early Mesozoic evolution, these terranes formed a series of related arcs and Sea of Japan-type backarcs which originated from and re-accreted to Laurentia (Colpron et al., 2007).

2.1 Yukon-Tanana Terrane

The Yukon-Tanana Terrane (YTT) spans eastern Alaska, central Yukon, and northwestern British Columbia (Fig. 2.1) and is the largest terrane of the Intermontane Belt. The YTT is divided into four distinct tectono-stratigraphic assemblages (Colpron et al., 2006b). The pre-Late Devonian Snowcap assemblage is the oldest unit in the YTT and forms the basement to successor assemblages (Colpron et al., 2006b). It consists of amphibolite-facies psammitic, pelitic, and calc-silicate schist, quartzite, marble and minor amphibolite and ultramafic rocks (Colpron et al., 2006a,b). U-Pb analyses of detrital zircon in the Snowcap assemblage indicate that these sediments were derived, at least in part, from the Laurentian craton (Piercey and Colpron, 2009). These lithological units and detrital zircon data indicate the Snowcap assemblage likely formed on the passive margin of Laurentia (Piercey and Colpron, 2009).

The Snowcap assemblage is unconformably overlain by continental arc volcanic and volcanoclastic rocks and cogenetic plutonic rocks of the Late Devonian to Early Mississippian Finlayson, Middle Mississippian to Early Permian Klinkit, and Middle to Late Permian Klondike assemblages (Colpron et al., 2006b).

Volcanism in the YTT is divided into five cycles (Piercey et al., 2006). The first cycle is the Mid-Late Devonian Ecstall cycle consisting of felsic and mafic intrusive rocks associated with variable metasediments. The second cycle is the Late Devonian-Early Mississippian Finlayson cycle consisting primarily of mafic and felsic volcanic rocks. The third cycle is the Early Mississippian Wolverine Cycle consisting primarily of felsic intrusive and volcanic

rocks. The fourth cycle is the Late Mississippian Little Salmon Cycle consisting primarily of intermediate and mafic intrusive and volcanic rocks. The final cycle is the Pennsylvanian-Early Permian Klinkit cycle consisting of variable volcanic and sedimentary rocks.

The protracted and complex development of the YTT and the northern Cordillera has resulted in multiple, overprinting deformation and metamorphic events in the YTT from ca. 365 Ma to ca. 115 Ma (Table 2.1). Metamorphism in the YTT varied across the terrane and over time and includes high-pressure low-temperature, medium-pressure, and low pressure-high temperature events. The structural complexity of this terrane and difficulties in determining precise pressure temperature (P-T) paths make it difficult to interpret the significance of these metamorphic events in the broader tectonic context.

2.2 Atlin Lake area

The YTT in the Atlin Lake area (Fig 2.2) is divided into two metamorphic suites. These are the Florence Range suite and the Boundary Ranges suite which are separated by the folded Wann River Shear Zone (Currie and Parrish, 1993; Currie, 1994; Currie and Parrish, 1997). The upper age limit of this shear zone is constrained by the ca. 185 Ma crystallization age of the youngest rocks deformed by this shearing event, the intrusive Tagish Lake suite located within the Wann River Shear Zone (Currie and Parrish, 1993). The lower age limit is provided by ca. 170 Ma U-Pb titanite and rutile dates interpreted as post-deformation cooling ages (Currie and Parrish, 1993). The region is intruded by Cretaceous to Tertiary Coast Belt plutonic rocks (< 127 Ma; U-Pb zircon) (Currie, 1992b, 1994).

2.2.1 Boundary Ranges suite

The Boundary Ranges suite (BRS) (Fig. 2.3A-C) consists of a wide range of lithological units, including muscovite-biotite-chlorite $\pm$ garnet schist, chlorite-actinolite schist, and felsic gneiss with rare marble, calcsilicate gneiss, and metagabbro (Currie and Parrish, 1997). The BRS was metamorphosed at upper-greenschist to lower amphibolite facies conditions and qualitatively shows less retrogression and overprinting than the Florence Range Suite. Felsic orthogneisses of the BRS range from ca. 366 Ma to 352 Ma (U-Pb zircon) (Currie and Parrish, 1997) and a ca. 270 Ma (U-Pb zircon) hornblende-plagioclase gneiss of intermediate composition, the Wann River Gneiss was identified in the Wann River Shear Zone (Currie, 1992a). The 191-181 Ma (U-Pb zircon) Tagish Lake suite crosscuts most of the BRS (Currie, 1992a; Currie and Parrish, 1997). The BRS has previously been included within the Stikinia terrane by Currie and Parrish (1997) and within the YTT by Mihalynuk (1999) but neither of these correlations adequately address the age and compositional diversity of the BRS. If the BRS is grouped in the YTT, the ages and lithologies best fit the descriptions of the Ecstall Cycle continental arc volcanism (Piercey et al., 2006) that predates the Finlayson cycle magmatism.

Timing and P-T conditions of metamorphism in the BRS are poorly constrained. Peak temperatures were estimated to be 500-600°C using biotite-garnet thermometry (Mihalynuk, 1999) but metamorphic pressures were not determined, and the timing of metamorphism is only constrained to post-270 Ma, the U-Pb zircon crystallization age of the metamorphosed Wann River Gneiss at the top of the BRS (Currie, 1992a, 1994).

2.2.2 Florence Range suite

The Florence Range suite (FRS) (Fig. 2.3D-E) has been correlated to the Snowcap assemblage (Nelson et al., 2006). Similar to the Snowcap, FRS is mostly composed of upper amphibolite facies biotite-muscovite schist with layers of metapelite, metapsammite, quartzite, marble, calcsilicate gneiss, and amphibolite. Local partial melting is inferred from the occurrence of leucosome in some metapelitic rocks, which has been dated at ca. 177 Ma (multi-grain U/Pb ID-TIMS on zircon and monazite: Currie (1994)). Retrograde mineral assemblages, such as chlorite and biotite replacing garnet porphyroblasts, are common in this suite.

In-situ laser-ablation split-stream monazite petrochronology on the same sample suite as this study documents three metamorphic events at P-T conditions loosely constrained based on Al_2SiO_5 polymorph stability (Soucy La Roche et al., in review). A Barrovian-type M1 metamorphic event is characterized by 270-240 Ma prograde metamorphism up to the kyanite stability field and a 240-215 Ma retrograde path. A Barrovian-type M2 event is characterised by renewed garnet growth to unquantified peak P-T conditions at 195-185 Ma, decompression and heating in the suprasolidus sillimanite stability field at 185-170Ma and cooling at 170-120 Ma. A M3 low pressure heating pulse in the andalusite and cordierite stability fields was also identified at < 120 Ma.

2.3 Sample locations

The samples in this study are part of a larger suite collected in the summer of 2018. The selected samples are representative of both the FRS and BRS with large enough geographic and structural distance between them to provide an understanding of metamorphism across the entire exposed suites. They were chosen as the least retrogressed samples with the fewest signs of garnet resorption. The locations of these samples are shown in figure 2.2. Sample locations and observed mineralogies are shown in table 2.2.

Figure 2.1: Terrane map of Yukon and northern BC, dashed box indicates the extent of the study area in Fig. 2.2. Modified after Colpron and Nelson (2020)

Figure 2.2: Map of the study area with sample localities (18ZE-R- prefix removed for clarity). Modified after Cui et al. (2019). Wann River Shear Zone drawn based on Currie and Parrish (1997) and our field observations.

Figure 2.3: Field photos of rocks from the Boundary Ranges Suite (A,B,C) and Florence Range Suite (D,E,F). (A) graphite garnet-chlorite-white mica schist with garnets up to 1 cm in diameter. Outcrop photo of 18ZE-R-14C. (B): Crenulated chlorite-muscovite-biotite schist. (C): Wann River Gneiss composed primarily of plagioclase and amphibole. (D): Deformed felsic dike crosscutting marble. (E): Garnet white mica gneiss with garnet partially replaced by biotite. (F): Rotated quartzite clast in marble

Table 2.1: Summary of published constraints on metamorphic events in the Yukon-Tanana terrane

Timespan of Metamorphism	Facies	Tectonic Setting	References
Early Mississippian (ca. 365-340 Ma)	Blueschist - Eclogite	Subduction and slab rollback	Erdmer et al. (1998), Berman et al. (2007), Mihalynuk et al. (2006), Devine et al. (2006)
Middle to late Permian (ca. 270-250)	Greenschist - Amphibolite; Eclogite	Subduction and collision with Laurentia	Petrie et al. (2016), Creaser et al. (1997), Philippot et al. (2001), Beranek and Mortensen (2011)
Middle Triassic (ca. 240 Ma)	Hornblende Hornfels - Upper Amphibolite	Intra-arc shortening or extension	Berman et al. (2007), Gaidies et al. (2020)
Early Jurassic (ca. 200-175 Ma)	Middle Amphibolite - Upper Amphibolite; Eclogite	Collision with Laurentia or Stikinia	Kellett et al. (2018), Berman et al. (2007), Currie (1994), Knight et al. (2013), Gaidies et al. (2020)
Middle to late Jurassic (ca. 170-140 Ma)	Middle Amphibolite	Slab rollback, extension and contact metamorphism, and foreland propagation of deformation	Berman et al. (2007), Staples et al. (2014)
Early Cretaceous (ca. 120-115 Ma)	Amphibolite	Slab rollback, extension, and exhumation and contact metamorphism	Berman et al. (2007), Staples et al. (2013)

Table 2.2: Sample mineralogies and coordinates.

Sample	Mineralogy	Latitude	Longitude
Boundary Ranges Suite			
18ZE-R-11A	Qz, WM ^a , Grt, Chl ^b , And, Pl, Ilm, Rt, Py, Ccp	59.063684	-133.989565
18ZE-R-14A	Pl, WM, Chl, Grt, Qz, Ilm	59.067150	-134.026806
18ZE-R-14B	Qz, Pl, Chl, Grt, Wm, Rt, Ilm	59.067150	-134.026806
18ZE-R-14C	WM, Chl, Grt, Pl, Qz, Ilm, Py, Ccp	59.067150	-134.026806
18ZE-R-16	Bt, WM, Pl, Qz, Grt, Ep, Chl, Ilm, Rt, Py, Ccp	59.068284	-134.031324
18ZE-R-73C	Pl, Bt, Qz, Grt, Chl, Ilm, Py, Rt, Ccp	59.105988	-134.115637
Florence Range Suite			
18ZE-R-77A	Bt, Qz, WM, Pl, Grt, Rt, Py, Ccp, Ilm	59.107245	-134.139384
18ZE-R-81	Bt, Pl, Qz, Grt, Kfs, Sil ^c , Po, Ilm, Ccp, Rt	59.106124	-134.159390
18ZE-R-49B	WM, Bt, Qz, Sil, Pl, Chl ^b , Py, Ilm, Ccp	59.140091	-134.180355
18ZE-R-71	Qz, Bt, Pl, Grt, Gr, Chl ^b	59.217766	-134.273863

Mineral abbreviations from Whitney and Evans (2010) except *a*: WM = White mica. *b*: Retrograde chlorite. *c*: Sillimanite pseudomorphed by white mica

3. Methods

3.1 XRF

Hand samples with no obvious compositional layering were crushed and chips that contained surface alteration or quartz veins were removed by hand before being powdered. The major element whole rock chemical compositions of the samples were obtained at ActLabs (Ancaster, Ontario) using X-ray fluorescence (XRF) analysis following lithium borate fusion using the technique described in Norrish and Hutton (1969). Samples were baked at 1000°C for two hours after which weight loss was measured to calculate loss on ignition (LOI). A portion of the baked sample weighing 0.75 g was mixed with 9.75 g of a mixture of lithium metaborate, lithium tetraborate, and lithium bromide. This mixture was fused in a Pt crucible and casted in a Pt mold to create a disc. The discs were analyzed on a Panalytical Axios Advanced wavelength dispersive XRF. The detection limit for the major elements was 0.01 wt%

3.2 XR- μ CT

The sizes, shapes, and spatial distributions of garnet porphyroblasts in the samples were determined by high resolution X-ray micro-computed tomography (XR- μ CT) using a Skyscan 1173 at the Carleton University Department of Earth Sciences XR- μ CT lab. Rock volumes of 20-60 cm³ were scanned with a polychromatic X-ray beam from a source with a voltage of 131 kV and current of 61 μ A with a 0.25 mm brass filter. The samples were rotated at a step size of 0.3° for a 180° rotation. The resulting X-ray images were processed using the SkyScan NRecon software to reconstruct the internal 3D structure of the sample. Further post-processing and 3D visualization was done using the program Blob3D (Ketcham, 2005). Postprocessing involved segmentation of garnet using greyscale thresholding and removal of isolated pixel islands and holes resulting from noise. Small inclusions in garnet typically less than four pixels and inclusions with similar greyscale values as garnet were segmented as garnet, resulting in an overestimation of garnet volume. Blob3D was used to quantify the size, abundance, and spatial distribution of garnet porphyroblasts. Crystal size distributions (CSDs) were produced from these data assuming the geometry of each crystal is a sphere and calculating the radius from the crystal volume. These data were also used to select the largest garnet. Central sections were cut along the long axis of these garnets.

3.3 EPMA

Compositional maps and quantitative line profiles of centrally sectioned garnets were acquired at the Geological Survey of Canada (Ottawa, Ontario) using the JEOL JXA-8230

electron probe micro-analyzer (EPMA) equipped with 5 vertical wavelength-dispersive spectrometers running ProbeForEPMA software (Donovan, 2020). The operating conditions for the line profiles were 20 kV accelerating voltage and 20nA current with a focused probe. On-peak count times were 10s and off-peak count times were 5s. Calibration standards were a mix of well-characterized natural and synthetic minerals. The correction procedure follows that of Armstrong (1988). The run conditions for the garnet maps varied from sample to sample and are outlined in table 3.1.

3.4 SEM

Minerals that could not be effectively identified using transmitted and reflected light microscopy were identified with the Tescan Mira3 Field Emission Scanning Electron microscope (SEM) equipped with an X-MAX 80 Silicon Drift Detector energy dispersive spectrometer (EDS) at the Geological Survey of Canada (Ottawa, Ontario). Mineral identification was done using the AZtec Energy 3.2 microanalysis software. The SEM operated at a standard working distance of 15mm with a voltage set at 20 kV and a probe current of 400-1000 pA.

Additional compositional maps of garnets were collected using EDS. These maps have a pixel size of 3.3-3.9 μm with a dwell time of 15 ms per spot.

3.5 LA-ICPMS

The trace element compositions of garnets were mapped and quantified using the laser ablation inductively coupled mass spectrometer (LA-ICPMS) at the Geological Survey of Canada

(Ottawa, Ontario). These maps were carried out using a photon Machines Analyte G2 excimer laser ablation system (λ : 193 nm), with a Helex II 2-volume ablation cell, and an Agilent 7700x quadrupole ICP-MS. The methodology used follows closely to that described in Gaidies et al. (2020). Spot sizes ranged from 8 to 25 μm with scanning speeds of 8 to 50 $\mu\text{m/s}$. Maps generated at a spot size of $> 8 \mu\text{m}$ would advance one equivalent spot diameter in 0.5 s. The map of 18ZE-R-73C-S using a spot size of 8 μm would advance one equivalent spot diameter in 1.0 s. Each spot diameter included two or four measurements of each atomic mass of interest for samples with spot size $> 8 \mu\text{m}$ and 8 μm respectively. The program XMapTools (Lenari, 2019) is utilized herein to generate compositional maps.

3.6 Phase equilibrium modelling

Thermodynamic modelling was done using THERIAK-DOMINO software (de Capitani and Petrakakis, 2010) and thermodynamic data of Holland and Powell (1998), with solution models as in Gaidies et al. (2015) and silicate melt models from White et al. (2001). Silicate melt models were only included in the simulations for samples assessed to have likely reached temperatures necessary for melting given their mineral contents and microstructures (49B, 71, 81). Pseudosections and mineral composition isopleths were calculated using the $\text{MnO-Na}_2\text{O-CaO-K}_2\text{O-FeO-MgO-Al}_2\text{O}_3\text{-SiO}_2\text{-C-H}_2\text{O-TiO}_2$ system with H_2O and C in excess. The excess H_2O and C results in a C-O-H fluid in equilibrium with graphite at all pressures and temperatures in the investigated P-T range. 18ZE-R-16 was modelled with no C and the

following fO_2 buffer:

This buffer was chosen because all of these phases are likely present across large parts of the relevant P-T conditions for this sample. This fO_2 buffer was necessary because of the presence of the Fe^{+3} -bearing epidote both in the matrix and included in garnet. This buffer was chosen over the hematite-magnetite fO_2 buffer because of the lack of observable hematite in the sample and the destabilization of garnet-bearing assemblages resulting from the higher fO_2 associated with such a buffer. Modelling of sample 18ZE-R-49B was done by removing all P and the corresponding amount of Ca assuming that P is only present in apatite in this sample. This was done because the bulk rock composition of this sample has the lowest Ca/P molar ratio and a higher modal abundance of apatite compared to the other samples in this study resulting in a more significant change in the bulk rock composition.

All the modelling done in this thesis was performed using the Graham cluster supported by Compute Canada (<http://www.computecanada.ca>) and Compute Ontario (<https://computeontario.ca/>). The application of high-performance computing was essential to efficiently compute the large number of pseudosections and isopleth plots of this study.

3.7 THERIA_G modelling

Garnet growth modelling was done using THERIA_G (Gaidies et al., 2008) for 18ZE-R-11A and 18ZE-R-16 using the same thermodynamic data, solution models, and fluid composition

as for the THERIAK-DOMINO calculations. The kinetic data used to calculate intragranular diffusion of Mn, Mg, and Fe in garnet was obtained from Chakraborty and Ganguly (1992). The tracer diffusion coefficient of Ca, D_{Ca}^* was set to $\frac{D_{Fe}^*}{2}$ after Loomis et al. (1985) and Florence and Spear (1991).

3.8 Diffusion modelling

Major component diffusion in garnet of 18ZE-R-16 and 18ZE-R-14B after garnet growth was modelled using the same diffusion parameters as for the THERIA-G calculations. The diffusion models were run assuming a spherical geometry of garnet using the Crank-Nicholson scheme and Dirichlet boundary conditions (Crank, 1975). The spacing of the time-distance grid used in the diffusion simulations is 10000 years and 20 μm for 18ZE-R-14B, 5000 years and 25 μm for 18ZE-R-16 diff1, and 2500 years and 25 μm for 18ZE-R-16 diff2.

3.9 Lu-Hf garnet-whole rock age dating

Sample 18ZE-R-73C was fragmented using the SelFrag at the Geological Survey of Canada (Ottawa, Ontario). Individual garnets were picked and separated into two size groups (< 1.2 mm and > 1.7 mm diameter) to be dated separately. The other samples were crushed with a Rocklabs hydraulic press and garnets were hand picked from the coarse-crush. Individual garnet fragments were handpicked from a single magnetic fraction under a binocular microscope. Average grain sizes were ~ 3 mm for 18ZE-R-71, 2-3 mm for 18ZE-R-77A, and ~ 1.5 mm for 18ZE-R-14B. Sample preparation and Lu-Hf isolation were carried out as described

in Cutts and Smit (2018). Isotope measurements were performed at the Pacific Centre for Isotopic and Geochemical Research, University of British Columbia using Nu instruments Nu (#021) plasma multicollector ICP-MS and the methodology described in Cutts and Smit (2018) .

Table 3.1: EPMA run conditions for garnet maps

Sample	Accelerating Voltage (kV)	Current (nA)	Pixel Size (μm)	Number of Passes	Counting Time (ms)	Elements Analyzed
18ZE-R-73C	20	200	5	2	50/25	Si, Mn, Ca, Y, Mg/Al, Fe, Ti
18ZE-R-14B	20	200	5	2	50/25	Si, Mn, Ca, Y, Mg/Al, Fe, Ti
18ZE-R-73C-2	20	100	5	2	50/25	Si, Mn, Ca, Y, Mg/Al, Fe, Ti
18ZE-R-77A	20	100	8	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-81	20	100	10	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-11A	20	100	10	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-71	20	100	10	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-16	20	200	10	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-49B	20	200	10	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-14A	20	200	10	1	100	Si, Mn, Ca, Y, Mg
18ZE-R-14C	20	200	12	1	100	Si, Mn, Ca, Y, Mg

4. Results

4.1 Whole rock chemical compositions

The whole rock chemical compositions of each sample analyzed in this study are shown in table 4.1. The average metapelite of Symmes and Ferry (1991) is plotted for comparison. Compared to the average metapelite, these samples are all enriched in MnO and FeO. According to their positions in an AFM plot (Fig. 4.1) (Thompson, 1957) the Boundary Ranges samples tend to be more Al-rich and K-poor than the average metapelite and most of the Florence range samples. Sample 18ZE-R-71 appears anomalous in its composition and plots below the F-M tie-line and outside of the range of the AFM plot and is not plotted.

4.2 Petrography

4.2.1 Boundary Ranges Suite

4.2.1.1 18ZE-R-11A

This is an andalusite-plagioclase-chlorite-garnet-bearing white mica schist. The matrix is composed primarily of xenoblastic quartz and parallel platy white mica and chlorite defining

mm-scale compositional banding. Foliation-parallel ilmenite needles up to 0.8 mm long are scattered throughout the matrix and are partially replaced by rutile. The matrix also contains minor pyrite and chalcopyrite and trace amounts of zircon and Fe-oxide. The Fe-oxide commonly replace pyrite and chalcopyrite.

Andalusite porphyroblasts are typically subidioblastic and separated from the matrix by thin ($\sim 10 \mu\text{m}$) white mica rims. Some andalusite grains are partially or completely replaced by fine grained white mica or plagioclase and chlorite (Fig. 4.2A).

Garnet porphyroblasts range from 1-4mm in diameter. They commonly display one or two idioblastic faces, but replacement by quartz (Fig. 4.2B) or chlorite, plagioclase, and white mica is most common. Inclusions in garnet are primarily quartz and ilmenite with occasional zoisite or clinozoisite. These inclusions display a sigmoidal pattern which is often truncated along a straight internal boundary (Fig. 4.2C).

The scanned sample contains 262 garnets making up 4.2% of the total rock volume with a density of 5.25 garnets/cm³ and an average sphericity of 0.46. A crystal size distribution (CSD) plot (Fig. 4.3A) shows a bimodal distribution.

4.2.1.2 18ZE-R-14A

This is a garnet-bearing chlorite, white mica, plagioclase schist. The matrix is composed primarily of subidioblastic to xenoblastic plagioclase grains 0.1-0.5 mm in diameter aligned with foliation-parallel white mica and chlorite with xenoblastic quartz and accessory ilmenite. Plagioclase grains contain spiral inclusion trails of uncertain composition (Fig. 4.2E), likely chlorite, white mica and ilmenite.

Garnet occurs as subidioblastic porphyroblasts (Fig. 4.2D) 0.6-4 mm in diameter that

contain ilmenite and plagioclase inclusions up to 0.3 mm in size. Occasionally, plagioclase inclusions are separated from garnet by a thin layer of quartz. Inclusions with high birefringence are too fine-grained to be identified optically, and form a spiral pattern (Fig. 4.2D). Some garnet grains have rims partially replaced by chlorite. Irregular grain boundaries are only observed adjacent to plagioclase which appears to have been impinged on garnet during its growth.

The scanned sample contains 910 garnets making up 7.2% of the total rock volume with a density of 17.9 garnets/cm³ and an average sphericity of 0.52. A CSD plot (Fig. 4.3) shows a left-skewed log-normal distribution. Inspection of the 3D isolated garnets (e.g. Fig. 4.4A) illustrates the irregular shape of garnets in this sample. Impingement of garnet on garnet is also apparent in the 3D visualization (Fig. 4.4B).

4.2.1.3 18ZE-R-14B

This is a garnet-bearing white mica, chlorite, plagioclase schist. The matrix is mostly composed of foliation-parallel chlorite, white mica, elongate xenoblastic quartz and plagioclase, and rutile needles. Plagioclase also occurs as subidioblastic porphyroblasts which are up to 0.5mm across. The sample is somewhat heterogenous with 1 mm thick quartz-rich bands interspersed throughout the matrix.

Garnet porphyroblasts range from 0.1 to 2.5 mm and are subidioblastic to idioblastic and highly fractured (Fig. 4.2F). They contain inclusions of quartz, white mica, chlorite, and occasionally rutile. Both garnet and plagioclase porphyroblasts have quartz pressure shadows.

The scanned sample contains 756 garnets making up 1.9% of the total rock volume with

a density of 38.6 garnets/cm³ and an average sphericity of 0.61. A CSD plot (Fig. 4.3) shows a log-normal distribution.

4.2.1.4 18ZE-R-14C

This sample is a plagioclase, garnet, chlorite, white mica schist. The matrix is composed of foliation-parallel chlorite, white-mica, elongate xenoblastic plagioclase and quartz, and accessory ilmenite. Randomly oriented chlorite mats occur in clusters with partly sericitized plagioclase throughout the matrix (Fig. 4.2H) which are frequently seen partially replacing garnet. Also present throughout the matrix are trace amounts of graphite, pyrite, chalcopyrite, and zircon. Trace amounts of monazite are present in a vein-like structure that is sub-parallel with the foliation.

Garnet forms idioblastic porphyroblasts (Fig. 4.2G) 0.5 - 7 mm in diameter. The inclusions consist of fine grained white mica, zoned plagioclase < 0.5 mm across, and ilmenite < 0.6 mm long. The ilmenite inclusions form a spiral pattern. Thin (< 0.05 mm) cracks filled with chlorite and white mica are abundant.

The scanned sample contains 147 garnets making up 17.2% of the total rock volume with a density of 4.30 garnets/cm³ and an average sphericity of 0.46. The CSD plot (Fig. 4.3) shows no clear trends.

4.2.1.5 18ZE-R-16

This is an epidote and garnet bearing plagioclase, white mica, biotite schist. The crenulated foliation is defined by biotite and white mica. Finer grained biotite, white mica, and minor chlorite form anastomosed layers around xenoblastic plagioclase and quartz grains (Fig.

4.2J). The rock appears somewhat heterogenous with quartz-rich domains pinching in and out between biotite and white mica rich domains. Plagioclase occurs as xenoblastic grains within the matrix and subidioblastic porphyroblasts up to 0.8 mm in diameter. Plagioclase porphyroblasts contain inclusions of epidote and clinozoisite. Minor chlorite appears primary but it is typically seen replacing biotite, occasionally with relict biotite grains within larger chlorite clusters. Garnet porphyroblasts are rare ranging from 0.4-4 mm in diameter (Fig. 4.2I). They are subidioblastic to idioblastic and typically elongate parallel to the foliation. Garnet contains slightly sigmoidal inclusion trails of quartz, white mica and epidote. The matrix contains minor ilmenite, epidote, and pyrite and trace chalcopyrite.

The scanned sample contains 56 garnets making up 1.5% of the total rock volume with a density of 1.72 garnets/cm³ and an average sphericity of 0.52. The CSD plot (Fig. 4.3) shows a log-normal distribution.

4.2.1.6 18ZE-R-73C

This is a garnet, biotite, plagioclase schist. The matrix is composed of plagioclase, biotite, quartz and accessory ilmenite, pyrite, pyrrhotite, and apatite. Biotite is platy and defines a weak foliation. Plagioclase reaches up to 0.8 mm in diameter and is composed of concentrically-zoned cores overgrown by unzoned xenoblastic plagioclase. Chlorite commonly occurs as overgrowths on garnet and biotite but rare porphyroblasts up to 0.3 mm are present as well.

Subidioblastic and rounded garnet porphyroblasts occur in two size groups, the majority of them fall in the small size group (Fig. 4.2K) < 1.4 mm in diameter and a small portion fall in the larger size group (Fig. 4.3L) 1.4 - 4 mm in diameter. The garnets of the larger

size group are commonly irregularly shaped compared to those in the smaller size group which are spherical and idioblastic. Inclusions of ilmenite and quartz are common in garnet independent of its size but are more abundant in the larger garnet grains. The inclusions in the larger garnet grains display a weak spiral pattern (Fig. 4.2D).

Due to the bimodal size distribution of garnet, size and spatial data were collected in two parts for this sample. Garnets over 1.4mm^3 were counted across the entire rock volume for a total of 56 garnets making up 1.2% of the total rock volume with a density of 1.18 garnets/ cm^3 and an average sphericity of 0.55. The CSD plot (Fig. 4.3) of these larger garnets does appear to have a log-normal distribution. Garnets of all sizes were counted across a smaller subvolume consisting of a 1.6 mm thick segment along the long axis of the cylindrical sample. The subvolume contains 1911 garnets and make up 4.0% of that subvolume with a density of 1016 garnets/ cm^3 and an average sphericity of 0.88. The CSD plot of the garnets in this subvolume (Fig. 4.3) shows a log-normal distribution with an apparent upper cut-off at ~ 0.6 mm radius.

4.2.2 Florence Range Suite

4.2.2.1 18ZE-R-77A

This is a garnet-bearing plagioclase, white mica, biotite schist. The matrix is composed of xenoblastic quartz and plagioclase, foliation parallel biotite and white mica, minor rutile, pyrite, Fe-oxide, apatite, and trace monazite, zircon, and xenotime. Quartz-rich domains pinch in and out between mica-rich domains. Some plagioclase grains reach up to 1.6 mm in length and display concentric zoning. The Fe-oxide in the matrix is frequently observed

replacing pyrite and is likely a result of late oxidation of sulfide.

Garnet porphyroblasts are subidioblastic (Fig. 4.5A) ranging from 0.5 to 2.5 mm in diameter. Garnet edges are locally replaced by plagioclase and biotite. The garnet porphyroblasts contain abundant plagioclase, quartz, ilmenite, biotite, white mica, and rare apatite inclusions. Some of the larger quartz, plagioclase, and biotite inclusions form linear inclusion trails (Fig. 4.5B) at moderate angle to the matrix foliation. Up to 0.3 mm wide cracks in garnet are filled with plagioclase, biotite, and quartz.

The scanned sample contains 481 garnets making up 5.5% of the total rock volume with a density of 9.33 garnets/cm³ and an average sphericity of 0.42. A CSD plot (Fig. 4.6) shows a log-normal distribution. The XR- μ CT imaging indicates that a majority of garnets contain these < 0.3 mm wide filled cracks (Fig. 4.7).

4.2.2.2 18ZE-R-81

This is a garnet-bearing biotite, plagioclase schist. The matrix is composed of foliation parallel biotite, elongate, xenoblastic quartz and plagioclase, accessory ilmenite, alkali feldspar, pyrite, and rutile, and trace apatite, tourmaline, zircon, monazite, and allanite. White mica rarely occurs as primary, foliation parallel crystals with biotite. It most commonly occurs as fine grained, randomly oriented mats replacing and pseudomorphing garnet and sillimanite. No traces of sillimanite have been observed but pseudomorphs of prismatic sillimanite indicates it was at one point stable (Fig. 4.5E).

Garnet typically occurs as subidioblastic, rounded porphyroblasts (Fig. 4.5C) 0.2 - 5 mm in diameter. They commonly contain inclusions of quartz, white mica, pyrite, and ilmenite. These frequently form inclusion trails that are parallel or subparallel with the

matrix foliation. Very rarely, garnet can be observed showing an atoll shape (Fig. 4.5D), the interior of which is primarily plagioclase.

The scanned sample contains 2630 garnets making up 5.2% of the total rock volume with a density of 80.5 garnets/cm³ and an average sphericity of 0.75. A CSD plot (Fig. 4.6) shows a log-normal distribution.

4.2.2.3 18ZE-R-49B

This sample is a garnet and sillimanite-bearing biotite, white mica schist with complex and unique textural features. A sinistral C-S fabric is defined by sillimanite and biotite. White mica usually occurs as fine-grained masses throughout the matrix but also as randomly oriented coarse grained crystals, usually replacing biotite with quartz and feldspar. Biotite is commonly rimmed and replaced by sillimanite (Fig. 4.5G) or intergrown with white mica. Randomly oriented biotite locally replaces garnet edges. Sillimanite occurs throughout the matrix and is mostly fibrous but few prismatic grains have also been observed. Chlorite partially replaces biotite and garnet. The matrix contains minor amounts of pyrite, ilmenite, apatite, plagioclase, and trace amounts of cordierite, chalcopyrite, monazite, zircon, xenotime, and allanite.

Garnet porphyroblasts (Fig. 4.5F) range from 1.5-8 mm in diameter. They occur within quartzofeldspathic lenses and contain abundant inclusions of biotite, quartz, white mica, plagioclase, staurolite, ilmenite, apatite, zircon, and rarely kyanite. Where preferentially oriented, the inclusions are at a high angle to the matrix foliation. Kyanite inclusions in garnet occur with biotite, and one kyanite inclusion contains a staurolite inclusion. Some biotite inclusions in garnet show a symplectite-like intergrowth with quartz, plagioclase and

white mica. The staurolite inclusions are up to 0.4 mm long and commonly associated with biotite and quartz (Fig. 4.5H).

The scanned sample contains 31 garnets making up 2.5% of the total rock volume with a density of 0.89 garnets/cm³ and an average sphericity of 0.51. This is not enough garnets to produce a meaningful CSD plot.

4.2.2.4 18ZE-R-71

This is a garnet and plagioclase-bearing graphite, biotite schist. The matrix is predominantly composed of xenoblastic quartz with single grains up to 2mm in length. The foliation is defined by platy graphite and biotite that occasionally has thin plagioclase rims. Plagioclase occurs as xenoblastic grains up to 1.5mm in length with concentric zoning apparent under crossed-polars. Also present in the matrix is trace zircon, monazite, allanite, pyrite, and chalcopyrite. Garnet porphyroblasts are rounded and subidioblastic (Fig. 4.5I) and range from 1.2 to 4mm in diameter. Garnet is partially replaced by chlorite and biotite at the rim and within abundant fractures. Garnet contains inclusions of quartz which show a weak spiral pattern.

The scanned sample contains 332 garnets making up 7.9% of the total rock volume with a density of 5.66 garnets/cm³ and an average sphericity of 0.73. A CSD plot (Fig. 4.6) shows a log-normal distribution.

4.3 Major element chemical composition of garnet

4.3.1 Boundary Ranges Suite

The major element distribution maps of garnet in the BRS samples (Fig. 4.8, 4.9, and 4.10) and the line profiles (Fig. 4.13) show concentric zoning with X_{Ca} and X_{Mn} highs in the cores and lows in the rims, as well as X_{Mg} and X_{Fe} lows in the cores and highs in the rims (core compositions in Table 4.2). 18ZE-R-11A (Fig. 4.8) shows a significant change in the chemical gradient 0.37-0.4mm from the rim where X_{Mn} and X_{Ca} noticeably increase (outlined in Fig. 4.8B). This increase is associated with a textural discontinuity in the garnet inclusions. 18ZE-R-14A shows two distinct positive peaks in X_{Ca} and X_{Mn} and negative peaks in X_{Fe} and X_{Mg} at its core. A small compositional discontinuity is visible in 18ZE-R-14B in both the spessartine and almandine components, it is most obvious in the line profile at ~ 0.9 and 1.8 mm.

Annuli are present in the X_{Ca} zoning pattern of 18ZE-R-73C (Fig. 4.10). This is more apparent in the rim of the larger garnet (73C-L) and throughout the entirety of the smaller garnet (73C-S) (Fig. 4.10, A and B respectively). The X_{Ca} zoning in the core of 73C-L is patchy with lows in X_{Ca} often corresponding with cracks and inclusions in the core. A sharp but small change in X_{Ca} can be used to demarcate two generations of garnet growth in 73C-L (G1 and G2 in Figs. 4.17 and 4.13). Differences between the profiles of the large and small garnet of 18ZE-R-73C are apparent (73C-L and 73C-S respectively) (Fig. 4.15). X_{Ca} and X_{Mg} are higher and X_{Fe} and X_{Mn} are lower in the core of 73C-S compared to the core of 73C-L. Near the rims the compositions approach the same values with X_{Fe} and

X_{Ca} lining up ~ 0.3 mm from the rim and X_{Mn} and X_{Mg} lining up ~ 0.1 mm from the rim. Before these synchronizations occur, the concentration gradients are steeper in garnet of 73C-S compared to that in 73C-L. It is also apparent that the radius of 73C-S is close to equal the length of the G2 portion of garnet radius in 73C-L.

4.3.2 Florence Range Suite

The major element distribution maps of garnet in the FRS samples (Figs. 4.11 and 4.12) and the line profiles (Fig. 4.14) show concentric zoning with X_{Ca} and X_{Mn} highs in the core and lows in the rim, as well as X_{Mg} and X_{Fe} low in the core and high in the rim (core compositions in Table 4.2). The garnets of the FRS are more homogenous than those of the BRS, with almost completely flat profiles in all the FRS samples except 18ZE-R-77A which shows well preserved but still smooth zoning patterns. 18ZE-R-49B (Fig. 4.12) exhibits a sharp increase in X_{Ca} 0.6-1.0 mm from the rim (outlined in Fig. 4.12B).

Spikes in X_{Mn} and X_{Fe} and dips in X_{Mg} are present at the outer edges of the garnets. These are most likely a result of ion-exchange and Mn backdiffusion (Kohn and Spear, 2000). These spikes also appear at the edges of cracks and embayments in the garnets which affected zoning patterns in 18ZE-R-77A, 18ZE-R-81, and 18ZE-R-49B (Fig. 4.11A,B and 4.12).

4.4 Trace element garnet chemistry

4.4.1 Boundary Ranges Suite

In 18ZE-R-14B and 18ZE-R-73C Lu and Y maps (Fig. 4.16A-C) show similar zoning patterns. 14B, 73C-L, and 73C-S each have multiple annuli but 73C-L has patchy zoning in its core. In 14B, Lu is highest in the core and decreases towards the rim. Y has a similar trend but contains a large spike in concentration close to the rim. In 73C-L the Lu and Y concentrations are highest about 0.6 mm from the rim when the annuli begin to appear, 73C-S exhibits similar concentric annuli with the highest Lu and Y concentrations near the core of the garnet.

V, Sm, Eu, and Gd maps of 73C-L and 73C-S emphasize two distinct regions in 73C-L separated by sharp changes in concentration (Fig. 4.17). The garnet core (G1 in Figs. 4.17 and 4.13) is characterized by high homogenous V, low homogeneous Sm, Eu, Gd and patchy Y and Lu. This core has several straight crystal faces, but also shows irregular embayments. It is overgrown by an idioblastic rim (G2 in Figs. 4.17 and 4.13) characterized by concentrically-zoned V decreasing towards the rim, oscillatory-zoned and relatively high Sm, Eu, Gd, Lu and Y. Similar patterns are apparent on a smaller scale in 73C-S.

4.4.2 Florence Range Suite

In sample 77A, Lu concentration is highest in the core and decreases towards the rim with one concentric annulus near the rim with elevated Lu concentrations (Fig. 4.16D). This annulus is truncated by the resorbed edges of the garnet (top and bottom of the image). Y

concentrations show the same pattern but the highest Y concentration is within the annulus near the rim. There are also elevated Y concentrations along the crack that cuts vertically across garnet on the right side of the image. Sample 71 shows perfect concentric zoning in Lu and Y decreasing from core to rim (Fig. 4.16E).

In sample 18ZE-R-49B, there are two distinct regions demarcated by a sharp change in concentration of trace elements (Fig. 4.18, Appendix C) that coincides with variations in major elements (e.g. Ca, Fig. 4.12). The boundary between these two regions is generally irregular, but rare straight segments are characteristic of former crystal faces. In the inner region (G1 in Figs. 4.12 and 4.14), Li, Na, and P increase in concentration towards the rim and sharply decreases in the outer region (G2 in Figs. 4.12 and 4.14). Sc, Zr, Y, Gd, and Lu show patchy zoning in the inner region. The outer region is marked by a sharp increase in concentration of these elements that decreases towards the rim. The zoning pattern of these elements is parallel to the boundary between the inner and outer region.

4.5 Lu-Hf garnet-whole rock ages

Timing of metamorphism was determined using Lu-Hf garnet dates (Table 4.3, Fig. 4.19). Samples 18ZE-R-77A and 18ZE-R-14B yield equivalent dates within error (190.9 ± 3.3 Ma and 192.4 ± 0.4 respectively). This corresponds to the oldest monazite dates documented in 18ZE-R-77A by Soucy La Roche et al. (in review). 18ZE-R-71 has a younger date at 185.3 ± 1.1 Ma. The Lu in these samples is strongly fractionated into the core (Fig. 4.16), suggesting these dates represent the early stages of garnet nucleation and growth in both the Florence Range and Boundary Ranges suite. The younger date in 18ZE-R-71 might be due

to diachronous burial of the FRS from the WRSZ. Alternatively, the date could represent the crystallization age of a younger generation of garnet (Smit et al., 2013), resulting from dating garnets smaller and thus younger than the first garnets to nucleate (Table 4.3). Whereas garnets dated in the other samples are closer in size to the largest garnet (60-70% of the size in terms of diameter), the garnet dated in 18ZE-R-71 have a diameter approximately equal to half that of the largest garnet in the sample.

Sample 18ZE-R-73C is approximately 10 Myr older than 18ZE-R-14B and 18ZE-R-77A with a date of 201.7 ± 2.8 Ma. In this sample, Lu fractionated more strongly into the rim of the larger garnets and the core of the smaller garnets indicating that the date reflects a stage later in the garnet growth history. Large and small garnets were dated separately, fall on the same isochron, and yield equivalent dates within error (202.4 ± 5.7 Ma and 201.6 ± 9.7 Ma for the large and small fractions, respectively, Fig. 4.19). Equivalent dates for both fractions indicate that any difference in timing of growth, if present, must be within the analytical uncertainty. There is no clear reason why this sample is older than the other dated samples. The simplest explanation is that it may have been part of a sliver distinct from the BRS and the FRS, that was structurally entrained within the WRSZ. This sliver would need to have been metamorphosed earlier before being moved to its current position at the top of the BRS.

4.6 Equilibrium phase relations and P-T conditions of initial garnet growth

The pseudosections and garnet isopleth plots discussed in this section represent phase relations and garnet compositions at thermodynamic equilibrium. This assumes that every component in the model system for a given sample is available for any phase following the equilibrium constraints. However, since garnet sequesters the components it requires for growth, making them unavailable for other reactions, its crystallization modifies the effective bulk rock composition (EBRC) and changes the equilibrium phase relations and mineral compositions (Hollister, 1966). Therefore, these plots are representations of the phase relations and garnet compositions before and at the initial stage of garnet growth in the respective sample. To determine the subsequent P-T evolution of the sample during metamorphism, chemical fractionation of garnet and its impact on the EBRC need to be considered (See section 5).

In the core isopleth plots, the pyrope isopleth is frequently shown not to be intersecting with the almandine, grossular, and spessartine isopleths. The pyrope content in these garnet cores with preserved growth zoning is always low ($< 3.5\%$). With lower concentrations of any component, small variations in predicted garnet chemistry can have significant effects on where an isopleth will be plotted. For example, if the model predicts 1.5% pyrope at the intersection of the other three isopleths but the measured pyrope content is 2%, that isopleth can be up to 15°C higher than the intersection point. This is compounded by the fact that the spacing between pyrope isopleths is typically large compared to the spacing of

other isopleths. We still include all isopleths in our analysis, but it is important to consider when interpreting the apparent precision of these P-T estimates.

4.6.1 Boundary Ranges Suite

4.6.1.1 18ZE-R-11A

This pseudosection (Fig. 4.20A) has many fields that aid in the interpretation of this petrologically complex sample. The garnet core isopleths intersect at a point at the garnet-in curve at $\sim 505^{\circ}\text{C}$ and 480 MPa. The predicted assemblage at this point is Fsp, Ilm, Grt, Cld, Chl, WM, and Qz and differs from the observed mineral assemblage (Table 2.2) which has andalusite and does not contain chloritoid. This indicates that chloritoid left the assemblage at a later point in the metamorphic history of the rock.

4.6.1.2 18ZE-R-14A

The garnet core isopleths do not intersect in the considered P-T space (Fig. 4.20B) indicating that our thermodynamic model is not able to predict the garnet core composition. However, the grossular, almandine, and pyrope isopleths come close at 480 - 490 $^{\circ}\text{C}$ and ~ 590 MPa in the predicted stability field of Fsp, Ilm, Grt, Chl, WM, and Qz. This mineral assemblage is stable between 460 and 510 $^{\circ}\text{C}$ and 560 and 680 MPa and corresponds to the observed mineral assemblage (Table 2.2). However, it is unlikely that the P-T path of the sample was restricted to this small P-T window after the initial growth of garnet. The high modal abundance of zoned plagioclase ($\sim 50\%$ of the rock volume) in this sample reflects chemical disequilibrium across the rock sample which likely affected the phase relations during garnet

growth. However, this fractionation effect has not been considered in this study due to modelling limitations and is the most likely reason the garnet core isopleths do not intersect.

4.6.1.3 18ZE-R-14B

The garnet core isopleths for spessartine, grossular, and almandine nearly intersect at a point (Fig. 4.21A) at $\sim 490^{\circ}\text{C}$ and 550 MPa. This intersection point is $\sim 15^{\circ}\text{C}$ and 50 MPa above the garnet-in curve. When pyrope is included, the intersection point becomes an intersection area at $T = 480 - 490^{\circ}\text{C}$ and $P = 510 - 550$ MPa. The lower limit of this intersection area is closer to the garnet-in curve but still above it by $\sim 5^{\circ}\text{C}$ and 10 MPa. The assemblage that corresponds to this intersection area is Fsp, Ilm, Grt, Chl, WM, Bt, and Qz and differs from the observed mineral assemblage (Table 2.2) which lacks biotite, possibly indicating that biotite left the assemblage at a later point in the metamorphic history of the rock.

4.6.1.4 18ZE-R-14C

The garnet core isopleths for spessartine, grossular, and almandine nearly intersect at a point (Fig. 4.21B) at $\sim 485^{\circ}\text{C}$ and 450 MPa. This intersection point is $\sim 10^{\circ}\text{C}$ and 50 MPa above the garnet-in curve. When pyrope is included, the intersection point becomes an intersection area at $T = 485 - 500^{\circ}\text{C}$ and $P = 450 - 680$ MPa. This isopleth intersection area spans multiple fields, but the predicted assemblage at the spessartine, grossular, and almandine intersection is Fsp, Ilm, Grt, Chl, WM, and Qz. This does correspond to the observed assemblage (Table 2.2), as does the field directly above this with the assemblage Fsp, Ilm, Grt, Chl, (2)WM, and Qz. These two fields have a P-T range of $465 - 570^{\circ}\text{C}$ and 330 - 760 MPa.

4.6.1.5 18ZE-R-16

Only the garnet core isopleths for grossular and almandine intersect at a point on the garnet in curve (Fig. 4.22A). The isopleth for the spessartine content at the core is at too low a pressure to intersect at this point but a small variation in spessartine content shown as an isopleth with a concentration 5% lower (0.2649 at the dotted line vs. 0.2788 at the dashed line on Fig. 4.22A) intersects at the same point as grossular and almandine at $\sim 505^{\circ}\text{C}$ and 480 MPa. This intersection point lies in the predicted stability field of Fsp, Ilm, Grt, Chl, WM, Bt, and Qz and it is at the edge of a similar field that also contains epidote, which corresponds to the observed assemblage (Table 2.2) and the field spans a P-T range of 500 - 565°C and 460 - 820 MPa.

4.6.1.6 18ZE-R-73C

This pseudosection (Fig. 4.22B) has a few large fields that commonly span 100°C and 400 MPa intervals. This sample is also unique in its prediction of talc at low pressure and higher temperature ($> 600^{\circ}\text{C}$, < 500 MPa). The intersection area of the core isopleths is large, with a P-T range of $520 - 555^{\circ}\text{C}$ and 410 - 830 MPa. At its lowest P-T bound this intersection area is $\sim 20^{\circ}\text{C}$ higher than the garnet-in curve. This intersection area overlaps four fields corresponding with three assemblages: Fsp, Ilm, Grt, Chl, Bt, and Qz; Fsp, Ilm, Grt, Chl, WM, Bt, and Qz; Fsp, Ilm, Grt, Chl, (2) WM, Bt, and Qz. The first assemblage best matches the assemblage observed in the sample (Table 2.2) and only fails to predict rutile. This stability field corresponds to a P-T range of $490 - 650^{\circ}\text{C}$ and 200 - 830 MPa.

In summary, the BRS samples show garnet core isopleth intersections at moderate temperatures and pressures between 480 and 505 °C and 450 and 550 MPa, indicating a geothermal gradient of ca. 25 to 30 °C/km typical of Barrovian-type metamorphism in continental crust of common composition. The assemblages predicted at these P-T conditions are similar and typically contain Fsp, Ilm, Grt, Chl, Wm, Qz $\pm$ Bt.

4.6.2 Florence Range Suite

Samples 18ZE-R-81, 18ZE-R-49B (G1, Fig. 4.14 and 4.12B), and 18ZE-R-71 have relaxed compositional profiles as a result of diffusion. The zoning profile of 81 and 71 are almost completely flat. These relaxed profiles suggest that growth zoning in these samples has been modified and therefore the core composition no longer represents the chemical composition of garnet when it crystallized. Therefore the garnet core isopleth intersection areas of these samples are less reliable representations of the sample's P-T history.

4.6.2.1 18ZE-R-77A

This sample is characterized by the most pronounced growth zoning of FRS samples and as a result, the garnet core isopleths for spessartine, almandine, and grossular nearly intersect at a point (Fig. 4.23A) at $\sim$ 505°C and 550 MPa. When the pyrope isopleth is included, it becomes an intersection area with a P-T range of 505-510 °C and 540-590 MPa. The lower bounds of this intersection area are $\sim$ 10°C and 50 MPa above the garnet-in curve. This gap is likely a result of small modifications of the garnet composition by diffusion. The intersection area lies in the predicted stability field of Fsp, Ilm, Grt, Chl, WM, Bt, and Qz

and differs from the observed assemblage (Table 2.2) which lacks chlorite and contains rutile. This indicates that chlorite left the assemblage at a later point in the metamorphic history of the rock.

4.6.2.2 18ZE-R-81

The garnet core isopleths of this sample (Fig. 4.23B) have an isopleth intersection area with a P-T range of 565-580 °C and 630 - 700 MPa. This lies in the predicted stability field of Fsp, Ilm, Grt, Chl, WM, Bt, and Qz and differs from the observed assemblage (Table 2.2) which contains pseudomorphed sillimanite, alkali feldspar, and rutile and lacks chlorite.

4.6.2.3 18ZE-R-49B

The garnet core isopleths for spessartine, pyrope, and almandine intersect at a point (Fig. 4.24A) at 690 °C and 280 MPa. This lies at the edge of the stability fields of (2)Fsp, Ilm, Grt, Bt, Sil, and Qz and (2)Fsp, Ilm, Grt, Bt, Crd, Sil, and Qz. These differ from the observed assemblage (Table 2.2) which contains white mica. The grossular isopleth does not intersect with any other isopleth in the considered P-T space.

4.6.2.4 18ZE-R-71

This pseudosection is dominated by three large fields that span more than 200 °C and 500 MPa (Fig. 4.24B). The garnet core isopleths for spessartine, pyrope, and grossular have an intersection area with a P-T range of 610-690 °C and 420 - 700 MPa. This intersection area lies in the stability fields of (2)Fsp, Ilm, Grt, WM, Bt, and Qz and (2)Fsp, Ilm, Grt, Bt, and Qz and differs from the observed assemblage (Table 2.2) which lacks alkali feldspar and

white mica.

Figure 4.1: AFM plot after Thompson (1957) for the samples in this study (except 18ZE-R-71, which falls outside plot area) as well as average metapelite from Symmes and Ferry (1991)

Figure 4.2 (*preceding page*): Photomicrographs and BSE images of Boundary Ranges Suite samples, abbreviations after Whitney and Evans (2010), WM = White mica. **(A):** 18ZE-R-11A andalusite porphyroblast being replaced by Pl + Chl, also with a thin WM rim (XPL). **(B):** 18ZE-R-11A Grt partially replaced by Qz (PPL). **(C):** 18ZE-R-11A BSE photo of Grt, dashed lines indicate inclusion trails within Grt, solid lines indicate discontinuity of these inclusion trails. **(D):** 18ZE-R-14A typical irregularly shaped Grt porphyroblast with fine grained inclusion trails (PPL). **(E):** 18ZE-R-14A matrix Pl crystals with fine grained inclusion trails (PPL). **(F):** 18ZE-R-14B typical idioblastic Grt porphyroblast (PPL). **(G):** 18ZE-R-14C, typical idoblastic Grt porphyroblast with Pl and Ilm inclusions (PPL). **(H):** 18ZE-R-14C patchy Chl + Pl region in matrix (PPL). **(I):** 18ZE-R-16 typical idioblastic Grt porphyroblasts (PPL). **(J):** 18ZE-R-16 anastomosed Bt layers around xenoblastic Qz and Pl (PPL). **(K):** 18ZE-R-73C typical idioblastic Grt porphyroblasts of the smaller Grt size class (PPL). **(L):** 18ZE-R-73C hypidioblastic Grt of the larger Grt size class with Ilm + Qz inclusion trails (PPL).

Figure 4.3 (*preceding page*): Volume normalized crystal size distribution (CSD) plots of Boundary Ranges suite samples: **(A)**: 18ZE-R-11A, **(B)**: 18ZE-R-14A, **(C)**: 18ZE-R-14B, **(D)**: 18ZE-R-14C, **(E)**: 18ZE-R-16, **(F)**: Larger size class of 18ZE-R-73C, **(G)**: Smaller size class of 18ZE-R-73C

Figure 4.4: **(A)**: 3D view of a garnet from 18ZE-R-14A produced using Blob3D illustrating the irregular form typical in this sample. **(B)**: 3D view of multiple garnets impinging upon one another in 18ZE-R-14A

Figure 4.5: Photomicrographs of Florence Range Suite samples, abbreviations after Whitney and Evans (2010), WM = White mica. **(A):** 18ZE-R-77A typical hypidioblastic Grt porphyroblasts with WM, Pl, and Bt inclusions (PPL). **(B):** 18ZE-R-77A Qz + Pl + Bt cracks cutting across garnet (XPL) **(C):** 18ZE-R-81 typical hypidioblastic Grt porphyroblasts (PPL). **(D):** 18ZE-R-81 rare atoll Grt filled with Pl + Chl (PPL). **(E):** 18ZE-R-81 WM pseudomorphing prismatic Sil, no relict Sil is observed in this sample (XPL) **(F):** 18ZE-R-49B Grt rich with inclusions of Bt, Qz, and WM (XPL) **(G):** 18ZE-R-49B Sil replacing Bt in matrix (PPL). **(H):** 18ZE-R-49B St + Bt inclusions in Grt (PPL). **(I):** 18ZE-R-71 typical hypidioblastic Grt porphyroblast (PPL).

Figure 4.6: Volume normalized crystal size distribution (CSD) plots of Florence Range suite samples: **(A)**: 18ZE-R-77A, **(B)**: 18ZE-R-81, **(C)**: 18ZE-R-71

Figure 4.7: CT cross section of 18ZE-R-77A, arrows indicate filled cracks in garnets

Figure 4.8: (A): BSE image with Mn, Mg, Fe, and Ca composition maps of a centrally sectioned garnet from 18ZE-R-11A. Line on BSE photo indicates location of quantitative profile (Fig. 4.13). (B): Sketched outline of 18ZE-R-11A indicating extent of the inner G1 and outer G2 garnet generations

Figure 4.9: BSE image with Mn, Mg, and Ca composition maps of centrally sectioned garnets from the Boundary Ranges Suite (Except 18ZE-R-11A and 18ZE-R-73C). Lines on BSE photos indicate location of quantitative profiles (Fig. 4.13). (A): 18ZE-R-14A, dashed line indicates separation between two distinct chemical cores G-A and G-B, (B): 18ZE-R-14B, (C): 18ZE-R-14C, (D): 18ZE-R-16

Figure 4.10: BSE image with Mn, Mg, and Ca composition maps of centrally sectioned garnets from 18ZE-R-73C. Lines on BSE photos indicate location of quantitative profiles (Fig. 4.13). (A): 18ZE-R-73C-L, a garnet from the larger garnet size class in this sample. (B): 18ZE-R-73C-S, a garnet from the smaller garnet size class in this sample.

Figure 4.11: BSE image with Mn, Mg, and Ca composition maps of centrally sectioned garnets from the Florence Range Suite (Except 18ZE-R-49B). Lines on BSE photos indicate location of quantitative profiles (Fig. 4.14). (A): 18ZE-R-77A, (B):18ZE-R-81, (C): 18ZE-R-71

Figure 4.12: (A): BSE image with Mn, Mg, Y, and Ca composition maps of a centrally sectioned garnet from 18ZE-R-49B. Lines on BSE photo indicate location of quantitative profiles (Fig. 4.14). (B): Sketched outline of 18ZE-R-49B indicating extent of the inner G1 and outer G2 garnet generations

Figure 4.13: Major element compositional profiles for the garnets of Boundary Ranges samples along the lines shown in figures 4.8, 4.9, and 4.10.

Figure 4.14: Major element compositional profiles for the garnets of Florence Range samples along the lines shown in figures 4.11 and 4.12

Figure 4.15: Scaled comparison of major element compositional profiles for the large (73C-L) and small (73C-S) garnet size classes in 18ZE-R-73C

Figure 4.16: Lu and Y LA-ICPMS maps of (A): 18ZE-R-14B, (B)18ZE-R-73C-L, C)18ZE-R-73C-S, D) 18ZE-R-77A, E)18ZE-R-71

Figure 4.17: V, Sm, Eu, and Gd LA-ICPMS maps of (A): 18ZE-R-73C -L with sketched outline indicating extent of the inner G1 and outer G2 garnet generations and (B): 18ZE-R-73C-S

Figure 4.18: Li, Na, P, Sc, Zr, Y, Gd, and Lu LA-ICPMS maps of 18ZE-R-49B

Figure 4.19: Lu-Hf isochron plots for samples listed in table 4.3

Figure 4.20 (*preceding page*): Calculated pseudosections and garnet core isopleths abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-11A: 1 = Fsp Cld Chl WM Qz Rt, 2 = Fsp Ilm Grt Bt Crd Sil Qz, 3 = Ilm Cld Chl (2)WM Czo Qz Rt, 4 = Fsp Ilm Grt Bt St And Qz, 5 = Ilm Grt Cld Chl (2)WM Czo Qz Rt, 6 = Ilm Grt Cld Chl (2)WM Czo Qz, 7 = Fsp Grt Chl (2)WM St Qz Rt, 8 = Fsp Grt Chl WM St Qz Rt, 9 = Fsp Ilm Grt WM Bt St Ky Qz, 10 = Fsp Grt WM Bt St Ky Qz Rt, 11 = Fsp Grt (2)WM Bt Ky Qz Rt **(B)** 18ZE-R-14A: 1 = Fsp Ilm Grt Chl (2)WM Bt Qz, 2 = Fsp Ilm Chl (2)WM Czo Qz , 3 = Fsp Ilm Grt Chl WM Qz , 4 = Fsp Ilm Grt Chl (2)WM Qz , 5 = Fsp Ilm Grt WM Bt Ky Qz, 6 = Fsp Ilm Grt WM Bt Qz, 7 = Fsp Ilm Grt WM Bt Qz Rt, 8 = Fsp Ilm Grt (2)WM Bt Qz Rt, 9 = Fsp Grt WM Bt Qz Rt

Figure 4.21 (*preceding page*): Calculated pseudosections and garnet core isopleths abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-14B: 1 = Fsp Ilm Grt Chl Bt Crd Qz , 2 = Fsp Ilm Grt Bt Crd And Qz, 3 = Fsp Ilm Chl WM Qz, 4 = Fsp Ilm Chl WM Czo Qz, 5 = Fsp Ilm Chl (2)WM Czo Qz, 6 = Fsp Ilm Grt Chl WM Qz, 7 = Fsp Ilm Grt Chl (2)WM Czo Qz Rt, 8 = Fsp Ilm Grt Chl (2)WM Qz, 9 = Fsp Ilm Grt Chl WM Bt Czo Qz Rt, 10 = Fsp Grt Chl Bt St Qz Rt **(B)** 18ZE-R-14C: 1 = Fsp Ilm Cld Chl WM Bt Qz, 2 = Fsp Ilm WM Bt And Qz, 3 = (2)Fsp Ilm Bt And Qz, 4 = Fsp Ilm Grt WM Bt Sil, 5 = Fsp Ilm Grt WM Qz, 6 = Fsp Ilm Grt WM St Qz, 7 = Fsp Ilm Grt WM St, 8 = Fsp Ilm Grt WM St Ky, 9 = Fsp Ilm Grt WM Qz Rt, 10 = Fsp Ilm Grt WM Bt Qz Rt, 11 = Ilm Grt Chl (2)WM Czo Qz, 12 = Ilm Grt Chl (2)WM Bt Qz Rt

Figure 4.22 (preceding page): Calculated pseudosections and garnet core isopleths abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-16: 1 = Fsp Ilm Ep (2)WM Bt Qz Rt , 2 = Fsp Ilm Ep Grt (2)WM Bt Qz Rt, 3 = Fsp Ilm Grt WM Bt Qz Rt **(B)** 18ZE-R-73C: 1 = Fsp Ilm Chl Bt Qz , 2 = Fsp Ilm Chl WM Bt Czo Qz Rt, 3 = Fsp Ilm Chl WM Bt Czo Qz Rt, 4 = Fsp Ilm Grt Chl WM Bt Qz Rt, 5 = Fsp Ilm Grt Chl Bt Qz Rt

Figure 4.23 (*preceding page*): Calculated pseudosections and garnet core isopleths abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-77A: 1 = Fsp Ilm Grt Chl (2)WM Bt Qz, 2 = Ilm Grt (2)WM Bt Czo Qz, 3 = Fsp Ilm Grt (2)WM Bt Czo Qz, 4 = Ilm Grt Chl (2)WM Bt Qz Rt, 5 = Ilm Grt Chl (2)WM Bt Qz, 6 = Fsp Ilm Grt (2)WM Bt Qz Rt **(B)** 18ZE-R-81, 1 = Fsp Ilm Chl Bt Qz, 2 = Fsp Ilm Grt Chl WM Bt Czo Qz Rt, 3 = Fsp Grt Chl Bt St Qz Rt, 4 = Fsp Grt Bt St Qz Rt, 5 = Fsp Grt WM Bt Ky Qz Rt, 6 = Fsp Ilm Grt Bt Qz Rt, 7 = Fsp Ilm Grt Bt Melt Qz Rt, 8 = Fsp Grt Bt Melt Ky Qz Rt

Figure 4.24 (*preceding page*): Calculated pseudosections and garnet core isopleths abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-49B: 1 = Fsp Ilm Chl WM Bt St Qz, 2 = (2)Fsp Ilm Grt Crd Sil Qz, 3 = (2)Fsp Ilm Grt Crd Sil, 4 = Fsp Ilm Grt Crd Sil Qz, 5 = (2)Fsp Ilm Grt Bt Melt Sil Qz, 6 = Fsp Ilm Grt Chl WM Bt Czo Qz, 7 = Fsp Ilm Grt WM Bt Melt Sil Qz, 8 = Ilm Grt Bt Melt Sil Qz, 9 = Ilm Chl (2)WM Czo Qz Rt, 10 = Ilm Grt Chl WM Czo Qz, 11 = Fsp Ilm Grt WM Bt Qz, 12 = Ilm Grt WM Bt Melt Qz Rt **(B)** 18ZE-R-71: 1 = (2)Fsp Ilm Grt Bt Melt Qz, 2 = Ilm Grt Bt Melt Qz

Table 4.1: Bulk rock chemical compositions in oxide weight % of the samples analyzed in this study, and the average pelite from Symmes and Ferry (1991)

Sample	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MnO	MgO	CaO	Na ₂ O	K ₂ O	TiO ₂	P ₂ O ₅	LOI	Σ
Boundary Ranges Suite												
18ZE-R-11A	59.32	19.01	9.75	0.18	3.06	1.09	0.97	2.27	1.09	0.13	4.01	100.88
18ZE-R-14A	54.76	19.38	12.43	0.17	2.13	1.78	4.74	1.21	1.33	0.42	2.09	100.44
18ZE-R-14B	62.01	17.03	8.19	0.20	2.55	2.23	3.73	1.07	0.77	0.22	2.52	100.52
18ZE-R-14C	43.52	27.72	13.02	0.17	1.31	2.31	2.43	3.89	2.03	0.39	3.62	100.41
18ZE-R-16	52.82	20.39	9.79	0.19	3.70	2.55	2.37	4.61	0.90	0.21	2.45	99.98
18ZE-R-73C	61.08	15.10	11.21	0.19	3.55	2.91	2.66	0.78	0.71	0.17	1.65	100.01
Florence Range Suite												
18ZE-R-77A	61.66	15.94	11.50	0.12	2.39	1.17	1.78	3.54	0.80	0.06	1.52	100.48
18ZE-R-81	56.11	18.30	10.03	0.13	3.74	3.75	3.04	2.14	0.99	0.23	1.35	99.81
18ZE-R-49B	51.37	24.39	11.21	0.05	2.44	0.41	0.64	5.96	1.07	0.13	2.76	100.43
18ZE-R-71	67.28	12.09	8.73	0.15	1.45	0.85	0.48	6.24	0.46	0.23	2.03	99.99
Av. Pelite	59.77	16.57	6.53	0.07	2.62	2.17	1.73	3.53	0.00	0.00	7.65	100.64

Table 4.2: Garnet core composition in oxide weight % of the samples analyzed in this study

Sample	SiO ₂	TiO ₂	Al ₂ O ₃	FeO	MnO	MgO	CaO
18ZE-R-11A	36.98	0.1420	20.46	25.81	8.764	0.892	7.295
18ZE-R-14A	37.53	0.1712	20.93	23.13	9.811	0.280	9.435
18ZE-R-14B	36.06	0.1467	20.79	20.65	9.966	0.416	10.493
18ZE-R-14C	36.23	0.0945	19.67	27.27	5.088	0.389	7.848
18ZE-R-16	37.65	0.1627	20.78	20.63	12.44	0.630	8.982
18ZE-R-73C-L	36.26	0.0322	20.90	28.35	7.969	1.790	4.248
18ZE-R-73C-S	37.67	0.0603	21.81	27.29	6.398	3.308	5.499
18ZE-R-77A	36.54	0.1607	20.72	26.20	5.975	0.600	9.053
18ZE-R-81	37.32	0.0380	20.91	32.68	1.459	3.501	3.879
18ZE-R-49B	37.15	0.0078	21.12	37.43	1.452	2.698	0.921
18ZE-R-71	34.10	0.0039	19.98	34.20	2.379	1.004	2.853

Table 4.3: Summary of Lu-Hf garnet dates

Sample	Lu-Hf age (Ma)	2 σ (Ma)	(¹⁷⁶ Hf/ ¹⁷⁷ Hf) _i	2 σ	MSWD	<i>n</i>	Dated garnet diameter (mm)	Largest garnet diameter (mm)
Boundary Ranges Suite								
18ZE-R-14B	192.4	0.4	0.282053	0.000017	1.8	4	1.5	2.4
18ZE-R-73C-S	202.4	5.7	0.282131	0.000017	1.19	4	< 1.2	1.4
18ZE-R-73C-L	201.6	9.7	0.282128	0.000053	2.3	4	1.7 - 3.5	4.2
18ZE-R-73C all	201.7	2.8	0.282131	0.000015	1.40	7	-	-
Florence Range Suite								
18ZE-R-77A	190.9	3.3	0.281991	0.000028	1.3	5	2 - 3	4.4
18ZE-R-71	185.3	1.1	0.281482	0.000047	2.5	4	3	5.8

The (¹⁷⁶Hf/¹⁷⁷Hf)_i is the calculated initial ¹⁷⁶Hf/¹⁷⁷Hf before decay began. The MSWD is the mean squared weighted deviation and indicates the degree of scatter in the data where a higher value means greater scatter.

5. Discussion

Determining P-T paths with garnet core isopleth intersections and peak assemblage fields is not very effective for many of these samples. Many of the fields associated with the peak assemblages of these samples are large and provide imprecise constraints on pressure and temperature, and most of the FRS samples have core compositions modified by diffusion and do not reflect the P-T conditions at the onset of garnet growth.

Due to the common occurrence of garnet, its slow intracrystalline diffusion, and well constrained solution models, garnet growth modelling presents an effective solution to this issue. Tools such as THERIA_G (Gaidies et al., 2008) can provide precise P-T paths by matching predicted garnet zoning with observed garnet zoning. Several factors make garnet growth modelling a challenge with the samples in this study. For most FRS samples, the core composition has been significantly modified by diffusion. While diffusion is accounted for in THERIA_G, the resulting profiles become less path-dependent with higher degree of modification. Based on the extent of modification of garnet in samples 81, 49B, and 71, confidently determining a P-T path from their zoning can be challenging. The BRS garnets that were analyzed have not been altered by diffusion based on the preservation of small but systematic changes in composition of fast-diffusing elements (Mn and Fe; Chakraborty

and Ganguly 1991) such as the abrupt change in spessartine and almandine composition from G1 to G2 in 18ZE-R-11A (Figs. 4.13, 4.8B) and the abrupt change in spessartine and almandine content in 18ZE-R-14B at ~ 0.9 and 1.8 mm on the line profile (Fig 4.13). Sample 77A has been less affected by diffusion than the other FRS samples. The challenge with these samples is that only two of them (11A and 16) provide core isopleth intersection points at the garnet-in curve. The rest have isopleth intersection areas > 10 °C and 50 MPa higher than the garnet-in curve. For 18ZE-R-77A, this might be explained with modification by diffusion but for the other samples this presents a challenge.

Several scenarios may explain the differences in P-T conditions between garnet core isopleth intersections and garnet-in curves: (1) Reaction overstepping, where this gap is a result of an energy barrier to nucleation of garnet (e.g. Pattison and Tinkham, 2009; Gaidies et al., 2011; Pattison et al., 2011; Gaidies, 2017; Spear and Wolfe, 2019). (2) The sequestration of components into other phases such as plagioclase before and during garnet crystallization. The high modal abundance of zoned plagioclase in many of these samples makes it a likely culprit. Other phases such as ilmenite have been observed to sequester Mn which if taken into account can raise the garnet-in curve by up to 50 °C and 150 MPa (McCarron et al., 2019). (3) The thermodynamic data does not adequately describe the phases observed, especially given the samples are not average metapelites and are enriched in MnO. (4) The chemical system was not closed and some degree of metasomatism occurred, changing the bulk rock composition during or after garnet crystallization.

We lack the data to account for these scenarios but the problem is still present and prevents us from estimating the P-T evolution during the metamorphism of most samples in this study. To sidestep these issues, we developed the G_FRAC garnet fractionation model

which provides rough estimates of the associated evolution of the effective bulk rock composition (EBRC) on the basis of the 3D distribution of the garnet volume in the studied samples and the compositional zoning of their largest garnet crystals. As opposed to previous garnet fractionation approaches (e.g. Konrad-Schmolke et al., 2008a; Moynihan and Pattison, 2013; Robyr et al., 2014), knowledge of the thermodynamic phase relations during garnet growth is not required for G_FRAC modelling. Instead, this model is employed with the assumption that the discrepancies between observed and predicted garnet composition and mineral content of garnet growth forward models reflect inappropriate EBRC predictions and that the aforementioned scenarios have a relatively minor impact on P-T estimates. The EBRC obtained from G_FRAC modelling may then be used with software such as THERIAK-DOMINO (de Capitani and Petrakakis, 2010), Perple_X (Connolly, 2005), or THERMOCALC (Powell and Holland, 1988) to calculate the progression of metamorphic phase equilibria during garnet crystallization.

5.1 G_FRAC

We developed G_FRAC to simulate fractionation associated with garnet growth. This is an inverse model that combines measured garnet volumes from XR- μ CT data with garnet composition profiles from EPMA data to estimate the change of the EBRC during garnet crystallization, assuming that internal metasomatism (Spear, 1988) from intracrystalline garnet diffusion did not significantly modify the EBRC.

The composition profile of garnet is ideally a central section through the long axis of the biggest garnet. G_FRAC assumes the composition of all other garnets in the sample using

this profile, such that the composition of garnet at a distance d from the rim is the same in all grains (as observed in George and Gaidies (2017)). The composition at the largest distance d , i.e. in the core of the largest garnet, is only observable in that garnet. This relationship is dependent on several assumptions:

1. All garnets are spheres
2. All garnets in the sample grow at the same radial rate for a given P-T step
3. Resorption or post-growth ion-exchange reactions involving garnet only occurred inward from the outer edge on all garnets and equally from all sides

Following these assumptions is that the largest garnet nucleated first and the smallest garnet nucleated last.

5.1.1 Model setup

G_FRAC models fractionation based on the volumetric distribution data provided from an XR- μ CT scan of a single sample. It therefore requires the absolute number of moles of each component to be calculated for that scanned volume. G_FRAC uses the rock density, sample volume, and bulk rock composition to do this calculation based on the assumption that these properties did not change after the onset of garnet crystallization in the sample.

There will typically be a discrepancy between the length of the profile from core to rim and the radius of the biggest garnet obtained from CT scanning because the measured composition profile might not be a cut through the perfect center of the biggest garnet or the garnet might not be a perfect sphere. G_FRAC accounts for this in two ways: inward extrapolation or stretching.

If the composition profile was not measured in the biggest garnet, it can be assumed that the typically homogeneous core composition of the second or third biggest garnet is the same as the biggest garnet. In this situation it is appropriate to take an average of the first three points of the profile measured at the core and extrapolate that inward to match the radius of the biggest garnet. This will maintain the length scale at the rim of the garnets. This correction was used for samples where a central section was cut through the second, third, or fourth largest garnet instead of the first largest and the length of the profile is not longer than the diameter of the calculated radius of the largest garnet. The only sample in which a central section was not cut across the largest garnet is 18ZE-R-14A.

Otherwise, if the composition profile is measured in the biggest garnet but is not along the longest axis or the garnet is non-spherical then it is more appropriate to stretch the profile. This will modify the distance between every point in the profile. This correction was used for every sample where a central section was cut through the largest garnet in the sample or the length of the profile is longer than the diameter of the calculated radius of the largest garnet. This correction was applied to all samples except 18ZE-R-14A.

There is also the possibility that the measured profile is off-center. If this is the case then it is more likely due to the geometric core of garnet is not in the same location in the garnet as the chemical core. Error in sample preparation is possible, however the central sections were matched as closely as possible to the CT images, so error is unlikely to be more than the size of a pixel (i.e. 20 - 50 μm). In either case, garnet core compositions were typically homogeneous indicating that the measured compositions at the core are representative of the initial stages of garnet growth.

Once the profile is fitted to match the radius of the largest garnet in the data-set, a

linear interpolation is done between each point in the profile. This interpolated profile is used to calculate the composition of each garnet shell. The normal thickness of each shell dr is calculated by $dr = R/3000$, where R is the radius of the largest garnet. The composition of each shell is equal to the average composition of the left and right side of the increment on the profile that the shell corresponds to.

5.1.2 Model algorithm

1. Nucleate the first garnet with radius $r = dr$ with the left side of the shell at $x = 0$ on the composition profile
2. Add a shell with a thickness of dr to the garnet
3. Continue adding shells, progressing through the chemical profile until the following condition is met: $r_{g1} + dr \geq r_{G1} - r_{G2}$ where r_{g1} is the radius of the biggest garnet at the current model step, r_{G1} is the final radius of the biggest garnet calculated from its measured volume, and r_{G2} is the final radius of the second biggest garnet calculated from its measured volume
4. Add a shell to the first garnet with a thickness $dr_a = r_{G1} - r_{G2} - r_{g1}$
5. Add another shell of the normal thickness dr
6. Nucleate a new garnet with radius $r = dr$ with the same composition of the outermost shell of the other garnets in the system
7. Go back to step 2 and add the shells to every garnet present in the system. The nucleation parameter will always check the n^{th} garnet against the $(n + 1)^{th}$ garnet

where n is the smallest garnet currently present in the system.

8. Stop adding shells once $r_{g1} = r_{G1}$

These steps are illustrated in figure 5.1.

For each shell added on each individual garnet, G_FRAC tracks the absolute number of moles of each component in that shell. The amount of moles n for component i in a given garnet shell k ($n_{i,k}$) is derived from the following equations:

$$n_{i,k} = \frac{m_{i,k}}{M_i} \quad (5.1)$$

$$f_{i,k} = \frac{X_{i,k}M_i}{\sum_{j=1}^p X_{j,k}M_j} \quad (5.2)$$

$$m_{i,k} = f_{i,k}m_k \quad (5.3)$$

Where $m_{i,k}$ is the mass of component i in shell k , $f_{i,k}$ is the mass fraction of component i in shell k , $X_{i,k}$ and $X_{j,k}$ are the molar fraction of components i and j in shell k , M_i and M_j are the molar mass of components i and j , p is the total number of components in garnet, and m_k is the mass of garnet shell k

The mass fraction of a component in a given garnet shell can only be determined if m_k is known. If the volume V of garnet shell k is known and a value for the density of garnet ρ_{grt} is chosen then m_k can be determined with $m_k = V_k\rho_{grt}$. The value for density used in the models in this thesis is 4.19 g/cm³ (Nesse, 2013).

Equation 5.3 can then be substituted into equation 5.1 to get:

$$n_{i,k} = \frac{f_{i,k}m_k}{M_i} \quad (5.4)$$

Equation 5.2 can then be substituted into equation 5.4 to get:

$$n_{i,k} = \frac{X_{i,k}M_im_k}{M_i \sum_{j=1}^p X_{j,k}M_j}$$

Which simplifies to:

$$n_{i,k} = \frac{X_{i,k}m_k}{\sum_{j=1}^p X_{j,k}M_j} \quad (5.5)$$

With equation 5.5, the total moles of each component in all the garnet present at a given model step can be calculated:

$$n_{i,tot} = \sum_{s=1}^t \left(\sum_{k=1}^l n_{i,k} \right)_s \quad (5.6)$$

Where s is a given garnet that is present in the current model step, t is the total number of garnets present in the current model step, and l is the total number of shells within garnet s for the current model step. EBRC is calculated simply by removing $n_{i,tot}$ from the initial bulk rock composition. G.FRAC does this calculation and outputs an effective bulk rock composition at regular radial intervals of the biggest garnet. It also records the garnet

composition at these intervals to be modelled with this EBRC.

5.1.3 Output

The program produces a series of THERIAK-DOMINO (de Capitani and Petrakakis, 2010) script files to model garnet isopleths at different intervals along the given garnet composition profile. G_FRAC itself calculates EBRC after garnet fractionation, it does not run any thermodynamic models. Therefore, the output of G_FRAC is independent of any thermodynamic database and not restricted by potential errors that might occur as a result of inaccuracies in the database.

5.2 Model results and P-T paths

G_FRAC modelling provides useful results for every sample of this study except 18ZE-R-73C for which we were unable to effectively predict garnet composition with THERIAK-DOMINO. Garnet isopleth intersection areas for each sample in the BRS and FRS at different stages of chemical fractionation associated with progressive garnet crystallization are shown in figures 5.2 and 5.3 respectively. The profiles used for these models and intervals of each stage of fractionation are shown in figures 5.4 and 5.5.

5.2.1 Boundary Ranges Suite

5.2.1.1 18ZE-R-11A

The microstructural discontinuities within garnet that coincide with the abrupt changes in chemical composition suggest two separate garnet growth events (forming G1 and G2 in Figs.

4.8B and 4.13). These garnets have had multiple stages of growth and resorption, producing irregular garnet shapes with uncertain amounts of garnet missing from the calculation of volume. The resorption results in an underestimation of volume removed. This will also result in garnets being removed from the EBRC at a later stage of fractionation than reality. Despite this, an apparent P-T path is produced which aligns well with the other samples of the BRS (Fig. 5.2).

It is likely that this is not a reflection of the robustness of the G_FRAC model and more a reflection on the effectiveness of the garnet solution model used in this study. This sample is one of only two samples which has a garnet core isopleth intersection at or very close to the garnet-in curve prior to any fractionation (Fig. 4.20A). This is a good indication that the solution models and thermodynamic database used are effective for thermodynamic modelling of this sample. Isopleth intersection areas of this sample remain tight for early stages of garnet fractionation but grow larger at later stages. At stages 16 and 17 (Fig. 5.4), which are the final two stages before the G2 garnet, the isopleths are so far apart that no reasonable isopleth intersection area can be determined (left out of Fig. 5.2). The tight isopleth intersection along most of the calculated P-T path suggests that the error produced by removing a lower volume of garnet at early stages of fractionation is not significant. The most likely reason for this is the lower volume of garnet removed does not affect the EBRC enough to change where the garnet isopleths plot. The stages within garnet G2 are also excluded because we do not consider them reliable representations of the true P-T conditions of the sample at their time of growth because we cannot account for the changes in EBRC from resorption of garnet before G2 growth.

The isopleth intersection area corresponding to the last stage plotted (stage 15, Fig. 5.4)

on figure 5.2 has a P-T range of 540 to 555 °C and 600 to 660 MPa and overlaps eight fields on the pseudosection (Fig. 5.6A) with assemblages of Grt, Chl, WM, Qz $\pm$ St, Cld, Czo, Fsp, Ilm, Rt. This intersection area overlaps with the staurolite-in reaction so the appearance of staurolite might be the reason why the G1 garnet was partially resorbed. While no staurolite is observed, it is likely that the low-pressure overprint consumed any staurolite that formed after G1 garnet grew and before the growth of G2 garnet initiated. The low pressure overprint in this sample makes it challenging to assess what the peak assemblage was and estimate peak P-T conditions. Based on the similarity of the predicted P-T path of this sample with other samples in the BRS (Fig. 5.2), it is unlikely the peak P-T conditions extended more than 15 °C past the upper temperature limit of the isopleth intersection area of stage 15.

This pseudosection also provides some insight into the low pressure overprint. The key mineral in the low-pressure overprint is andalusite. Andalusite does not appear to be growing at the expense of garnet, so it is possible the outer garnet (G2 in Figs. 4.8B and 4.13) formed during this low pressure event as well. This provides constraints to the andalusite and garnet bearing fields in the lower portion of the pseudosection (Fig. 5.6A). The lack of biotite in the observed assemblage restricts this further to a small field of Fsp, Ilm, Grt, Chl, WM, And, and Qz and differs from the observed assemblage (Table 2.2) which contains rutile. This rutile is relatively low in abundance and could be relict from the earlier higher pressure event. This field restricts the peak P-T conditions of the low pressure event to a P-T range of 505 to 515 °C and 200 to 230 MPa.

5.2.1.2 18ZE-R-14A

The garnet isopleths do not intersect until the 4th stage of garnet fractionation (Fig. 5.4), which is the first isopleth intersection area shown in figure 5.2. At stage 7, the spessartine isopleth begins to diverge further away from the other isopleths until it disappears from the plot completely in stage 8. The isopleth intersection areas used in stage 8 and later are therefore only using the almandine, grossular, and pyrope isopleths. The final fractionation stage is left out from figure 5.2 as well because the almandine isopleth begins to diverge too much to plot a reasonable isopleth intersection area. The isopleth intersection area of the last stage plotted (stage 10) on figure 5.2 has a P-T range of ~ 545 °C and 620 to 750 MPa and lies in the predicted stability field (pseudosection in Fig. 5.6B) of Fsp, Ilm, Grt, Chl, WM, Bt, and Qz and differs from the observed mineral assemblage (Table 2.2), which lacks biotite.

This sample is problematic for several reasons. It is likely there is another process modifying the EBRC of the sample that is unaccounted for in our models. One possible culprit is the high modal abundance of zoned plagioclase within this sample. Plagioclase is also frequently included in garnet, which both sequesters plagioclase and increases the apparent volume of garnet calculated based on the CT scan. Both of these features would reasonably affect the EBRC, removing the Ca available for garnet growth.

Another possible issue with this sample is the shape of garnet. Due to apparent impingement of garnet growth by plagioclase, many of the garnets in this sample deviate far from the ideal spherical garnet shape, often appearing in irregular clusters. Garnet impingement is commonly seen in this sample, evident in the major element map and line profile (G-A

and G-B in Figs. 4.9A and 4.13) and the 3D intersection of multiple garnet crystals (Fig. 4.4). As a result, the measured garnet volumes may not be entirely appropriate for modelling fractionation during garnet growth.

Despite these issues, the calculated P-T path follows the same trend as the other BRS samples and has overlapping isopleth intersection areas for the final stages of growth with samples 14B and 14C that were collected at the same outcrop.

5.2.1.3 18ZE-R-14B

This sample produced the most consistently small isopleth intersection areas between 14A, 14B, and 14C (Fig. 5.2). This sample contains the lowest volume of garnet with the most consistently euhedral or spherical shape between the three. Since this sample best meets model assumptions, we consider the P-T path of this sample to be the most reliable of the three. The isopleth intersection area at the final stage of fractionation has a P-T range of 550 to 610 °C and 680 to 890 MPa and lies within the predicted stability field (pseudosection in Fig. 5.7A) of Fsp, Ilm, Grt, Chl, WM, Bt, Qz $\pm$ rutile and differs from the observed assemblage, which lacks biotite (Table 2.2).

The primary issue observed in this sample is the increasing distance between the isopleth intersection area and the garnet-in curve. This discrepancy is observed even before fractionation with the ~ 15 °C and 50 MPa gap between the garnet core isopleth intersection area and the garnet-in curve. This issue is discussed in more detail at the beginning of section 5. It is reasonable to assume that this “error” would be propagated as progressively lower volumes of garnet are removed than would be predicted with THERIAK-DOMINO. The other possible factor is the exclusion of cut garnets at the edge of the sample that would

reduce the volume of garnet removed from the EBRC. While the volume added by these may seem negligible, it is possible that this exaggerates the issue further.

5.2.1.4 18ZE-R-14C

For the first 7 of 12 fractionation stages, the grossular, spessartine, and almandine isopleths intersect at a point above the garnet in curve. In the final five stages, the spessartine isopleth diverges. Stage 8 and onward on figure 5.2 show only the intersection between grossular, pyrope, and almandine isopleths. The isopleth intersection at the final stage of fractionation has a P-T range of ~ 550 °C and 650 to 720 MPa and overlaps two fields that contain the predicted assemblage (pseudosection in Fig. 5.7B) of Fsp Ilm Grt Chl (2)WM Qz $\pm$ Bt. The lower pressure field, which lacks biotite, is identical to the observed mineral assemblage (Table 2.2).

It is important to note that the garnets in this sample contain a high volume of ilmenite inclusions. This is another sequestration process that is not accounted for in these models and if incorporated, would likely result in raising the garnet-in curve to a higher pressure and temperature due to removal of important garnet forming components Mn and Fe.

The low number of garnets combined with the high volume introduces more potential sources of error. Many garnets were cut along the edges of the scanned sample and the measured volumes do not reflect the true sizes of garnet. Since we do not correct for partially cut garnets, the model was run with the edge garnets removed from the calculation, providing an underestimation of garnet removal, likely contributing to the gap between isopleth intersections and the garnet-in reaction.

5.2.1.5 18ZE-R-16

The P-T path calculated for this sample provides a P-T path very similar to 18ZE-R-11A. This P-T path continuously straddles the epidote-in reaction line and crosses it several times. At each stage of fractionation the garnet isopleth intersection areas stay relatively close to the garnet in curve ($< 100^{\circ}\text{C}$ and 100 MPa) compared to the other samples in this study. The isopleth intersection areas remain small, covering a $< 10^{\circ}\text{C}$ and 30 MPa span except for when it is in the epidote-bearing field and the spacing between grossular isopleths is large, up to 100 MPa difference in pressure with a 5% increase or decrease in grossular content. The isopleth intersection at the final stage of fractionation has a P-T range of 555 to 565 $^{\circ}\text{C}$ and 650 to 680 MPa and lies in the predicted stability field (pseudosection in Fig. 5.8A) of Fsp, Ilm, Grt, Chl, WM, Bt, and Qz. This differs from the observed mineral assemblage (Table 2.2), which contains epidote, and rutile but the isopleth intersection area is only 30 MPa below the epidote-in reaction and rutile is low in abundance in this sample.

5.2.1.6 18ZE-R-73C

Using G_FRAC did not aid in determining P-T paths for this sample. The large phase stability fields in the pseudosection, older date, and multiple garnet growth events makes an enigmatic sample. This challenge is further compounded by the apparent lack of equilibrium between different garnets in the sample, which is seen in the comparison between the major element profile of 73C-L and 73C-S (Fig. 4.15). The higher Ca and lower Fe in the core of 73C-S and the differences between their profiles until the outer 0.3 mm indicates that a significant portion of the garnet growth history in this sample was not interface controlled

growth but dominated by another process such as diffusion (e.g. Kretz, 1974; Lasaga, 1986; Carlson, 1989; Carlson and Denison, 1992). This is beyond the constraints of G_FRAC and THERIA_G and presents a modelling challenge beyond the scope of this study.

5.2.2 Florence Range Suite

5.2.2.1 18ZE-R-77A

Since this sample has the best preserved garnet growth zoning in the FRS, it is key to document the P-T history of the FRS. The isopleth intersection areas remain small ($< 15^{\circ}\text{C}$ and 50 MPa span, Fig. 5.3) until the final three stages of fractionation (Fig. 5.5) where the spessartine isopleth begins to diverge and move off the plot in the second last stage. The intersection areas of the other three isopleths remain small however. The final isopleth intersection area has a P-T range of 605 to 615 $^{\circ}\text{C}$ and 980 to 1010 MPa and lies in the stability field (pseudosection in Fig. 5.8B) of Fsp, Ilm, Grt, WM, Bt, and Qz and differs from the observed mineral assemblage (Table 2.2) which contains rutile. The apparent P-T path follows the same trend as those seen in the BRS however it shows a higher peak P and T than those samples.

From the major and trace element maps (Figs. 4.11A, 4.16D) and profiles (Fig. 4.14), it can be inferred that there has been some degree of garnet resorption. While the garnets in this sample have appeared to maintain their form and the resorption does not seem significant, this still results in a loss of volume that will result in underestimations of garnet removal in G_FRAC. In addition the annulus seen near the rim of the garnet in the Lu and Y maps (Fig. 4.16D) has been truncated on the resorbed edges of the garnet. With the

annulus as an indicator of extent of resorption, it is apparent the composition profile we measured does not reflect the full extent of garnet growth in this sample. This means some portion of the metamorphic history is not recorded and the sample may have a higher peak P and T than shown in figure 5.3.

This Lu and Y annulus is seen in the other REEs (Appendix C) and exhibits the shape of a euhedral garnet suggesting there was no resorption prior to the formation of the annulus. It corresponds to a change in inclusion density with no observed changes in the major element composition, indicating this annulus is a result of a reaction along the same P-T path. In the trace element maps of P (Appendix C) there are many P rich inclusions before the annulus and none past it, and the annulus coincides with an increase in P concentration in garnet. The likely culprit of this is the apatite-out reaction which would supply some of the REE needed to form this annulus. While the P-T conditions of formation for the garnet past the annulus cannot be determined with this dataset, the edge of the profile used in this model lines up with the annulus and can provide a P-T constraint for an apatite-out reaction.

5.2.2.2 18ZE-R-81

Only the isopleth intersection area after the final stage of fractionation is displayed on figure 5.3. Due to the mostly homogenous composition of these garnets, we only assessed the very edge of the garnet as an accurate representation of its composition at equilibrium. The composition of the garnet rim that we used to calculate a P-T point has been modified by resorption and re-equilibrium with the matrix during Mg-Fe exchange and Mn back diffusion (Fig. 4.14). The hypidioblastic shape of the majority of garnets in this sample suggests that resorption has not modified their size and shape too significantly or that it has acted at an

approximately equal rate on all sides of each garnet. This indicates that the outer edge likely represents equilibrium along a retrograde path. In figure 5.3 two polygons are displayed for this sample with the dashed line indicating the extent of the pyrope, grossular, and almandine intersection area and the larger including spessartine. The isopleth intersection area at the final stage of fractionation has a P-T range of 585 to 615 °C and 400 to 700 MPa and overlaps two fields in the pseudosection (Fig. 5.9A), which have predicted stable mineral assemblages of Fsp, Ilm, Grt, Bt, St, Qz, $\pm$ Chl. This differs from the observed assemblage (Table 2.2) which lacks staurolite and contains white mica and alkali feldspar. The white mica is mostly retrograde, seen locally replacing garnet and pseudomorphing sillimanite. This replacement of garnet is rare and the extent is variable ranging from partial to complete replacement. It is likely this replacement reaction was strongly influenced by local equilibrium later along the retrograde path. The isopleth intersection area shown in figure 4.14 would therefore represent equilibrium of garnet with the matrix on a sample scale. While no staurolite is present in the sample, the isopleth intersection area is right at the high pressure edge of another field with a stable assemblage of Fsp, Ilm, Grt, Bt, Sil, and Qz. This sample does contain pseudomorphs of sillimanite, so this could be a reasonable P-T constraint on the last point of garnet-matrix equilibrium.

5.2.2.3 18ZE-R-49B

This is a complex sample which has experienced multiple stages of garnet growth based on the zoning patterns of Ca, Fe, and trace elements (Figs. 4.12, 4.14, 4.18). Monazite inclusions in garnet from this sample have been dated at 270-217 Ma in contrast to monazite in the matrix, which yields 190-175 Ma dates, suggesting that at least this sample experienced two

separate metamorphic events (Soucy La Roche et al., in review).

Due to the presence of staurolite and kyanite inclusions in the G1 garnet we do not consider the isopleth intersection point in figure 4.24A a realistic point along its P-T path as the formation of those phases would require a steeper P-T path. The presence of kyanite inclusions restricts the possible peak assemblage of the first metamorphic event to three fields with assemblages of Ilm, Grt, WM, Bt, Ky, and Qz; Fsp, Ilm, Grt, WM, Bt, Ky, and Qz; and Ilm, Grt, WM, Bt, Melt, Ky, and Qz. These fields correspond to a P-T range of 640 - 750 °C and 680 - 900 MPa.

Due to the low number of garnets in this sample and their large size, we included the partially cut garnets in the fractionation model. Removing them would have resulted in a significant reduction in total garnet volume and the error introduced because of this was assessed to be more significant than the error of using the sizes of cut garnets.

The relaxed compositional profile in the first generation of garnet (G1 in Figs. 4.12B and 4.14) means its composition is not reflective of its original growth zoning. For this reason, we ignore garnet G1 and only show isopleth intersection areas for G2 garnet. The isopleth intersection areas for this sample shown in Figure 5.3 correspond to stages 20 and 24 in the fractionation sequence (Fig. 5.5). Stage 20 is the first model stage of the G2 garnet. The isopleth intersection area of stage 20 is shown with a dashed outline in figure 5.3. At stage 20, the isopleths do not completely intersect (Fig. 5.10A) so we plotted the region where the predicted pyrope, grossular, and almandine contents closest match the observed garnet composition. Diffusion appears to have modified the concentration of spessartine more significantly than the other components which is why they are given more weight in determining the P-T conditions at stage 20. This intersection has a P-T range of 700 to 715

°C and 680 to 750 MPa and lies in the field with a predicted stable assemblages of Fsp, Ilm, Grt, WM, Bt, Melt, Sil, and Qz. This lines up well with the observed mineral assemblage (Table 2.2). In addition, the presence of garnets within quartzofeldspathic lenses and the homogenous composition of G2 except at the interface with G1 or the matrix indicates that it grew in the presence of melt since the chemical gradient between G1 and G2 rules out diffusion as a possible cause of homogenization. The strong enrichment in REEs and HFSEs and depletion in LILEs in G2 compared to G1 (Fig. 4.18) provide further evidence of garnet growth in the presence of melt (Gaidies et al., 2020).

The final stage (stage 24) of fractionation is when all other garnet is removed from the thermodynamically effective chemical system. The garnet isopleths at this stage intersect at a point on the garnet-in curve (Fig. 5.10B), indicating a remarkable match with the observed garnet rim composition at the P-T point of $\sim 610^{\circ}\text{C}$ and ~ 490 MPa. The associated phase equilibrium calculations point to an assemblage composed of Fsp, Ilm, Grt, WM, Bt, Sil, and Qz. This also closely matches the observed matrix assemblage (Table 2.2) with the absence of cordierite. Cordierite is rare and very likely a low pressure overprint similar to the one observed in 18ZE-R-11A. This isopleth intersection area also aligns well with the one observed in 18ZE-R-81.

5.2.2.4 18ZE-R-71

Like 18ZE-R-81, only the isopleth intersection area associated with the final fractionation stage is displayed on figure 5.3. Due to the mostly homogenous composition of these garnets, we only assessed the very edge of the garnet as an accurate representation of its composition at equilibrium. The composition of the garnet rim that we used to calculate a P-T point has

been modified by resorption and re-equilibrium with the matrix during Mg-Fe exchange and Mn back diffusion (Fig. 4.14). The hypidioblastic to idioblastic shape of all the garnets in this sample suggests that resorption did not modify size and shape of garnet too significantly. The isopleth intersection area at the final stage of fractionation is at the garnet in curve with a P-T range of 675 to 700 °C and 570 to 730 MPa and overlaps two fields on the pseudosection (Fig. 5.9B), which contain predicted stable assemblages of (2)Fsp, Ilm, Grt, Bt, Qz, $\pm$ WM. White mica is not present in the observed assemblage but the lower pressure field does not contain white mica. This field is still not a perfect match though because alkali-feldspar or ilmenite were not observed in the sample.

The isopleth intersection area records a higher P and T than 18ZE-R-81 but lines up close to the approximated isopleth intersection area of stage 20 in 18ZE-R-49B. The limited resorption likely contributed to the preservation of garnet composition at a higher temperature compared to 81 and 49B. Being at a higher temperature, around 700 °C, there was likely some diffusion after this last point of equilibrium. This would modify the observed composition and introduce inaccuracies and is a possible reason why the isopleth intersection area provides a large range of possible temperatures and pressures.

5.3 Comparison with forward modelling

THERIA_G models were produced using the P-T paths determined with the use of G_FRAC and THERIAK-DOMINO (Table 5.1). The THERIA_G models produced for 18ZE-R-11A and 18ZE-R-16 were effectively able to predict the garnet zoning observed in both samples after they were rescaled to be the same length as the sphere-normalized diameter of the

largest garnet. Due to the garnet overgrowth on 18ZE-R-11A, the displayed zoning profile (Fig. 5.14) does not extend across the whole garnet radius. The fit of the THERIA_G profile also gets worse as it comes closer to the rim of the G1 garnet. This is similar to what we observe in the G_FRAC models. The THERIA_G model of 18ZE-R-16 fits the observed profile almost perfectly along this path (Fig. 5.15).

We were not able to use THERIA_G to accurately model garnet growth in any other sample. For the reasons discussed in the beginning of section 5, the rest of the samples had other factors that were uncertain and unaccounted for and prevented us from applying the forward model. Therefore these two samples serve as a calibration for G_FRAC to confirm that the results we get from it are consistent with results we get from forward modelling.

5.4 Discussion on G_FRAC

Linking the EBRC predictions of G_FRAC with THERIAK-DOMINO calculations permitted the estimation of prograde and retrograde P-T points in the sample suite. Reproducing garnet zoning using THERIA_G following the same paths as predicted with G_FRAC and THERIAK-DOMINO shows this method provides similar results to well established methods. This has allowed us to expand the P-T dataset from these samples suites and provides the added benefit of being able to predict retrograde P-T points in garnet-bearing samples.

The weakness of G_FRAC is that it does not account for diffusion during growth and the resulting internal metasomatism. Significant modification of garnet composition by diffusion results in the loss of information from the core. This modification does not render G_FRAC useless. In this study, it is obvious that the FRS has reached higher temperatures than the

BRS resulting in garnets that are almost unmodified by diffusion in the BRS and garnets that are almost completely homogenized in the FRS with regards to their major component concentrations. In those cases where garnets are nearly homogenized (Samples 49B, 71, and 81) much of the information that would have been preserved in the garnet zoning has been lost. The outer edge of the garnets in these samples would still be in equilibrium with the matrix during their growth. While diffusion and resorption do occur, the composition of the outer edge measured today should still be close to representative of the last point of equilibrium. In this case removing the inner portions of the garnet which would not have interacted with the matrix would provide the EBRC at this last point of equilibrium.

In the other scenario, where diffusion has modified the composition profile of garnet but not to the point where the core has been obviously modified as in sample 18ZE-R-77A the question becomes how reliable is the produced P-T path? To address this, we have run diffusion simulations using diffusion coefficients of Chakraborty and Ganguly (1992) on samples 18ZE-R-16 and 18ZE-R-14B from the BRS (since no unaltered profiles exist in the FRS) at conditions similar to what we expect 18ZE-R-77A experienced (Fig. 5.11). These diffused profiles were then used for new G_FRAC models to compare with the original unmodified versions. While the conditions (Table 5.2) for diffusion were chosen to be representative of those experienced by 18ZE-R-77A, they were varied between the two samples to produce different types of profiles:

1. A thin core which has been slightly modified by diffusion with some information from the core lost (18ZE-R-16, diff1)
2. A thin core which has been significantly modified by diffusion with more information

from the core lost (18ZE-R-16, diff2)

3. A wide core which has not been modified by diffusion (18ZE-R-14B, diff1)
4. A wide core which has been significantly modified by diffusion, with some information from the core lost (18ZE-R-14B, diff2)

These diffused profiles were used for G_FRAC models using the same initial bulk rock composition and garnet size statistics as their respective samples. The comparisons between the respective isopleth intersection areas calculated with THERIAK-DOMINO (Fig. 5.12, 5.13) show diffusion did not modify the resulting path significantly. Loss of information at the core in both cases for 18ZE-R-16 and diff2 for 18ZE-R-14B results in a truncation of the apparent P-T path at the beginning, but the rest of the path is close to the original. One important difference to note is the increased distance between the garnet-in curve and the isopleth intersection area.

The undiffused and diffused profile models yield consistent results indicating that this method is robust. Even if diffusion has modified the core composition of the largest garnet in 18ZE-R-77A, the P-T path determined with G_FRAC and THERIAK-DOMINO must still follow closely with the path that we would observe if diffusion could not occur. It is still important to consider that this does not account for internal metasomatism that would occur during growth.

Since it does not consider diffusion, G_FRAC also does not account for the fact that smaller garnets are more significantly altered by diffusion than large garnets. This will result in an over estimation of spessartine removal and an under estimation of almandine removal which both would result in too large a shift of the garnet-in reaction up P and T during

garnet growth. The persistently expanding gap between the garnet isopleth intersection areas and the garnet-in curve observed in this study seems to imply that diffusion in smaller crystals has a minor influence on the P-T estimates obtained.

This gap has multiple possible explanations. In garnets with more relaxed profiles like in 18ZE-R-77A, it might be a result of diffusion but if that were the only reason then THERIA_G could be used to model the diffusion. Other explanations include:

1. Reduced volume of garnet removed because partially cut garnets in scanned sample were not included
2. Reduced volume of garnet due to resorption
3. Unaccounted for sequestration in garnet inclusions
4. Propagation of “error” with the presence of a gap prior to garnet fractionation and consistently removing less garnet than the model predicts

5.5 Tectonic Implications

New garnet Lu-Hf isochron age data on the BRS provide the only radiometric constraints on the timing of metamorphism and allows comparison to the conditions and timing of metamorphism in the adjacent FRS and the Yukon-Tanana terrane (Table 2.1). The oldest Lu-Hf age in the BRS was obtained from a Grt-Pl-Bt schist (18ZE-R-73C) in the Wann River Shear Zone. This 201.7 ± 2.8 Ma age is significantly younger than the Permian-Triassic population of monazite and xenotime in the Florence Range, and significantly older than then Early Jurassic Lu-Hf garnet ages from BRS and FRS, and monazite and xenotime in

the FRS (Soucy La Roche et al., in review). The complexity of this sample (see section 5.2.1.6) makes it difficult to constrain the reasons for discrepancy relative to other samples, though there are several possible explanations, the simplest being that this rock was separate from the rest of the BRS and was metamorphosed 10 Myr earlier before being juxtaposed with the BRS as a structural sliver within the WRSZ.

Other Lu-Hf isochron garnet dates from BRS (18ZE-R-14B: 192.4 ± 0.4) and FRS (18ZE-R-77A: 190.9 ± 3.3) indicate that both suites were undergoing coeval metamorphism and garnet crystallization at ca. 191 Ma. The metamorphism may have been more protracted in the FRS with Lu-Hf isochron dates ~ 5 Myr later (18ZE-R-71: 185.3 ± 1.1). Protracted metamorphism is supported by early Jurassic monazite inclusions in garnet rims and matrix monazite interpreted to have crystallized synchronously with garnet in the FRS (Soucy La Roche et al., in review) and overlaps with emplacement of the Tagish Lake Suite at 191-181 Ma (Currie and Parrish, 1997). Our data indicate that the FRS and BRS were metamorphosed at the same time and followed parallel and overlapping P-T paths (Figs. 5.2 and 5.3) with the FRS reaching a greater depth (Peak P ~ 1000 MPa) than the BRS (peak P $\sim 700 - 800$ MPa)

The peak P of ~ 1000 MPa estimated for the FRS from sample 18ZE-R-77A is too high for sillimanite and alkali feldspar crystallization observed in other samples in the FRS (18ZE-R-49B, 18ZE-R-81) unless there was significant decompression and heating after garnet crystallized. From our models, we estimate the peak T of these samples to be between 700 and 730 °C. The timing of decompression and heating in the FRS given by Soucy La Roche et al. (in review) aligns with the timing of the Wann River Shear Zone from Currie and Parrish (1993) at 185-170 Ma. It was likely during this period that the FRS was brought

from greater depth to its current relative position with the BRS.

The estimated P-T paths of these samples provide similar metamorphic constraints to other Early Jurassic metamorphic events documented in the Yukon Tanana Terrane (e.g. Berman et al., 2007; Gaidies et al., 2020).

Figure 5.1: Illustration of steps in the G_FRAC algorithm described in section 5.1.2

Figure 5.2: Garnet isopleth intersection areas of Boundary Ranges suite samples estimated with THERIAK-DOMINO after each G_FRAC fractionation stage (Fig. 5.4). Fractionation stages plotted for each sample are 18ZE-R-11A: 0, 2, 4, 6, 8, 10, 12 to 15, 18ZE-R-14A: 0 to 10, 18ZE-R-14B: 0 to 12, 18ZE-R-14C: 0 to 12, 18ZE-R-16: 0 to 10. Stage 0 are the models prior to any garnet fractionation (Figs. 4.20-4.22)

Figure 5.3: Garnet isopleth intersection areas of Florence Range suite samples estimated with THERIAK-DOMINO after each G.FRAC fractionation stage (Fig. 5.5). Fractionation stages plotted for each sample are 18ZE-R-77A: 0 to 11, 18ZE-R-81: 13, 18ZE-R-49B: 20 and 24, 18ZE-R-71: 10. Stage 0 are the models prior to any garnet fractionation (Fig. 4.23). The isopleth intersection area of 18ZE-R-81 shows a dashed line indicating the extent of the pyrope, almandine, and grossular isopleth intersection area on the right side. The dashed circle represents stage 20 of 18ZE-R-49B and represents the general area the isopleths come close to touching but do not intersect.

Figure 5.4: BRS profiles used in G.FRAC models. Everything to the left of the vertical dashed lines represent the garnet that has been fractionated at each stage

Figure 5.5: FRS profiles used in G.FRAC models. Everything to the left of the vertical dashed lines represent the garnet that has been fractionated at each stage

Figure 5.6 (preceding page): Calculated pseudosections and garnet isopleths. Abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-11A stage 15: 1 = Fsp Cld Chl WM Qz Rt, 2 = Fsp Ilm Grt Bt Crd Sil Qz, 3 = Ilm Cld Chl (2)WM Czo Qz Rt, 4 = Fsp Ilm Grt Bt St And Qz, 5 = Ilm Grt Cld Chl (2)WM Czo Qz Rt, 6 = Fsp Ilm Grt Chl Bt St Qz, 7 = Fsp Grt Chl (2)WM St Qz Rt, 8 = Fsp Grt Chl WM St Qz Rt, 9 = Fsp Ilm Grt WM Bt St Ky Qz, 10 = Fsp Grt WM Bt St Ky Qz Rt, 11 = Fsp Grt (2)WM Bt Ky Qz Rt **(B)** 18ZE-R-14A stage 10: 1 = Fsp Ilm Grt Chl (2)WM Bt Qz, 2 = Fsp Ilm Chl (2)WM Qz, 3 = Fsp Ilm Grt Chl WM Qz, 4 = Fsp Ilm Grt WM Bt Ky Qz, 5 = Fsp Grt Chl WM Bt Czo Qz Rt

Table 5.1: Pressure-temperature-time paths used in THERIA_G models for 18ZE-R-11A and 18ZE-R-16

18ZE-R-11A			18ZE-R-16		
T (°C)	P (MPa)	t (Myr)	T (°C)	P (MPa)	t (Myr)
450	300.0	0	450	300.0	0
505	494.0	5.5	502	469.3	5.2
508	502.4	5.8	504	481.8	5.4
510	503.7	6	507	485.3	5.7
513	524.8	6.3	509	496.7	5.9
518	542.0	6.8	513	518.7	6.3
528	571.1	7.8	518	533.0	6.8
541	594.9	8.1	523	565.8	7.3
549	610.7	8.9	532	588.4	8.2
553	646.4	9.3	544	640.1	9.4
555	659.6	9.5	553	646.5	10.3
562	687.3	10.2	556	667.8	10.6
535	300.0	13.2	535	300.0	13.6

Table 5.2: P-T-t conditions of diffusion simulations of 18ZE-R-14B and 18ZE-R-16

Diffusion Model	T (°C)	P (MPa)	t (Myr)
14B diff1	650	1000	4
14B diff2	650	1000	20
16 diff1	680	900	20
16 diff2	700	900	20

Figure 5.7 (preceding page): Calculated pseudosections and garnet isopleths. Abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-14B stage 12: 1 = Fsp Ilm Grt Chl Bt Crd Qz, 2 = Fsp Ilm Grt Bt Crd And Qz, 3 = Fsp Ilm Chl WM Czo Qz Rt, 4 = Fsp Ilm Chl WM Czo Qz, 5 = Fsp Ilm Grt Chl WM Czo Qz, 6 = Fsp Ilm Grt Chl WM Qz, 7 = Fsp Ilm Grt WM Bt St Ky Qz, 8 = Fsp Ilm Grt WM Bt Ky Qz, 9 = Fsp Ilm Grt Chl (2)WM Czo Qz Rt, 10 = Fsp Ilm Grt Chl WM Bt Czo Qz Rt, 11 = Fsp Ilm Grt Chl WM Bt Czo Qz, 12 = Fsp Ilm Grt Chl WM Bt Qz Rt, 13 = Fsp Grt Chl Bt St Qz Rt, 14 = Fsp Grt Bt St Qz Rt, 15 = Fsp Grt WM Bt Ky Qz Rt **(B)** 18ZE-R-14C stage 12: 1 = Fsp Ilm WM Bt St Qz, 2 = Fsp Ilm Grt WM Bt And Qz, 3 = Fsp Ilm Chl (2)WM Qz Rt, 4 = Ilm Chl (2)WM Bt Czo Qz Rt, 5 = Ilm Chl (2)WM Bt Czo Qz, 6 = Fsp Ilm Grt (2)WM Bt Czo Qz, 7 = Fsp Ilm Grt WM Bt Ky Rt, 8 = Fsp Grt WM Bt Ky Rt

Figure 5.8 (preceding page): Calculated pseudosections and garnet isopleths. Abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-16 stage 10: 1 = Fsp Ilm Grt Chl WM Bt Qz, 2 = Fsp Ilm Ep (2)WM Bt Qz, 3 = Fsp Ilm Ep Grt (2)WM Bt Qz, 4 = Fsp Ilm Ep Grt (2)WM Bt Qz Rt, 5 = Fsp Ilm Grt WM Bt Qz Rt **(B)** 18ZE-R-77A stage 11: 1 = Fsp Ilm WM Bt St Qz, 2 = Fsp Ilm Grt Chl WM Bt Czo Qz, 3 = Fsp Ilm (2)WM Bt Czo Qz Rt, 4 = Fsp Ilm (2)WM Bt Czo Qz, 5 = Fsp Ilm Grt (2)WM Bt Czo Qz Rt

Figure 5.9 (*preceding page*): Calculated pseudosections and garnet isopleths. Abbreviations after Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-81 stage 13: 1 = Fsp Ilm Grt Chl Bt Crd Qz, 2 = Fsp Chl WM Bt Qz Rt, 3 = Fsp Ilm Grt Chl Bt Qz, 4 = Fsp Ilm Grt Chl Bt Sil Qz, 5 = Fsp Ilm Grt Bt Sil Qz, 6 = Fsp Ilm Chl WM Bt Czo Qz Rt, 7 = Fsp Ilm Grt Bt St Qz, 8 = Fsp Ilm Grt Chl WM Bt Czo Qz, 9 = Fsp Ilm Grt Bt Ky Qz, 10 = Fsp Ilm Grt Chl WM Bt Czo Qz Rt, 11 = Fsp Grt Bt St Qz Rt, 12 = Fsp Grt Bt Ky Qz Rt, 13 = Fsp Ilm Grt Bt Qz Rt, 14 = Fsp Ilm Grt Bt Melt Qz Rt **(B)** 18ZE-R-71 stage 10: 1 = (2)Fsp Ilm WM Bt Qz Rt, 2 = (2)Fsp Ilm Bt Crd Qz, 3 = (2)Fsp Ilm Grt Bt Melt Qz, 4 = Fsp Ilm Grt Bt Melt Qz, 5 = (2)Fsp Ilm Grt WM Bt Qz Rt, 6 = (2)Fsp Ilm Grt WM Bt Melt Qz, 7 = Ilm Grt Bt Melt Qz, 8 = Fsp Ilm Grt WM Bt Qz Rt, 9 = Fsp Ilm Grt WM Bt Melt Qz Rt

Figure 5.10 (preceding page): Calculated pseudosections and garnet isopleths. Abbreviations Whitney and Evans (2010), WM = White mica. **(A)** 18ZE-R-49B stage 20: 1 = Fsp Ilm Chl WM Bt St Qz, 2 = (2)Fsp Ilm Bt Crd And Qz, 3 = (2)Fsp Ilm Grt Crd Sil, 4 = (2)Fsp Ilm Grt Crd Sil Qz, 5 = Fsp Ilm Grt Crd Sil Qz, 6 = (2)Fsp Ilm Grt Bt Melt Sil Qz, 7 = Ilm Chl WM Bt Czo Qz Rt, 8 = Fsp Ilm Grt WM Bt Melt Sil Qz, 9 = Ilm Grt Bt Melt Sil Qz, 10 = Fsp Ilm Grt WM Bt Ky Qz, 11 = Ilm Grt WM Bt Melt Sil Qz, 12 = Ilm Chl (2)WM Bt Czo Qz Rt, 13 = Ilm Chl (2)WM Czo Qz Rt, 14 = Fsp Ilm Grt WM Bt Qz, 15 = Ilm Grt WM Bt Melt Qz Rt **(B)** 18ZE-R-49B stage 24: 1 = Fsp Ilm Chl WM Bt St Qz, 2 = (2)Fsp Ilm Bt Crd And Qz, 3 = (2)Fsp Ilm Grt Crd Sil, 4 = (2)Fsp Ilm Grt Crd Sil Qz, 5 = Fsp Ilm Grt Crd Sil Qz, 6 = (2)Fsp Ilm Grt Bt Melt Sil Qz, 7 = Ilm Chl WM Bt Czo Qz Rt, 8 = Fsp Ilm Grt WM Bt St Qz, 9 = Fsp Ilm Grt WM Bt Melt Sil Qz, 10 = Ilm Grt Bt Melt Sil Qz, 11 = Chl (2)WM Bt Czo Qz Rt, 12 = Ilm Chl (2)WM Bt Czo Qz Rt, 13 = Ilm Chl (2)WM Czo Qz Rt, 14 = Ilm Grt WM Bt Qz, 15 = Ilm Grt WM Bt Melt Qz Rt

Figure 5.11: Spessartine profiles after diffusion for 18ZE-R-14B and 18ZE-R-16. Conditions to produce these profiles in Table 5.2

Figure 5.12: Garnet isopleth intersection areas of 18ZE-R-14B after the profile has been altered by diffusion (Fig. 5.11) estimated with THERIAK-DOMINO after each G_FRAC fractionation stage

Figure 5.13: Garnet isopleth intersection areas of 18ZE-R-16 after the profile has been altered by diffusion (Fig. 5.11) estimated with THERIAK-DOMINO after each G_FRAC fractionation stage

Figure 5.14: Predicted composition of garnet in 18ZE-R-11A from THERIA_G model along same path as predicted with G_FRAC (Table 5.1). The measured profile is rescaled to the sphere-normalized diameter of the largest garnet in the sample

Figure 5.15: Predicted composition of garnet in 18ZE-R-16 from THERIA_G model along same path as predicted with G_FRAC (Table 5.1). The measured profile is rescaled to the sphere-normalized diameter of the largest garnet in the sample

6. Conclusions

G_FRAC provides an effective and versatile tool to use alongside THERIAK-DOMINO to extract P-T data. We have shown multiple different scenarios in which this tool can be used that extend beyond the possible uses of forward modelling techniques such as THERIA_G (Gaidies et al., 2008). This has allowed us to calculate prograde and retrograde P-T points on multiple samples that could not otherwise be modelled with THERIA_G. For the few samples that could be modelled effectively with THERIA_G, we have found good agreement with the prograde paths predicted with G_FRAC and THERIAK-DOMINO.

The calculated P-T paths and garnet dates show that metamorphism in the FRS and BRS occurred synchronously between 192 and 185 Ma along similar paths, with the BRS reaching peak P of ~ 700 MPa and peak T $> 550^{\circ}\text{C}$ and the FRS reaching peak P of ~ 1000 MPa and peak T $\sim 700^{\circ}\text{C}$. The temporal correlation of this Barrovian-type event with other Barrovian-type metamorphic events in the YTT (e.g. Berman et al., 2007; Gaidies et al., 2020) shows that this tectonic event occurred at approximately the same time across the entire YTT.

Future metamorphic studies can make use of G_FRAC for fast and flexible calculation of P-T paths. In combination with THERIA_G, these models can be produced with confidence

and accuracy. Further applications of these tools in the study of the Canadian Cordillera can build towards a more complete picture of the tectonic history of this geologically complex region.

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Appendices

A. Petrographic reports

A.1 18ZE-R-11A

Andalusite garnet bearing white mica schist. Foliation largely defined by white mica. There is weak compositional banding of quartz rich and mica rich bands. There appear to be some minor syn-metamorphic veinlets (Fig. A.1).

Mineral	Modal %	Size	Description
Quartz	41	<0.6mm	Xenoblastic grains in matrix, often segregated from white mica. Occur as replacement rims on garnet (Fig. A.3)
White Mica	37	<0.75mm	Primary muscovite follows the foliation. Might be two different generations of muscovite, some are very fine grained following the primary foliation but there are many larger grains which don't appear parallel with this foliation. Also occur as partial fine grained pseudomorphs of andalusite (Fig A.2).
Garnet	6	1-4mm	Occur as occasional porphyroblasts, don't appear to favour quartz rich or mica rich bands. Appear to be highly resorbed, many have one or two sharp, idioblastic faces, but the other grain boundaries are usually quite irregular. Inclusions are primarily quartz and ilmenite. Where resorption is evident, there are usually quartz or chlorite + plagioclase + white mica resorption rims. Multiple growth generations seen in inclusion patterns on garnet. S-shaped inclusion trails in garnet suggest syn-kinematic growth (Fig. A.4, also see central section)

Chlorite	5	<0.05mm	Appears retrograde, replaces garnet, and white mica. Often occurs with plagioclase and andalusite. Doesn't follow foliation when replacing garnet and white mica but does when it appears with andalusite or plagioclase.
Andalusite	4	0.2-3.5mm	Usually hypidioblastic, can have one or two straight edges usually in contact with matrix with very thin white mica rims. Irregular contacts with plagioclase and chlorite are typical
Plagioclase	4	<3.5mm	Appears to be replacing andalusite often appearing as large xenoblastic overgrowths on andalusite porphyroblasts (Fig. A.1
Opaque	2		
(ClinoZoisite	1	<0.2mm	Occur as inclusions in garnet
Calcite	Tr.	<0.25mm	Seen included in plagioclase

(a) PPL

(b) XPL

Figure A.1: Plagioclase replacing andalusite porphyroblasts

(a) PPL

(b) XPL

Figure A.2: White mica pseudomorphing andalusite

(a) PPL

(b) XPL

Figure A.3: Quartz pseudomorphing garnet rims in a possible replacement reaction

(a) PPL

(b) XPL

Figure A.4: S-shaped inclusion trails in garnet

A.2 18ZE-R-14A

Garnet bearing white mica plagioclase schist. Has a foliation defined by white mica, chlorite and plagioclase. Also contains deformed quartz veins, parallel to the foliation, not appearing to crosscut it.

Mineral	Modal %	Size	Description
Plagioclase	50	0.1 - 0.5mm	Occur as hypidioblastic to xenoblastic porphyroblasts within the matrix, contacts with WM, Chl, and quartz are hypidioblastic but contacts with other plagioclase grains are xenoblastic. Also occur as inclusions in garnet. Occasionally the garnet inclusions or grains in contact with garnet (possibly former inclusions prior to garnet resorption) show a very thin layer of quartz in between (Fig. A.5). Often contains spiralled inclusion trails of unknown minerals, appear to be very small grains of chlorite and white mica plus an opaque mineral. Usually these inclusions are parallel to the foliation but occasionally exhibit more complicated textures indicating syn-kinematic growth (Fig. A.6)
White Mica	20	< 0.5mm	Elongate and platy. Defines the foliation along with chlorite and plagioclase. Usually stable with chlorite. Sometimes included in plagioclase
Chlorite	12	< 0.5mm	Elongate and platy. Defines foliation along with white mica and plagioclase. Sometimes included in plagioclase. In some places, it seems like chlorite might be replacing white mica. Some retrograde chlorite on the more resorbed looking garnet. There is retrograde chlorite but it is not all retrograde.
Garnet	8	0.6 - 4mm	Occur as hypidioblastic porphyroblasts. Sharp edges are uncommon but present. No obvious resorption rims, but there is almost always a higher concentration of quartz and plagioclase next to the most irregular sections of garnet. Appears that large plagioclase grains and quartz might be impinging on garnet growth. Plagioclase appears as large inclusions and partial inclusions in garnet. Complex inclusion trails present in some garnet, very fine hard to identify, possibly epidote (Fig. A.7).

Quartz	7	0.01 - 0.6mm	Xenoblastic, occurs in veins and throughout matrix. In the matrix, it is usually associated with plagioclase and sometimes garnet
Opaque	3

(a) PPL

(b) XPL

Figure A.5: Plagioclase inclusions in garnet, quartz rims at interface

(a) PPL

(b) XPL

Figure A.6: Spiralled inclusion trails in plagioclase

(a) PPL

(b) XPL

(c) PPL, zoomed

(d) XPL, zoomed

Figure A.7: Inclusion trails in garnet

A.3 18ZE-R-14B

Somewhat heterogenous sample with sections of higher white mica and garnet occurrence. Foliation well defined by quartz, chlorite, and white mica. Matrix consists of quartz, plagioclase, chlorite, and white mica.

Mineral	Modal %	Size	Description
Quartz	60	< 0.6mm	Xenoblastic grains making up most of the matrix. Usually elongate and defining the foliation. Often appear on the sides of garnet as pressure shadows. Also appear in thick foliated veins of mostly quartz.
Plagioclase	25	< 0.5mm	Occurs as xenoblastic grains in matrix and as hypidioblastic porphyroblasts (Fig. A.8).
Chlorite	10	< 0.2mm	Elongate platy, defining foliation
Garnet	2	0.1-2.5mm	Porphyroblasts occur as hypidioblastic to idioblastic grains. Partly impinged by matrix material such as quartz (Fig. A.9). Impingement occurs more typically parallel to foliation. Highly fractured with inclusions of quartz, white mica, and chlorite.
White Mica	2	< 0.4mm	Elongate platy, defining foliation
Opaques	1		Rutile and Ilmenite

(a) PPL

(b) XPL

Figure A.8: Plagioclase porphyroblast in 18ZE-R-14B

(a) PPL

(b) XPL

Figure A.9: Garnet porphyroblast in 18ZE-R-14B

A.4 18ZE-R-14C

Messy rock that appears to have experienced a fair bit of retrogression and later alteration by fluid. Foliation defined by white mica. Mats of chlorite with sericitized plagioclase, likely a later fluid-mediated alteration, possibly related to vein-like structures with monazite present within. Likely contains graphite.

Mineral	Modal %	Size	Description
White Mica	38	< 0.7 mm	Primary matrix material, foliated and wraps around garnet. Platy shape, subidioblastic
Chlorite	25	< 0.3 mm	Typically occurs as retrograde, replacing garnet at some faces or as randomly oriented mats with plagioclase (Fig. A.10), appears to be crosscutting the rock in a vein possibly a fluid mediated reaction.
Garnet	17	0.4-7 mm	Euhedral prophyroblasts large and impinging on each other. Contains fine grained white mica inclusions, zoned plagioclase inclusions < 0.5mm, ilmenite inclusions in a spiral pattern < 0.6 mm long, and rare quartz inclusions (Fig. A.11). Partial replacement by chlorite on irregular edges. Highly fractured with cracks filled with chlorite and white mica.
Plagioclase	10	< 1mm	Included in garnet and throughout matrix, as subidioblastic to xenoblastic, irregular grains, show zoning under XPL. Also in large clumps with randomly oriented Chlorite near fractures, this plagioclase appears partly sericitized.
Quartz	6	< 2 mm	Xenoblastic throughout matrix and included in garnet
Ilmenite	4	< 1 mm	Idioblastic throughout matrix, foliation parallel except where included in garnet then it has a spiral pattern

(a) PPL

(b) XPL

Figure A.10: Chlorite mats and sericitized plagioclase in 18ZE-R-14C

(a) PPL

(b) XPL

Figure A.11: Garnet porphyroblast in 18ZE-R-14C

A.5 18ZE-R-16

Crenulated foliation structure defined by biotite and white mica. Finer grained biotite and white mica anastomose around sub-angular to sub-rounded plagioclase and quartz grains (Fig. A.12). Also present are quartz veins which are parallel to foliation in the rock.

Mineral	Modal %	Size	Description
Biotite	33	<0.9mm	Defines the foliation with white mica. Also crenulation cleavage present. Associated with white mica, epidote, and plagioclase. Might be replacing plagioclase in areas where it seems to anastomose around sub-rounded to sub-angular plagioclase fragments. Anastomosing biotite sometimes appears extremely fine grained and appears to cut through the rock like a deformed vein (Fig. A.13)
White Mica	23	<0.5mm	Defines the foliation with biotite. Also crenulation cleavage present. Associated with biotite, epidote, and plagioclase. Occasionally occurs within these regions of anastomosing biotite. Also occurs as inclusions in garnet
Plagioclase	23	0.02 - 0.8mm	Contain inclusions of epidote and zoisite (Fig. A.14). Some grains show signs of zoning in XPL. Associated with biotite and quartz. Appears hypidioblastic with biotite, looking subangular-subrounded. Looks more xenoblastic when with quartz with very irregular contacts
Quartz	15	0.01 - 1mm	Appears in quartz rich domains with plagioclase as xenoblastic grains. Also appears in veins of only quartz that have been deformed with the rest of the matrix. Also associated with garnet either in pressure shadows or with garnets present in these quartz rich domains.
Garnet	2	0.4 - 4mm	Appears as hypidioblastic-idioblastic porphyroblasts. Associated with biotite, plagioclase, and quartz. Not oriented with the foliation, one grain elongated perpendicular to the foliation (Fig. A.16). Contain inclusions of quartz, white mica and epidote that show s-shaped inclusion trails. Also contains occasional ilmenite inclusions.

Epidote	2	<0.1mm	Occurs in matrix with biotite and white mica (Fig. A.15). Also occurs as inclusions in plagioclase and garnet (Fig. A.14,A.16). Possible signs of zoning in XPL?
Chlorite	1	0.01 - 0.9mm	Appears to be mostly retrograde, seems to replace biotite. Relict biotite grains within larger chlorite clusters. It also does not follow the fabric in the rest of the rock. Some primary chlorite present with same orientation as the micas
Opaque	1		
Zoisite	Tr.	<0.15mm	Occur as inclusions in plagioclase (Fig. A.14)

Figure A.12: Biotite anastomosing around fragmented plagioclase

(a) PPL

(b) XPL

Figure A.13: Biotite “vein” cutting through thin section

(a) PPL

(b) XPL

Figure A.14: Epidote and zoisite inclusions in plagioclase

(a) PPL

(b) XPL

Figure A.15: Epidote in matrix

(a) PPL

(b) XPL

Figure A.16: Garnet with inclusions

A.6 18ZE-R-49B

It is moderately heterogenous, General foliation defined by sillimanite and biotite, white mica does not always follow this foliation and often appears randomly oriented

Mineral	Modal %	Size	Description
White Mica	35	<0.5mm	Throughout matrix. Occurs as fine grained material throughout, possibly pseudomorphing earlier minerals. Also occurs as coarser grained crystals, usually replacing biotite (Fig. A.17)
Biotite	25	<1mm	Appears throughout matrix as hypidioblastic and xenoblastic grains. Often appear to have “feathery” edges, could be getting resorbed as a result of melting reaction. Further evidence of this is apparent replacement of biotite by sillimanite (Fig. A.18). Also seen being replaced by white mica + quartz and feldspar (Fig. A.17) Complex intergrowths seen between individual biotite grains, could be exsolution but they have distinct orientations (Fig. A.19. Also occurs as inclusions in garnet, sometimes as symplectic intergrowths with quartz alongside plagioclase and white mica (Fig. A.20). Also seen as inclusions within staurolite inclusions in garnet.
Quartz	23	<1.5mm	Xenoblastic, occurs as inclusions in garnet and throughout matrix. Occurs as larger grains in more quartzo-felspathic rich bands.
Sillimanite	8	<1.2mm	Mostly fibrous, some prismatic grains, occurs in the matrix and associated with biotite and white mica. Often seen replacing biotite.

Garnet	5	1.5-8mm	Very large porphyroblasts present in matrix. They contain many inclusions of biotite, quartz, white mica, plagioclase, ilmenite, apatite, zircon, monazite and kyanite. The inclusions seem oriented roughly parallel to each other in a single garnet, but they are not parallel with the matrix foliation (Fig. A.21) Kyanite inclusions are very rare, only one found on SEM (not shown here) occurring with staurolite and biotite. Biotite seen symplectic with quartz beside plagioclase and white mica (Fig. A.20). Staurolite inclusions somewhat common, seen with biotite and also with biotite and quartz inclusions (Fig. A.22). Some resorption seen with replacement by chlorite + biotite. More obvious in hand sample is occurrence of garnet in quartzofeldspathic lenses.
Chlorite	4	<0.5mm	Seen replacing biotite and garnet. Often replaces biotite as one crystal
Staurolite	Tr.	0.05-0.4mm	Occurs only as inclusions in garnet (Fig. A.22), inclusions often irregular. Occurs with biotite, quartz, and kyanite. Sometimes seen with biotite inclusions.
Kyanite	Tr.		One inclusion seen in garnet
Cordierite	Tr?		Identified with EDS in another thin section, no “obvious” occurrence in this thin section. Seen with quartz, plagioclase, biotite, and chlorite.
Plagioclase	Tr?	<0.1mm	Not common or obvious, best identified with EDS. appears small and xenoblastic. Occurs as inclusions in garnet and in matrix with quartz, chlorite, biotite, and sometimes cordierite.

(a) PPL

(b) XPL

Figure A.17: White mica, quartz, and feldspar replacing a biotite grain

(a) PPL

(b) XPL

Figure A.18: Sillimanite shown replacing biotite

(a) PPL

(b) XPL

Figure A.19: Biotite and white mica intergrowths

(a) PPL

(b) XPL

Figure A.20: Biotite-quartz symplectite shown included in garnet. The biotite zones outward to muscovite

(a) PPL

(b) XPL

Figure A.21: Garnet with inclusions that show indication of preferred orientation in a different direction from matrix foliation

(a) PPL

(b) XPL

Figure A.22: Staurolite inclusions in garnet, occurring with biotite

A.7 18ZE-R-71

Foliation defined by biotite and graphite. Somewhat heterogenous with quartz rich lenses scattered among the matrix, often near garnet

Mineral	Modal %	Size	Description
Quartz	60	<2mm	Dominant matrix material. Xenoblastic, present throughout.
Biotite	20	<0.4mm	Red-brown biotite platy, throughout matrix. usually occurs with plagioclase. Sometimes rimmed by plagioclase (Fig. A.23)
Plagioclase	11	<1.5mm	Xenoblastic, associated with biotite. Zoning apparent in XPL
Garnet	4	1.2 - 4mm	Rounded, hypidioblastic porphyroblasts. Some edges are straight and well defined. Lots of fractures in the garnets filled with a green biotite and chlorite. The same material appears as very thin rims on the edge of the garnet, thicker at the more rounded edges. Contains inclusions of quartz which show slightly spiralled pattern (Fig. A.24)
Graphite	3	< 0.1mm	Hypidioblastic platy grains associated with biotite and plagioclase in the matrix.
Chlorite	2	< 0.05mm	Only retrograde on garnet in cracks and on rims with biotite.

(a) PPL

(b) XPL

Figure A.23: Rims of plagioclase on biotite in matrix of 71

(a) PPL

(b) XPL

Figure A.24: Inclusions in garnets

A.8 18ZE-R-73C

Weakly foliated, defined by biotite. Chlorite filled fracture visible in hand sample. Appears mostly homogenous with occasional quartz lenses.

Mineral	Modal %	Size	Description
Plagioclase	28	<0.8mm	Mostly xenoblastic grains in matrix although sometimes appear as hypidioblastic grains, possibly slightly resorbed porphyroblasts (Fig. A.25). Zoning obvious in XPL, possibly two generations of plagioclase growth.
Biotite	25	<0.4mm	Weakly foliated in matrix. Appear dark green with possible zoning apparent in PPL and XPL.
Quartz	30	< 0.5mm	Xenoblastic grains in matrix
Garnet	12	<4mm	Hypidioblastic, relatively round porphyroblasts. Made up mostly of small grains < 1.2mm but there are some very large grains >2mm. There have been two generations of growth. Contain inclusions of ilmenite and quartz. Inclusions appear with a spiral pattern in some grains (Fig. A.26). A lot of the smaller grains appear more idioblastic than the larger grains (Fig. A.27). Larger grains sometimes appear to be clusters of smaller grains, or perhaps relicts of older ones that grew “warts” of smaller grains on top (more obvious in three dimensions
Chlorite	4	<0.3mm	Mostly occurs as overgrowth on biotite or garnet, but occasional porphyroblasts are present (Fig. A.28)
Opaque	1		
Apatite	Tr.	<0.05mm	Small idioblastic grains sometimes present in matrix

(a) PPL

(b) XPL

Figure A.25: Plagioclase porphyroblasts in 73C

(a) PPL

(b) XPL

Figure A.26: Spiral shaped inclusion patterns in garnets of 73C

(a) PPL

(b) XPL

Figure A.27: Very small, idioblastic garnet in 73C

(a) PPL

(b) XPL

Figure A.28: Chlorite porphyroblast in 73C

A.9 18ZE-R-77A

High grade garnet bearing-white mica-biotite schist with matrix of foliated biotite and white mica and xenoblastic quartz and plagioclase.

Mineral	Modal %	Size	Description
Biotite	28	0.05 - 1.2mm	Platy grains defining foliation with white mica, the foliation “bends” around garnets. Associated with garnet plagioclase and white mica. Some biotite at rims of garnets does not follow the foliation and appears parallel to the garnet surface, could be retrograde (Fig. A.29). Biotite also occurs as inclusions in garnet. Largest biotite grains appear in domains with high amounts of biotite and white mica.
Quartz	25	0.01 - 6mm	Xenoblastic, Present throughout matrix but often concentrated in quartz rich domains. Associated with plagioclase, biotite, and white mica. Occurs as inclusion in garnet
White Mica	20	0.02 - 2mm	Platy grains defining foliation with biotite, the foliation “bends” around garnets. Associated with garnet, plagioclase, and biotite. Some white mica at rims of garnet does not follow the foliation and appears parallel to the garnet surface. White mica also occurs as inclusions in garnet. Largest grains appear in domains with high amounts of biotite and white mica
Plagioclase	18	0.02 - 1.6mm	Appears xenoblastic with quartz, occasionally hypidioblastic. Some grains show zoning in XPL. Frequently occurs as inclusions with garnet, often plucked out in thin section, some show signs of alteration to white mica. The inclusions are often hypidioblastic

Garnet	8	0.5 - 2.5mm	Hypidioblastic porphyroblasts. Some signs of resorption with plagioclase and biotite occasionally appearing to replace it at some margins. Appears otherwise unresorbed. Very inclusion rich with plagioclase being the most significant followed by quartz then ilmenite then biotite and white mica. Ilmenite inclusions extremely small ($< 0.05\text{mm}$) but very numerous (Fig. A.30). Sometimes present are parallel cracks filled in with plagioclase + biotite + quartz that crosscut the garnet, they appear to continue into the matrix but do not appear very discrete outside of the garnet (Fig. A.31). Linear inclusion trails in garnet align with these “veins” in the same garnet. These are possibly inclusion trails that persisted from a pre-existing foliation, or trails that occur as a result of primary compositional banding (Fig. A.32). The cracks could actually be preferential resorption of garnet along planes of greater diffusion rates.
Opaque	1		Contains magnetite, ilmenite, and pyrite
Apatite	Tr.	$< 0.05\text{mm}$	Occurs as inclusions in garnet, possibly in matrix too
Barite	Tr.		Seen with EDS

Figure A.29: Garnet in 77A with inclusions

Figure A.30: Small ilmenite inclusions in garnet

Figure A.31: Crack cutting through garnet

Figure A.32: Quartz inclusion trails and cracks possibly as a result of pre-existing foliation

A.10 18ZE-R-81

Mineral	Modal %	Size	Description
Quartz	35	< 0.3 mm	xenoblastic grains throughout the matrix elongated parallel to foliation
Plagioclase	30	< 0.3 mm	Xenoblastic zoned grains throughout matrix elongated parallel to foliation, occasionally with quartz inclusions
Biotite	27	< 2.5 mm	Foliation defining platy grains throughout matrix, occasionally with white mica and occasionally replaced by fine grained white mica
Garnet	5	0.2 -5 mm	Typically subidioblastic with a rounded shape (Fig. A.33). Contain inclusions of quartz and white mica < 0.1 mm. Occasionally some garnets look very irregular and resorbed, some partial or complete replacement by white mica. Very rarely appear as atoll garnets (Fig. A.34) filled primarily with plagioclase. Contain cracks containing white mica
White mica	3	< 0.2 mm	Appears in matrix as foliation parallel hypidioblastic grains same size as biotite. More commonly appears as fine grained masses replacing garnet, biotite, and pseudomorphing sillimanite (Fig. A.35)
Alkali Feldspar	2	< 1 mm	xenoblastic foliation parallel
Apatite	Tr.	< 0.1 mm	Idioblastic
Tourmaline	Tr	< 0.2 mm	Idioblastic grains rare in matrix

(a) PPL

(b) XPL

Figure A.33: Typical garnets in 81

(a) PPL

(b) XPL

Figure A.34: Atoll garnet in 81

(a) PPL

(b) XPL

Figure A.35: White mica pseudomorphing sillimanite in 81

B. EPMA Garnet profiles

Table B.1: 18ZE-R-11A EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.14277	0.07443	0.75651	0.02629
0.03604	0.16896	0.0716	0.73297	0.02647
0.07209	0.18478	0.06536	0.72205	0.0278
0.10813	0.19812	0.06286	0.70958	0.02944
0.14418	0.19926	0.06286	0.70682	0.03106
0.18022	0.1906	0.06196	0.71267	0.03477
0.21626	0.19864	0.05966	0.70517	0.03654
0.25231	0.21903	0.05791	0.68559	0.03746
0.28835	0.1972	0.05924	0.70119	0.04237
0.32439	0.19804	0.05907	0.70045	0.04244
0.36044	0.19318	0.06014	0.71406	0.03262
0.39648	0.2009	0.05952	0.71846	0.02112
0.43253	0.19976	0.05991	0.72073	0.01959
0.46857	0.19539	0.05924	0.72546	0.01991
0.50461	0.19776	0.05959	0.72158	0.02108
0.54066	0.1803	0.06305	0.73406	0.02259
0.5767	0.17505	0.06121	0.73723	0.02651
0.61274	0.18536	0.05711	0.72955	0.02798
0.64879	0.18084	0.05917	0.72948	0.03051
0.68483	0.18356	0.05795	0.726	0.0325
0.72088	0.2011	0.05865	0.70786	0.03239
0.75692	0.1906	0.05918	0.71428	0.03594
0.79296	0.18358	0.06141	0.71694	0.03807
0.82901	0.18209	0.06017	0.71771	0.04003
0.86505	0.16805	0.05849	0.72916	0.0443
0.90109	0.18711	0.0581	0.70881	0.04598
0.93714	0.18726	0.05765	0.70525	0.04984

0.97318	0.19837	0.05513	0.69797	0.04853
1.00923	0.19284	0.05479	0.69886	0.0535
1.04527	0.19458	0.05519	0.69456	0.05567
1.08131	0.20539	0.0538	0.68345	0.05736
1.11736	0.19044	0.05431	0.69317	0.06208
1.1534	0.19231	0.05149	0.68715	0.06906
1.18944	0.19487	0.0521	0.67853	0.07449
1.22549	0.19502	0.05129	0.67341	0.08028
1.26153	0.19965	0.05	0.66451	0.08584
1.29758	0.21039	0.05219	0.65227	0.08515
1.33362	0.21843	0.04874	0.64563	0.0872
1.36966	0.20888	0.04397	0.64409	0.10306
1.40571	0.22035	0.04437	0.63482	0.10047
1.44175	0.21523	0.04604	0.637	0.10173
1.4778	0.20553	0.04702	0.64288	0.10457
1.51384	0.20981	0.04632	0.62929	0.11458
1.54988	0.21632	0.04232	0.61894	0.12242
1.58593	0.21457	0.04063	0.62315	0.12164
1.62197	0.21374	0.04153	0.61774	0.12699
1.65801	0.20946	0.04495	0.6222	0.12339
1.69406	0.21423	0.04519	0.61063	0.12994
1.7301	0.20794	0.04179	0.60597	0.14431
1.76615	0.22642	0.04045	0.59795	0.13517
1.80219	0.22907	0.04168	0.59409	0.13516
1.83823	0.22044	0.04136	0.59503	0.14317
1.87428	0.20361	0.04051	0.59707	0.1588
1.91032	0.21413	0.03894	0.58823	0.1587
1.94636	0.21045	0.04462	0.60261	0.14232
1.98241	0.21382	0.05198	0.62173	0.11247
2.01845	0.21034	0.04983	0.62253	0.1173
2.0545	0.21703	0.04427	0.61045	0.12825
2.09054	0.22281	0.04527	0.60476	0.12716
2.12658	0.20846	0.04748	0.61018	0.13388
2.16263	0.20674	0.04282	0.59834	0.1521
2.19867	0.21354	0.03987	0.58646	0.16014
2.23471	0.21371	0.03907	0.57093	0.17629
2.27076	0.21231	0.0383	0.5732	0.1762
2.3068	0.2031	0.03862	0.58495	0.17333
2.34285	0.20637	0.03896	0.58428	0.17039
2.37889	0.22157	0.0352	0.55683	0.1864
2.41493	0.20988	0.03994	0.57767	0.17251
2.45098	0.22007	0.03975	0.57429	0.16589
2.48702	0.21553	0.0357	0.56185	0.18691
2.52306	0.22277	0.03518	0.55346	0.18859
2.55911	0.22336	0.03792	0.55257	0.18614

2.59515	0.22036	0.03598	0.55972	0.18394
2.6312	0.21819	0.03641	0.5651	0.1803
2.66724	0.22393	0.03368	0.55523	0.18715
2.70328	0.22277	0.03734	0.55335	0.18654
2.73933	0.21312	0.03454	0.56162	0.19072
2.77537	0.20836	0.03602	0.56402	0.19159
2.81142	0.2084	0.03483	0.56409	0.19269
2.84746	0.20484	0.03486	0.56575	0.19454
2.8835	0.20549	0.03582	0.56882	0.18986
2.91955	0.21881	0.03751	0.55801	0.18566
2.95559	0.21838	0.03445	0.56161	0.18556
2.99163	0.21932	0.0374	0.56166	0.18162
3.02768	0.20753	0.03814	0.56597	0.18837
3.06372	0.19994	0.03639	0.57526	0.18842
3.09977	0.2168	0.03719	0.56516	0.18086
3.13581	0.2279	0.03697	0.56013	0.175
3.17185	0.21281	0.03753	0.57015	0.17952
3.2079	0.21766	0.03556	0.57141	0.17538
3.24394	0.21651	0.03846	0.56948	0.17556
3.27998	0.21104	0.03587	0.57737	0.17571
3.31603	0.21859	0.03489	0.57646	0.17006
3.35207	0.21367	0.03822	0.5803	0.16781
3.38812	0.21589	0.03728	0.58119	0.16565
3.42416	0.2097	0.04169	0.58547	0.16314
3.4602	0.21631	0.04006	0.58251	0.16111
3.49625	0.21882	0.03982	0.58295	0.15841
3.53229	0.22185	0.03976	0.58494	0.15346
3.56833	0.2113	0.03853	0.59502	0.15514
3.60438	0.21616	0.04062	0.5918	0.15141
3.64042	0.21266	0.04207	0.59702	0.14825
3.67647	0.22491	0.03895	0.5949	0.14123
3.71251	0.2123	0.04127	0.6068	0.13963
3.74855	0.22093	0.04019	0.60491	0.13397
3.7846	0.22445	0.0398	0.60593	0.12982
3.82064	0.21082	0.04121	0.6181	0.12987
3.85669	0.21873	0.04071	0.61661	0.12395
3.89273	0.21684	0.04229	0.62184	0.11903
3.92877	0.21531	0.04496	0.62744	0.11229
3.96482	0.21561	0.04487	0.63538	0.10414
4.00086	0.21255	0.04402	0.64466	0.09877
4.0369	0.22149	0.04438	0.64115	0.09297
4.07295	0.21273	0.04635	0.64841	0.0925
4.10899	0.22834	0.0466	0.64091	0.08415
4.14504	0.20601	0.04817	0.66392	0.0819
4.18108	0.19265	0.05184	0.68081	0.07471

4.21712	0.20748	0.05105	0.6713	0.07016
4.25317	0.19991	0.05215	0.68003	0.06791
4.28921	0.19437	0.05356	0.69046	0.06161
4.32525	0.19795	0.05463	0.68959	0.05782
4.3613	0.1873	0.05462	0.70306	0.05502
4.39734	0.18153	0.054	0.71045	0.05402
4.43339	0.19154	0.05593	0.70278	0.04975
4.46943	0.18016	0.05662	0.71881	0.04441
4.50547	0.18062	0.05719	0.71973	0.04246
4.54152	0.1737	0.05984	0.72741	0.03905
4.57756	0.17507	0.06078	0.72422	0.03992
4.6136	0.19029	0.0577	0.71652	0.03548
4.64965	0.19547	0.05623	0.71483	0.03347
4.68569	0.19079	0.05969	0.71719	0.03233
4.72174	0.20321	0.0611	0.70497	0.03072
4.75778	0.19373	0.05766	0.71866	0.02995
4.79382	0.20919	0.05806	0.706	0.02675
4.82987	0.18581	0.05969	0.72739	0.02711
4.86591	0.19007	0.06264	0.72434	0.02296
4.90195	0.20919	0.05855	0.71053	0.02173
4.938	0.20016	0.05897	0.7212	0.01967
4.97404	0.19763	0.05923	0.72417	0.01897
5.01009	0.22141	0.05741	0.703	0.01818
5.04613	0.21697	0.05891	0.70536	0.01876
5.08217	0.2011	0.06141	0.70333	0.03417
5.11822	0.19888	0.05772	0.69698	0.04642
5.15426	0.20448	0.05831	0.69554	0.04167
5.19031	0.19927	0.06346	0.69816	0.03911
5.22635	0.20333	0.0621	0.69908	0.0355
5.26239	0.20326	0.06277	0.70019	0.03378
5.29844	0.19484	0.06436	0.71086	0.02994
5.33448	0.18824	0.06804	0.71674	0.02698
5.37052	0.17841	0.07125	0.72404	0.0263
5.40657	0.14537	0.07669	0.75362	0.02432

Table B.2: 18ZE-R-14A EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.126143	0.063599	0.807987	0.002271
0.029463	0.166734	0.060041	0.771305	0.001921
0.058926	0.166131	0.060951	0.771405	0.001512
0.08839	0.167853	0.059099	0.770685	0.002363
0.117853	0.166912	0.054973	0.776367	0.001747
0.147316	0.157539	0.058505	0.781343	0.002612

0.176779	0.158543	0.057764	0.782044	0.001649
0.206242	0.156296	0.05835	0.782701	0.002653
0.235705	0.168179	0.055457	0.773951	0.002413
0.265169	0.158854	0.055106	0.784086	0.001954
0.294632	0.145415	0.061313	0.790574	0.002699
0.324095	0.142652	0.05681	0.798522	0.002016
0.353558	0.154092	0.05704	0.786823	0.002045
0.383021	0.147206	0.057934	0.793295	0.001565
0.412484	0.138936	0.055412	0.80231	0.003342
0.441948	0.137847	0.053836	0.805302	0.003015
0.471411	0.16231	0.05244	0.781983	0.003267
0.500874	0.161183	0.050273	0.785632	0.002912
0.530337	0.159349	0.05024	0.787089	0.003323
0.5598	0.153898	0.04633	0.795878	0.003894
0.589263	0.148778	0.049046	0.798503	0.003672
0.618727	0.162107	0.050276	0.784333	0.003283
0.64819	0.158598	0.047955	0.789122	0.004325
0.677653	0.153151	0.046507	0.795847	0.004496
0.707116	0.149928	0.046479	0.798153	0.00544
0.736579	0.147851	0.047179	0.799969	0.005002
0.766043	0.155858	0.047159	0.791246	0.005737
0.795506	0.144645	0.044662	0.804932	0.00576
0.824969	0.159183	0.045053	0.788678	0.007086
0.854432	0.159122	0.042744	0.791262	0.006871
0.883895	0.160197	0.042603	0.788785	0.008416
0.913358	0.167364	0.041793	0.781534	0.009309
0.942822	0.161463	0.040356	0.787258	0.010923
0.972285	0.175048	0.040027	0.774424	0.010501
1.001748	0.167954	0.039878	0.77892	0.013248
1.031211	0.173294	0.040655	0.772065	0.013985
1.060674	0.174298	0.038392	0.770912	0.016398
1.090137	0.17134	0.041058	0.771262	0.016339
1.119601	0.180934	0.037907	0.764135	0.017024
1.149064	0.174156	0.03946	0.768101	0.018283
1.178527	0.182715	0.041858	0.7574	0.018027
1.20799	0.176814	0.042494	0.76303	0.017661
1.237453	0.198521	0.037492	0.738104	0.025883
1.266917	0.194097	0.036531	0.739229	0.030143
1.29638	0.196321	0.036473	0.732482	0.034724
1.325843	0.201861	0.034298	0.731051	0.03279
1.355306	0.189151	0.038044	0.741165	0.031639
1.384769	0.182955	0.034746	0.74388	0.038419
1.414232	0.185898	0.032623	0.740512	0.040967
1.443696	0.197343	0.029899	0.727233	0.045525
1.473159	0.195468	0.030887	0.727938	0.045706

1.502622	0.207537	0.028469	0.716372	0.047622
1.532085	0.213487	0.029566	0.705728	0.051218
1.561548	0.19685	0.031069	0.717076	0.055005
1.591011	0.198655	0.029332	0.71494	0.057073
1.620475	0.208978	0.027064	0.707021	0.056937
1.649938	0.199744	0.028192	0.709471	0.062593
1.679401	0.200173	0.029923	0.708257	0.061647
1.708864	0.195992	0.039632	0.718696	0.045679
1.738327	0.187998	0.043748	0.726865	0.041389
1.76779	0.181311	0.045239	0.729635	0.043815
1.797254	0.215685	0.034466	0.696036	0.053813
1.826717	0.23002	0.031821	0.675251	0.062908
1.85618	0.215067	0.039514	0.702074	0.043345
1.885643	0.2191	0.038552	0.688137	0.054212
1.915106	0.216347	0.032615	0.682993	0.068046
1.94457	0.232922	0.027948	0.65948	0.079649
1.974033	0.245262	0.027188	0.642742	0.084807
2.003496	0.240162	0.023985	0.640568	0.095284
2.032959	0.250748	0.023556	0.633808	0.091889
2.062422	0.244379	0.022692	0.634936	0.097993
2.091885	0.237521	0.021361	0.639272	0.101846
2.121349	0.240813	0.025516	0.633106	0.100566
2.150812	0.241689	0.033413	0.649612	0.075286
2.180275	0.25653	0.027749	0.62102	0.094702
2.209738	0.264675	0.021583	0.613147	0.100594
2.239201	0.249661	0.020126	0.616843	0.11337
2.268664	0.267475	0.018829	0.598951	0.114745
2.298128	0.269379	0.01791	0.59126	0.121451
2.327591	0.279918	0.017452	0.571819	0.130811
2.357054	0.269042	0.017371	0.58136	0.132226
2.386517	0.268662	0.021318	0.596788	0.113232
2.41598	0.238199	0.029815	0.649047	0.082938
2.445443	0.268898	0.036043	0.627779	0.06728
2.474907	0.247883	0.032359	0.62996	0.089798
2.50437	0.247173	0.026168	0.610389	0.11627
2.533833	0.238201	0.030999	0.638203	0.092597
2.563296	0.21064	0.04441	0.700775	0.044175
2.592759	0.204636	0.047376	0.713512	0.034476
2.622223	0.184065	0.050931	0.740923	0.024081
2.651686	0.175552	0.048503	0.750784	0.025161
2.681149	0.79362	0.004946	0.201434	0
2.710612	0.744194	0.01025	0.245556	0
2.740075	0.768868	0.011457	0.204082	0.015593
2.769538	0.800941	0.02476	0.1743	0
2.799002	0.8463	0	0.146539	0.007161

2.828465	0.760288	0.040978	0.198733	0
2.857928	0.150622	0.055416	0.780111	0.013852
2.887391	0.179732	0.035489	0.753738	0.031041
2.916854	0.206974	0.032938	0.715503	0.044584
2.946317	0.191236	0.031715	0.721666	0.055384
2.975781	0.190309	0.030503	0.718456	0.060732
3.005244	0.209613	0.029955	0.697795	0.062636
3.034707	0.236904	0.026655	0.670286	0.066155
3.06417	0.225769	0.025445	0.678533	0.070253
3.093633	0.239827	0.022978	0.660276	0.07692
3.123097	0.233491	0.02391	0.660042	0.082556
3.15256	0.232776	0.022731	0.656829	0.087664
3.182023	0.229982	0.021449	0.654188	0.094381
3.211486	0.230676	0.024425	0.644993	0.099906
3.240949	0.240791	0.021227	0.632762	0.10522
3.270412	0.226001	0.021898	0.642111	0.109989
3.299876	0.239902	0.020191	0.626593	0.113313
3.329339	0.255372	0.019933	0.60921	0.115485
3.358802	0.241891	0.020621	0.612256	0.125231
3.388265	0.266088	0.017979	0.588414	0.127519
3.417728	0.253987	0.017969	0.580533	0.147511
3.447191	0.26425	0.013928	0.543807	0.178015
3.476655	0.275511	0.011419	0.519744	0.193326
3.506118	0.2688	0.012436	0.515891	0.202873
3.535581	0.260688	0.013971	0.512816	0.212524
3.565044	0.257697	0.011226	0.509439	0.221637
3.594507	0.258181	0.012566	0.505104	0.224148
3.62397	0.263758	0.012095	0.500871	0.223276
3.653434	0.261697	0.013222	0.500148	0.224933
3.682897	0.268647	0.010759	0.496862	0.223732
3.71236	0.264802	0.010923	0.506608	0.217667
3.741823	0.267334	0.014745	0.509963	0.207958
3.771286	0.253751	0.016108	0.526063	0.204077
3.80075	0.269388	0.013186	0.520451	0.196975
3.830213	0.258526	0.013943	0.538597	0.188933
3.859676	0.258449	0.014002	0.545172	0.182377
3.889139	0.259139	0.015351	0.552882	0.172627
3.918602	0.267853	0.012793	0.553283	0.166071
3.948065	0.256471	0.017099	0.572996	0.153434
3.977529	0.25792	0.017498	0.590674	0.133908
4.006992	0.265287	0.01913	0.595838	0.119744
4.036455	0.246219	0.018395	0.622564	0.112823
4.065918	0.245934	0.022085	0.630092	0.10189
4.095381	0.231273	0.023408	0.649052	0.096268
4.124844	0.243253	0.024592	0.644533	0.087622

4.154308	0.22692	0.022658	0.66634	0.084083
4.183771	0.209523	0.025011	0.686669	0.078797
4.213234	0.203762	0.026764	0.692016	0.077458
4.242697	0.201929	0.027432	0.702674	0.067966
4.27216	0.214426	0.029365	0.695486	0.060724
4.301623	0.218084	0.027781	0.695318	0.058817
4.331087	0.205258	0.030124	0.710223	0.054395
4.36055	0.211664	0.030098	0.709816	0.048422
4.390013	0.196748	0.032699	0.727001	0.043552
4.419476	0.19623	0.031982	0.732424	0.039364
4.448939	0.174827	0.034484	0.756457	0.034233
4.478403	0.185921	0.032292	0.752237	0.029549
4.507866	0.17937	0.036617	0.75858	0.025433
4.537329	0.188314	0.036858	0.753964	0.020864
4.566792	0.169949	0.037302	0.774078	0.01867
4.596255	0.184672	0.038848	0.761836	0.014643
4.625718	0.163433	0.040457	0.783722	0.012388
4.655182	0.16309	0.043942	0.783671	0.009297
4.684645	0.162527	0.046355	0.782448	0.00867
4.714108	0.154577	0.048136	0.789229	0.008058
4.743571	0.162698	0.047641	0.783988	0.005673
4.773034	0.159215	0.048002	0.787968	0.004815
4.802497	0.160212	0.04848	0.787291	0.004018
4.831961	0.148434	0.050875	0.796819	0.003872
4.861424	0.132955	0.051251	0.811807	0.003987
4.890887	0.151074	0.049975	0.795568	0.003383
4.92035	0.139212	0.051896	0.80563	0.003262
4.949813	0.156866	0.051103	0.788903	0.003128
4.979277	0.160914	0.049979	0.786073	0.003035
5.00874	0.157681	0.05258	0.787631	0.002108
5.038203	0.149538	0.053449	0.794117	0.002896
5.067666	0.150459	0.053964	0.793021	0.002556
5.097129	0.147922	0.054485	0.795372	0.002222
5.126592	0.15149	0.055468	0.790568	0.002475
5.156056	0.149051	0.056283	0.792667	0.001999
5.185519	0.157316	0.056332	0.784667	0.001686
5.214982	0.158232	0.055205	0.784596	0.001966
5.244445	0.154497	0.056466	0.787434	0.001603
5.273908	0.160067	0.053308	0.78487	0.001755
5.303371	0.155954	0.060854	0.781158	0.002033
5.332835	0.164092	0.057212	0.776388	0.002309
5.362298	0.166431	0.058238	0.772836	0.002495
5.391761	0.386767	0.254648	0.342247	0.016339

Table B.3: 18ZE-R-14B EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.196471	0.069692	0.707631	0.026206
0.020481	0.221477	0.068147	0.685593	0.024783
0.040962	0.225297	0.063732	0.684722	0.02625
0.061443	0.216916	0.06276	0.692405	0.027919
0.081924	0.206398	0.063381	0.700047	0.030175
0.102405	0.212028	0.061424	0.693638	0.03291
0.122886	0.214166	0.06329	0.687342	0.035202
0.143367	0.209624	0.062996	0.689604	0.037776
0.163848	0.203347	0.063334	0.694202	0.039118
0.184329	0.208648	0.06328	0.687554	0.040519
0.20481	0.207057	0.061952	0.688338	0.042653
0.225291	0.206623	0.062046	0.688711	0.042621
0.245772	0.199526	0.065768	0.690008	0.044698
0.266253	0.2073	0.058219	0.687923	0.046558
0.368657	0.225984	0.056812	0.669334	0.04787
0.389138	0.222546	0.060913	0.665158	0.051383
0.409619	0.212332	0.055586	0.677818	0.054265
0.4301	0.221302	0.055493	0.6677	0.055506
0.450581	0.227138	0.055673	0.661592	0.055598
0.471062	0.217394	0.053901	0.669348	0.059357
0.491543	0.226283	0.054499	0.660583	0.058636
0.512024	0.235063	0.053381	0.651062	0.060494
0.532505	0.23489	0.053977	0.650228	0.060905
0.552986	0.230448	0.050657	0.65595	0.062945
0.573467	0.233569	0.05261	0.646898	0.066923
0.593948	0.234639	0.050732	0.645495	0.069135
0.614429	0.237767	0.050465	0.638527	0.073241
0.63491	0.231125	0.049165	0.639432	0.080278
0.655391	0.241775	0.046462	0.625732	0.086031
0.675872	0.245903	0.045939	0.61653	0.091629
0.696353	0.229326	0.048204	0.629742	0.092729
0.716834	0.21944	0.041692	0.621296	0.117572
0.737315	0.227043	0.042556	0.594184	0.136218
0.757796	0.230301	0.040442	0.588694	0.140563
0.778277	0.248927	0.037606	0.558886	0.154581
0.798758	0.240655	0.037813	0.557121	0.164412
0.819239	0.244379	0.037122	0.547229	0.17127
0.839719	0.239612	0.042875	0.542121	0.175392
0.8602	0.245218	0.029624	0.528635	0.196523
0.880681	0.250848	0.033478	0.50986	0.205814
0.901162	0.249476	0.029347	0.508712	0.212465

0.921643	0.268065	0.027255	0.488408	0.216272
0.942124	0.262828	0.023464	0.474177	0.239532
0.962605	0.24646	0.026473	0.481051	0.246016
0.983086	0.27626	0.026283	0.478762	0.218695
1.003567	0.295836	0.023429	0.461551	0.219184
1.024048	0.290402	0.020343	0.466559	0.222696
1.044529	0.295811	0.0184	0.46626	0.219528
1.06501	0.285653	0.020463	0.472553	0.221331
1.085491	0.277583	0.038245	0.47122	0.212953
1.105972	0.279492	0.019034	0.47242	0.229054
1.126453	0.281923	0.021544	0.466221	0.230313
1.146934	0.283236	0.021299	0.471277	0.224189
1.167415	0.28781	0.023322	0.468306	0.220563
1.187896	0.289093	0.020188	0.463412	0.227307
1.208377	0.279332	0.019542	0.46967	0.231457
1.228858	0.285028	0.018465	0.467934	0.228574
1.249339	0.296628	0.017929	0.462633	0.22281
1.26982	0.290181	0.017443	0.463039	0.229338
1.290301	0.290053	0.017739	0.462686	0.229522
1.310782	0.280469	0.018896	0.465956	0.23468
1.331263	0.299172	0.016523	0.459653	0.224652
1.351744	0.284642	0.018339	0.468878	0.228142
1.372224	0.281043	0.017041	0.467828	0.234089
1.392705	0.282084	0.019151	0.471783	0.226982
1.413186	0.288183	0.020369	0.468734	0.222714
1.433667	0.29387	0.018231	0.468779	0.21912
1.454148	0.28681	0.019289	0.469555	0.224347
1.474629	0.315167	0.017731	0.452558	0.214545
1.49511	0.291177	0.018974	0.465736	0.224113
1.515591	0.274963	0.021422	0.479656	0.223959
1.536072	0.292785	0.021106	0.470066	0.216043
1.556553	0.283865	0.020746	0.481297	0.214092
1.577034	0.274898	0.023561	0.489539	0.212002
1.597515	0.27724	0.026697	0.493178	0.202885
1.617996	0.264008	0.026203	0.505853	0.203936
1.638477	0.275973	0.026339	0.500633	0.197055
1.658958	0.263249	0.028588	0.517055	0.191108
1.679439	0.26123	0.025539	0.491358	0.221874
1.69992	0.274858	0.026485	0.475306	0.22335
1.720401	0.255669	0.030524	0.506354	0.207454
1.740882	0.236866	0.03321	0.547464	0.18246
1.761363	0.237077	0.035422	0.558837	0.168663
1.781844	0.24173	0.038658	0.565696	0.153917
1.802325	0.23672	0.042313	0.588074	0.132893
1.822806	0.245905	0.043928	0.591409	0.118758

1.843287	0.221699	0.045219	0.625433	0.107649
1.863768	0.255342	0.044259	0.607451	0.092948
1.884249	0.219613	0.056461	0.663754	0.060172
1.90473	0.230492	0.053626	0.649588	0.066294
1.92521	0.233601	0.051297	0.645045	0.070058
1.945691	0.23288	0.05198	0.651932	0.063209
1.966172	0.230621	0.055449	0.65189	0.062041
1.986653	0.224606	0.05677	0.663471	0.055154
2.007134	0.209108	0.057471	0.680487	0.052935
2.027615	0.206821	0.059777	0.681674	0.051728
2.048096	0.205498	0.057125	0.686277	0.0511
2.068577	0.203888	0.061664	0.683627	0.050822
2.089058	0.202236	0.059414	0.687231	0.05112
2.109539	0.199125	0.061898	0.689365	0.049612
2.13002	0.197497	0.062364	0.690452	0.049687
2.150501	0.195179	0.061327	0.694376	0.049119
2.170982	0.20329	0.062052	0.689079	0.04558
2.191463	0.216579	0.059999	0.680239	0.043183
2.211944	0.232299	0.059148	0.669593	0.03896
2.232425	0.21617	0.061115	0.684067	0.038649

Table B.4: 18ZE-R-14C EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.198233	0.059446	0.740118	0.002203
0.050853	0.184089	0.059781	0.753592	0.002539
0.101706	0.190964	0.052708	0.754043	0.002285
0.152559	0.194836	0.050843	0.752547	0.001774
0.203412	0.201032	0.047446	0.749722	0.0018
0.254264	0.185022	0.047138	0.766482	0.001358
0.305117	0.194266	0.04717	0.756793	0.001771
0.35597	0.206608	0.043304	0.748186	0.001902
0.406823	0.195404	0.043717	0.758315	0.002563
0.457676	0.203824	0.042552	0.751681	0.001943
0.508529	0.200529	0.041819	0.755737	0.001915
0.559382	0.199695	0.03988	0.758855	0.00157
0.610235	0.199817	0.039097	0.759072	0.002014
0.661088	0.201836	0.035845	0.760255	0.002063
0.71194	0.20491	0.037712	0.755194	0.002184
0.762793	0.213061	0.034408	0.749339	0.003192
0.813646	0.198487	0.037031	0.761484	0.002998
0.864499	0.20888	0.035172	0.752817	0.003131
0.915352	0.199741	0.034296	0.762472	0.00349
0.966205	0.21422	0.034034	0.747218	0.004527

1.017058	0.210515	0.032698	0.752026	0.004761
1.067911	0.219643	0.03177	0.743309	0.005277
1.118764	0.208129	0.031236	0.754736	0.005898
1.169616	0.12533	0.100681	0.769378	0.00461
1.220469	0.209275	0.028382	0.754332	0.00801
1.271322	0.211032	0.031455	0.74898	0.008534
1.322175	0.21931	0.028941	0.741787	0.009962
1.373028	0.207018	0.028619	0.753294	0.011069
1.423881	0.211147	0.028393	0.747416	0.013044
1.474734	0.203781	0.028978	0.750906	0.016335
1.525587	0.211271	0.028708	0.74326	0.016762
1.57644	0.208453	0.027755	0.744457	0.019334
1.627293	0.209376	0.028342	0.739345	0.022937
1.678145	0.208781	0.028633	0.734378	0.028207
1.728998	0.208688	0.041029	0.720308	0.029975
1.779851	0.254741	0.027511	0.685479	0.032269
1.830704	0.224933	0.029314	0.708867	0.036887
1.881557	0.235567	0.026032	0.696973	0.041428
1.93241	0.225684	0.024441	0.702444	0.047431
1.983263	0.234667	0.027217	0.688276	0.04984
2.034116	0.239474	0.022888	0.681584	0.056054
2.084969	0.216994	0.021282	0.703581	0.058143
2.135821	0.217629	0.023472	0.698483	0.060416
2.186674	0.224974	0.022407	0.690661	0.061958
2.237527	0.21864	0.02289	0.688572	0.069899
2.28838	0.235363	0.020622	0.675435	0.06858
2.339233	0.20155	0.056162	0.702156	0.040132
2.390086	0.224587	0.021573	0.67638	0.07746
2.440939	0.241173	0.021109	0.656352	0.081366
2.491792	0.221319	0.019661	0.670499	0.08852
2.542645	0.243938	0.021918	0.647552	0.086592
2.593497	0.230174	0.019285	0.659539	0.091002
2.64435	0.220732	0.020139	0.659809	0.09932
2.695203	0.225293	0.019011	0.649682	0.106014
2.746056	0.234582	0.017095	0.641084	0.107239
2.796909	0.234013	0.01797	0.637868	0.11015
2.847762	0.252327	0.016757	0.623433	0.107484
2.898615	0.254561	0.017947	0.621867	0.105626
2.949468	0.259141	0.015841	0.615088	0.10993
3.000321	0.248951	0.017016	0.622688	0.111345
3.051173	0.232618	0.018594	0.636865	0.111923
3.102026	0.256337	0.017137	0.618671	0.107855
3.152879	0.254138	0.018307	0.616336	0.11122
3.203732	0.260385	0.01685	0.612709	0.110057
3.254585	0.233811	0.016806	0.631737	0.117645

3.305438	0.242112	0.018423	0.621362	0.118104
3.356291	0.249278	0.016981	0.618375	0.115366
3.407144	0.262395	0.016456	0.606588	0.114562
3.457997	0.26372	0.015898	0.603448	0.116934
3.508849	0.268791	0.017017	0.600839	0.113353
3.559702	0.243797	0.016161	0.624658	0.115384
3.610555	0.232914	0.016049	0.631664	0.119373
3.661408	0.234235	0.01909	0.630619	0.116057
3.712261	0.244298	0.018269	0.627655	0.109778
3.763114	0.226013	0.018219	0.638503	0.117265
3.813967	0.243908	0.017492	0.624567	0.114033
3.86482	0.226877	0.017501	0.637343	0.118278
3.915673	0.234077	0.018322	0.634756	0.112845
3.966525	0.233998	0.016997	0.634272	0.114733
4.017378	0.238287	0.017471	0.631403	0.112839
4.068231	0.245375	0.017433	0.620927	0.116265
4.119084	0.248679	0.016481	0.618709	0.116131
4.169937	0.243493	0.016374	0.621567	0.118566
4.22079	0.227346	0.019359	0.63521	0.118085
4.271643	0.232973	0.018437	0.63103	0.117559
4.322496	0.238258	0.016708	0.632728	0.112306
4.373349	0.236528	0.017681	0.63766	0.108131
4.424201	0.227382	0.021773	0.64785	0.102995
4.475054	0.218621	0.02033	0.655128	0.105921
4.525907	0.22784	0.020025	0.650508	0.101627
4.57676	0.228993	0.020268	0.656709	0.09403
4.627613	0.235885	0.019781	0.651623	0.092712
4.678466	0.240621	0.018829	0.655197	0.085353
4.729319	0.224872	0.021714	0.665316	0.088098
4.780172	0.235503	0.01903	0.663158	0.08231
4.831025	0.221986	0.019629	0.678648	0.079737
4.881878	0.225099	0.021888	0.676387	0.076626
4.93273	0.230007	0.023058	0.673293	0.073642
4.983583	0.233344	0.020964	0.674683	0.071009
5.034436	0.232198	0.020059	0.679879	0.067863
5.085289	0.217383	0.022537	0.696754	0.063326
5.136142	0.22651	0.023058	0.6901	0.060331
5.186995	0.220342	0.023321	0.700073	0.056263
5.237848	0.205187	0.022322	0.71889	0.053601
5.288701	0.217297	0.023142	0.708005	0.051555
5.339554	0.212793	0.023903	0.718598	0.044706
5.390406	0.21969	0.027517	0.711288	0.041506
5.441259	0.240754	0.029035	0.694017	0.036194
5.492112	0.227177	0.024721	0.712526	0.035576
5.542965	0.225447	0.025109	0.715007	0.034437

5.593818	0.218297	0.025148	0.725125	0.031431
5.644671	0.219873	0.026193	0.72476	0.029173
5.695524	0.21346	0.025476	0.733373	0.027691
5.746377	0.194838	0.03622	0.743407	0.025535
5.79723	0.222818	0.025916	0.726	0.025266
5.848082	0.216869	0.028039	0.733803	0.021288
5.898935	0.220771	0.029076	0.729888	0.020265
5.949788	0.218109	0.0286	0.736382	0.016909
6.000641	0.207595	0.031997	0.744457	0.015951
6.051494	0.191048	0.028396	0.766924	0.013631
6.102347	0.183758	0.035062	0.769452	0.011727
6.1532	0.21378	0.027465	0.74873	0.010024
6.204053	0.196588	0.032909	0.76205	0.008453
6.254906	0.216994	0.030973	0.743826	0.008207
6.305758	0.209794	0.031823	0.751793	0.006591
6.356611	0.20542	0.034635	0.754923	0.005023
6.407464	0.21376	0.033389	0.749092	0.003759
6.458317	0.210809	0.038693	0.747523	0.002976
6.50917	0.205105	0.036146	0.756409	0.002339
6.560023	0.203023	0.037366	0.756798	0.002814
6.610876	0.20423	0.038294	0.755221	0.002254
6.661729	0.205285	0.037332	0.755296	0.002087
6.712582	0.207529	0.038657	0.751606	0.002209
6.763434	0.198665	0.04878	0.751021	0.001534
6.814287	0.208955	0.039808	0.749409	0.001827
6.86514	0.204356	0.043542	0.750169	0.001932
6.915993	0.203538	0.041844	0.752146	0.002472
6.966846	0.206131	0.044009	0.748101	0.001759
7.017699	0.197141	0.047116	0.753695	0.002048
7.068552	0.198476	0.0472	0.75245	0.001874
7.119405	0.197685	0.04895	0.750887	0.002478
7.170258	0.196922	0.050171	0.750927	0.00198
7.22111	0.191246	0.054188	0.752676	0.00189
7.271963	0.186758	0.057529	0.753681	0.002032
7.322816	0.190906	0.060612	0.746099	0.002383
7.373669	0.198494	0.063683	0.735529	0.002294

Table B.5: 18ZE-R-16 EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.239206	0.064948	0.627549	0.068296
0.025374	0.233982	0.065726	0.628836	0.071456
0.050747	0.211654	0.07063	0.636502	0.081213
0.076121	0.206838	0.071435	0.634821	0.086906

0.101495	0.215801	0.065396	0.627641	0.091163
0.126868	0.242087	0.061169	0.605058	0.091685
0.152242	0.233635	0.063412	0.609815	0.093138
0.177615	0.248104	0.060117	0.597925	0.093854
0.202989	0.24683	0.058328	0.598895	0.095947
0.228363	0.257359	0.055202	0.593264	0.094175
0.253736	0.246971	0.056199	0.598466	0.098364
0.27911	0.25909	0.054795	0.588361	0.097754
0.304484	0.265236	0.050843	0.584561	0.09936
0.329857	0.273714	0.050714	0.574089	0.101483
0.355231	0.268723	0.048839	0.58094	0.101498
0.380605	0.256475	0.049729	0.587134	0.106663
0.405978	0.254288	0.051649	0.588231	0.105832
0.431352	0.267397	0.045816	0.576363	0.110423
0.456726	0.267768	0.047164	0.572375	0.112693
0.482099	0.273627	0.044737	0.565613	0.116022
0.507473	0.270928	0.04316	0.56686	0.119052
0.532846	0.27771	0.044209	0.560744	0.117336
0.55822	0.268415	0.043453	0.560615	0.127516
0.583594	0.249118	0.044163	0.57154	0.135179
0.608967	0.244054	0.046011	0.572878	0.137056
0.634341	0.245638	0.042961	0.569418	0.141983
0.659715	0.42511	0.027145	0.436779	0.110966
0.685088	0.27915	0.039161	0.537491	0.144197
0.710462	0.244509	0.043001	0.556372	0.156118
0.735836	0.257685	0.042134	0.542411	0.157769
0.761209	0.25902	0.041248	0.540085	0.159646
0.786583	0.263953	0.037683	0.535958	0.162405
0.811956	0.256974	0.039455	0.535017	0.168554
0.83733	0.265813	0.036546	0.523808	0.173834
0.862704	0.273026	0.036877	0.515588	0.174509
0.888077	0.27013	0.036664	0.512045	0.181162
0.913451	0.254484	0.035998	0.51791	0.191607
0.938825	0.262561	0.033856	0.513428	0.190155
0.964198	0.255425	0.036177	0.515902	0.192496
0.989572	0.271866	0.033482	0.505867	0.188785
1.014946	0.259667	0.033424	0.50608	0.200829
1.040319	0.243148	0.03555	0.513355	0.207948
1.065693	0.247793	0.034416	0.502693	0.215097
1.091067	0.254856	0.0349	0.495586	0.214659
1.11644	0.251562	0.032492	0.496028	0.219919
1.141814	0.24923	0.033653	0.490152	0.226965
1.167187	0.251436	0.033453	0.489991	0.22512
1.192561	0.253048	0.032604	0.483532	0.230816
1.217935	0.260244	0.03071	0.47885	0.230196

1.243308	0.259599	0.031217	0.47822	0.230964
1.268682	0.25991	0.031146	0.476673	0.232271
1.294056	0.275284	0.030908	0.462085	0.231723
1.319429	0.248656	0.032323	0.47993	0.239091
1.344803	0.266677	0.029826	0.469047	0.23445
1.370177	0.256823	0.032124	0.473845	0.237208
1.39555	0.260181	0.032741	0.474035	0.233044
1.420924	0.261187	0.028066	0.470382	0.240365
1.446297	0.248631	0.029838	0.476063	0.245468
1.471671	0.258612	0.028768	0.47355	0.23907
1.497045	0.25407	0.029401	0.471581	0.244948
1.522418	0.256728	0.031069	0.474317	0.237886
1.547792	0.255619	0.033164	0.481044	0.230173
1.573166	0.258713	0.031754	0.478406	0.231127
1.598539	0.270668	0.025642	0.461409	0.242281
1.623913	0.257248	0.027925	0.459251	0.255576
1.649287	0.253757	0.029372	0.463398	0.253472
1.67466	0.264902	0.029734	0.465256	0.240109
1.700034	0.251872	0.027083	0.468871	0.252174
1.725408	0.278126	0.029149	0.44944	0.243284
1.750781	0.271923	0.026766	0.452914	0.248397
1.776155	0.258872	0.024741	0.446144	0.270243
1.801528	0.276974	0.024624	0.433816	0.264586
1.826902	0.28554	0.022981	0.427646	0.263833
1.852276	0.284157	0.020791	0.420359	0.274692
1.877649	0.278481	0.021724	0.425399	0.274397
1.903023	0.262781	0.021644	0.431259	0.284316
1.928397	0.250919	0.02449	0.449818	0.274774
1.95377	0.258612	0.024314	0.443532	0.273542
1.979144	0.267855	0.023164	0.435222	0.273759
2.004518	0.285988	0.021058	0.42077	0.272184
2.029891	0.275318	0.023252	0.427152	0.274279
2.055265	0.273476	0.023797	0.433443	0.269284
2.080639	0.279069	0.022745	0.438746	0.25944
2.106012	0.274225	0.023609	0.440913	0.261253
2.131386	0.276409	0.024304	0.444552	0.254735
2.156759	0.249894	0.027319	0.461441	0.261346
2.182133	0.258821	0.026969	0.452966	0.261243
2.207507	0.265864	0.027076	0.450276	0.256783
2.23288	0.271769	0.026152	0.450273	0.251807
2.258254	0.268671	0.027586	0.452404	0.25134
2.283628	0.266733	0.030066	0.454276	0.248925
2.309001	0.275186	0.029279	0.451103	0.244432
2.334375	0.254663	0.029976	0.466436	0.248924
2.359749	0.269152	0.030545	0.457007	0.243296

2.385122	0.273363	0.02808	0.454465	0.244092
2.410496	0.250125	0.029615	0.466357	0.253902
2.435869	0.244022	0.03222	0.474129	0.249629
2.461243	0.239193	0.031237	0.480154	0.249416
2.486617	0.255244	0.032607	0.473515	0.238634
2.51199	0.23093	0.034382	0.496656	0.238032
2.537364	0.253607	0.030774	0.474155	0.241464
2.562738	0.263592	0.032559	0.467867	0.235982
2.588111	0.268578	0.029469	0.466966	0.234987
2.613485	0.245418	0.033634	0.484198	0.23675
2.638859	0.264342	0.030592	0.467955	0.237112
2.664232	0.252647	0.029052	0.474428	0.243873
2.689606	0.272889	0.034256	0.464277	0.228578
2.71498	0.250753	0.03189	0.478259	0.239097
2.740353	0.251628	0.033909	0.48302	0.231443
2.765727	0.259216	0.037042	0.478384	0.225358
2.7911	0.267977	0.030856	0.476501	0.224665
2.816474	0.264109	0.036694	0.472945	0.226251
2.841848	0.25821	0.033102	0.476566	0.232121
2.867221	0.254556	0.032403	0.485602	0.227438
2.892595	0.23683	0.035	0.495793	0.232377
2.917969	0.2577	0.032085	0.48706	0.223154
2.943342	0.276549	0.031733	0.47596	0.215758
2.968716	0.243727	0.035483	0.496197	0.224592
2.99409	0.236625	0.035027	0.503	0.225348
3.019463	0.238766	0.03438	0.501497	0.225356
3.044837	0.247362	0.03487	0.503925	0.213843
3.07021	0.258206	0.03455	0.49573	0.211514
3.095584	0.247566	0.034556	0.506425	0.211453
3.120958	0.261721	0.035786	0.506027	0.196465
3.146331	0.264717	0.03228	0.49915	0.203853
3.171705	0.26015	0.036538	0.505516	0.197797
3.197079	0.251356	0.040365	0.507504	0.200775
3.222452	0.251715	0.03822	0.508218	0.201847
3.247826	0.256156	0.036073	0.509728	0.198043
3.2732	0.258011	0.037441	0.511336	0.193211
3.298573	0.248519	0.037215	0.519215	0.19505
3.323947	0.257804	0.037788	0.518107	0.186301
3.349321	0.257148	0.038371	0.517028	0.187452
3.374694	0.264544	0.036363	0.520464	0.178629
3.400068	0.275836	0.036927	0.513798	0.173439
3.425441	0.254585	0.036218	0.531195	0.178003
3.450815	0.269453	0.038994	0.521042	0.170511
3.476189	0.249335	0.039803	0.542989	0.167873
3.501562	0.244788	0.041274	0.546281	0.167656

3.526936	0.260564	0.039246	0.537863	0.162327
3.55231	0.263264	0.037451	0.537943	0.161342
3.577683	0.26889	0.039083	0.538622	0.153405
3.603057	0.264384	0.040441	0.544915	0.15026
3.628431	0.25806	0.04089	0.551709	0.14934
3.653804	0.256395	0.040985	0.560529	0.142091
3.679178	0.257436	0.042472	0.559776	0.140316
3.704551	0.270791	0.04253	0.552866	0.133814
3.729925	0.271629	0.043338	0.55575	0.129283
3.755299	0.272382	0.042578	0.559859	0.125181
3.780672	0.273345	0.042283	0.563497	0.120875
3.806046	0.268507	0.043054	0.569153	0.119286
3.83142	0.267929	0.047196	0.57283	0.112044
3.856793	0.271247	0.047981	0.571848	0.108924
3.882167	0.255278	0.049974	0.590963	0.103785
3.907541	0.245079	0.05663	0.596998	0.101293
3.932914	0.225743	0.06385	0.619946	0.09046
3.958288	0.253547	0.056349	0.601108	0.088996
3.983662	0.233053	0.062744	0.607058	0.097145
4.009035	0.218947	0.064411	0.623235	0.093407
4.034409	0.212679	0.064491	0.627462	0.095368
4.059782	0.217961	0.066609	0.622752	0.092678
4.085156	0.220337	0.067871	0.617521	0.09427
4.11053	0.223402	0.067403	0.617525	0.09167
4.135903	0.219229	0.067388	0.621899	0.091485
4.161277	0.223288	0.066616	0.62577	0.084326
4.186651	0.225606	0.066562	0.629593	0.078238
4.212024	0.225064	0.066468	0.631271	0.077197
4.237398	0.227659	0.065957	0.629926	0.076458
4.262772	0.221373	0.065793	0.638656	0.074178
4.288145	0.23018	0.068312	0.632116	0.069392
4.313519	0.224403	0.070987	0.638371	0.066239
4.338892	0.225221	0.068928	0.642498	0.063353

Table B.6: 18ZE-R-73C-L EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.070281	0.208151	0.697283	0.024285
0.015216	0.068846	0.205118	0.698279	0.027756
0.030432	0.069815	0.206014	0.694447	0.029725
0.045647	0.066807	0.197215	0.702391	0.033587
0.060863	0.067641	0.19342	0.700067	0.038872
0.076079	0.06706	0.189257	0.699221	0.044462
0.091295	0.066644	0.182425	0.703141	0.04779

0.106511	0.064613	0.18298	0.699116	0.053291
0.121726	0.068355	0.173209	0.699586	0.058851
0.136942	0.070033	0.169486	0.696435	0.064046
0.152158	0.070131	0.162861	0.693857	0.073151
0.167374	0.070388	0.157416	0.692281	0.079916
0.18259	0.073277	0.156685	0.689408	0.08063
0.197805	0.072409	0.150252	0.687242	0.090097
0.213021	0.072092	0.14295	0.689885	0.095073
0.228237	0.073028	0.140115	0.685594	0.101263
0.243453	0.072216	0.132873	0.688099	0.106813
0.258669	0.074085	0.127361	0.686875	0.111679
0.273884	0.076852	0.126277	0.68146	0.115412
0.2891	0.078954	0.123852	0.6765	0.120694
0.304316	0.079484	0.119476	0.678311	0.122729
0.319532	0.076761	0.114757	0.677898	0.130585
0.334747	0.079258	0.113483	0.671937	0.135322
0.349963	0.080045	0.115424	0.668377	0.136154
0.365179	0.087273	0.108365	0.667296	0.137066
0.380395	0.086766	0.104495	0.667305	0.141434
0.395611	0.083874	0.103175	0.670636	0.142315
0.410826	0.085443	0.101648	0.666286	0.146623
0.426042	0.088335	0.097074	0.665546	0.149045
0.441258	0.089706	0.094026	0.661219	0.15505
0.456474	0.090244	0.09461	0.659232	0.155914
0.47169	0.097369	0.088108	0.655362	0.159161
0.486905	0.100089	0.087988	0.651922	0.16
0.502121	0.096887	0.083581	0.656704	0.162829
0.517337	0.095034	0.081242	0.661232	0.162492
0.532553	0.097163	0.082592	0.655444	0.164802
0.547769	0.09605	0.079705	0.659721	0.164524
0.562984	0.094056	0.080505	0.657832	0.167607
0.5782	0.097733	0.076715	0.656509	0.169044
0.593416	0.099906	0.076802	0.653721	0.16957
0.608632	0.101554	0.077133	0.654374	0.166939
0.623848	0.10295	0.074006	0.652348	0.170696
0.639063	0.103943	0.072846	0.650086	0.173125
0.654279	0.103699	0.075142	0.648257	0.172902
0.669495	0.102657	0.077117	0.647175	0.173051
0.684711	0.104682	0.073198	0.646498	0.175621
0.699927	0.102446	0.07434	0.64829	0.174925
0.715142	0.106001	0.07231	0.648554	0.173134
0.730358	0.109699	0.072837	0.642432	0.175032
0.745574	0.112142	0.070021	0.642362	0.175475
0.76079	0.110293	0.070365	0.64366	0.175682
0.776006	0.11062	0.074397	0.638084	0.176899

0.791221	0.112746	0.068763	0.640324	0.178167
0.806437	0.115723	0.070395	0.635525	0.178357
0.821653	0.11359	0.069883	0.63653	0.179998
0.836869	0.116652	0.06929	0.634684	0.179374
0.852085	0.118071	0.069152	0.634819	0.177959
0.8673	0.119923	0.069115	0.63236	0.178602
0.882516	0.11552	0.067966	0.637171	0.179343
0.897732	0.117632	0.070101	0.633153	0.179114
0.912948	0.118904	0.070991	0.631634	0.178471
0.928164	0.122473	0.07076	0.629819	0.176948
0.943379	0.119351	0.071481	0.631577	0.177591
0.958595	0.117553	0.069082	0.633094	0.180271
0.973811	0.120965	0.07006	0.630293	0.178682
0.989027	0.121805	0.066792	0.631759	0.179644
1.004242	0.120806	0.070808	0.629234	0.179152
1.019458	0.118625	0.070495	0.631426	0.179454
1.034674	0.119358	0.069931	0.630577	0.180133
1.04989	0.121799	0.068802	0.629225	0.180174
1.065106	0.12033	0.068003	0.632427	0.179241
1.080321	0.120298	0.070031	0.628661	0.18101
1.095537	0.118938	0.068359	0.632732	0.179971
1.110753	0.113919	0.072109	0.633045	0.180928
1.125969	0.117145	0.071134	0.632613	0.179109
1.141185	0.117158	0.073326	0.632068	0.177449
1.1564	0.113446	0.070945	0.635995	0.179614
1.171616	0.112264	0.070451	0.638345	0.178939
1.186832	0.114224	0.070262	0.637755	0.177759
1.202048	0.112509	0.072511	0.636018	0.178962
1.217264	0.113975	0.07409	0.63301	0.178925
1.232479	0.113116	0.072183	0.636834	0.177867
1.247695	0.112416	0.073159	0.634981	0.179444
1.262911	0.113453	0.072792	0.634994	0.178762
1.278127	0.115452	0.071562	0.634123	0.178863
1.293343	0.116455	0.069427	0.636501	0.177618
1.308558	0.117799	0.069664	0.63529	0.177246
1.323774	0.1167	0.071892	0.634479	0.176929
1.33899	0.119568	0.070069	0.6338	0.176563
1.354206	0.109185	0.073053	0.63834	0.179421
1.369422	0.109306	0.07291	0.637036	0.180748
1.384637	0.108597	0.072199	0.63807	0.181134
1.399853	0.110094	0.073345	0.637839	0.178723
1.415069	0.109596	0.073352	0.635303	0.18175
1.430285	0.112174	0.072111	0.635858	0.179857
1.445501	0.110302	0.071952	0.637247	0.180499
1.460716	0.109618	0.072718	0.637455	0.18021

1.475932	0.11036	0.072927	0.636555	0.180158
1.491148	0.109415	0.072543	0.639603	0.178439
1.506364	0.108974	0.073554	0.639398	0.178075
1.52158	0.107084	0.07366	0.642133	0.177123
1.536795	0.107285	0.073773	0.638256	0.180686
1.552011	0.103028	0.073277	0.644586	0.179109
1.567227	0.103446	0.074661	0.643986	0.177907
1.582443	0.105747	0.075508	0.641063	0.177683
1.597659	0.104682	0.071972	0.64401	0.179336
1.612874	0.108472	0.072866	0.641144	0.177519
1.62809	0.107883	0.074667	0.641399	0.176052
1.643306	0.104397	0.073646	0.644569	0.177388
1.658522	0.104999	0.073273	0.643584	0.178144
1.673737	0.10708	0.077369	0.639712	0.17584
1.688953	0.10351	0.072379	0.645435	0.178676
1.704169	0.104633	0.074232	0.642712	0.178423
1.719385	0.103816	0.077385	0.642891	0.175908
1.734601	0.104389	0.074573	0.64627	0.174768
1.749816	0.10669	0.075002	0.644322	0.173987
1.765032	0.10982	0.07674	0.641072	0.172368
1.780248	0.10971	0.079128	0.639937	0.171225
1.795464	0.106653	0.076542	0.645159	0.171646
1.81068	0.103199	0.079964	0.643427	0.173411
1.825895	0.105313	0.079796	0.642886	0.172005
1.841111	0.104254	0.07936	0.644391	0.171995
1.856327	0.100704	0.082239	0.646459	0.170598
1.871543	0.102343	0.080323	0.646422	0.170912
1.886759	0.102863	0.084638	0.644496	0.168003
1.901974	0.102671	0.083202	0.643513	0.170614
1.91719	0.100982	0.082981	0.646878	0.169158
1.932406	0.104455	0.084044	0.645303	0.166199
1.947622	0.100464	0.084758	0.646156	0.168622
1.962838	0.09786	0.086566	0.646958	0.168616
1.978053	0.091758	0.087284	0.65318	0.167778
1.993269	0.085956	0.090272	0.657307	0.166465
2.008485	0.088868	0.092377	0.652892	0.165864
2.023701	0.087284	0.097138	0.649184	0.166395
2.038917	0.083365	0.09593	0.656071	0.164633
2.054132	0.078886	0.09927	0.660659	0.161185
2.069348	0.082921	0.100881	0.65906	0.157138
2.084564	0.079987	0.104046	0.658063	0.157904
2.09978	0.086393	0.108146	0.654358	0.151103
2.114996	0.083525	0.112329	0.656953	0.147194
2.130211	0.081718	0.111221	0.663244	0.143817
2.145427	0.079388	0.110878	0.665415	0.14432

2.160643	0.077794	0.115847	0.665851	0.140509
2.175859	0.081361	0.115103	0.66939	0.134146
2.191075	0.080481	0.123816	0.66322	0.132484
2.20629	0.078808	0.124773	0.666609	0.12981
2.221506	0.081009	0.128544	0.673308	0.117139
2.236722	0.080286	0.131609	0.674547	0.113558
2.251938	0.076226	0.134324	0.681131	0.108319
2.267154	0.075432	0.13616	0.686055	0.102353
2.282369	0.070292	0.145893	0.688864	0.094951
2.297585	0.06914	0.147481	0.689052	0.094328
2.312801	0.067336	0.152152	0.691722	0.08879
2.328017	0.071277	0.160736	0.689453	0.078534
2.343232	0.06805	0.163049	0.696044	0.072858
2.358448	0.068188	0.171993	0.698092	0.061727
2.373664	0.066338	0.176493	0.699669	0.0575
2.38888	0.063359	0.182795	0.699925	0.05392
2.404096	0.068963	0.186863	0.696492	0.047681
2.419311	0.071739	0.18778	0.697522	0.042959
2.434527	0.067335	0.197706	0.69665	0.038309
2.449743	0.06706	0.200198	0.697741	0.035001
2.464959	0.066346	0.201677	0.699291	0.032686
2.480175	0.069841	0.204336	0.698556	0.027267
2.49539	0.068848	0.211089	0.693943	0.026121
2.510606	0.073062	0.212291	0.690785	0.023863
2.525822	0.073333	0.199073	0.702814	0.02478

Table B.7: 18ZE-R-73C-S EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.069989	0.21002	0.686684	0.033307
0.010197	0.069293	0.21226	0.685055	0.033392
0.020394	0.069052	0.207243	0.688829	0.034876
0.030591	0.07015	0.200622	0.692074	0.037153
0.040788	0.067374	0.206149	0.686464	0.040013
0.050985	0.065477	0.202526	0.68952	0.042477
0.061182	0.063094	0.203646	0.689274	0.043986
0.07138	0.063876	0.201088	0.68961	0.045426
0.081577	0.059534	0.200932	0.69292	0.046615
0.091774	0.06526	0.196168	0.691149	0.047423
0.101971	0.074497	0.191838	0.682739	0.050925
0.112168	0.047824	0.32046	0.593397	0.038319
0.122365	0.079656	0.188613	0.677201	0.05453
0.132562	0.079371	0.192924	0.672015	0.05569
0.142759	0.077596	0.186938	0.676918	0.058548

0.152956	0.074827	0.188357	0.675524	0.061293
0.163153	0.076238	0.19033	0.669022	0.06441
0.17335	0.087556	0.175363	0.670053	0.067028
0.183547	0.081576	0.174358	0.672452	0.071615
0.193744	0.079974	0.171265	0.67492	0.073841
0.203941	0.082866	0.171262	0.670282	0.075591
0.214139	0.083704	0.17094	0.666086	0.07927
0.224336	0.09225	0.162982	0.663959	0.08081
0.234533	0.093972	0.162638	0.659622	0.083767
0.24473	0.092476	0.161674	0.658205	0.087645
0.254927	0.087673	0.162616	0.658457	0.091254
0.265124	0.091966	0.154316	0.660088	0.093631
0.275321	0.086889	0.155137	0.660069	0.097905
0.285518	0.088019	0.150505	0.660453	0.101023
0.295715	0.085084	0.152376	0.656372	0.106169
0.305912	0.093616	0.142869	0.651523	0.111992
0.316109	0.092228	0.139726	0.650407	0.117639
0.326306	0.102709	0.133923	0.64148	0.121887
0.336503	0.102319	0.132287	0.637945	0.127449
0.3467	0.103937	0.127372	0.637545	0.131146
0.356898	0.123817	0.116868	0.621531	0.137784
0.367095	0.133053	0.115842	0.613152	0.137954
0.377292	0.139174	0.109251	0.610544	0.14103
0.387489	0.14939	0.107164	0.601639	0.141807
0.397686	0.151797	0.103892	0.593061	0.15125
0.407883	0.15307	0.101654	0.590173	0.155104
0.41808	0.161973	0.099086	0.586204	0.152737
0.428277	0.16813	0.094025	0.581138	0.156707
0.438474	0.175941	0.089899	0.578145	0.156015
0.448671	0.171811	0.0906	0.578245	0.159344
0.458868	0.14594	0.097664	0.590886	0.16551
0.469065	0.144135	0.093421	0.59415	0.168295
0.479262	0.144618	0.095954	0.590473	0.168955
0.48946	0.14618	0.100793	0.587118	0.165909
0.499657	0.153189	0.091898	0.591517	0.163396
0.509854	0.152733	0.09458	0.587261	0.165425
0.520051	0.160553	0.095003	0.584072	0.160373
0.530248	0.160029	0.094966	0.583127	0.161879
0.540445	0.160225	0.098345	0.586188	0.155242
0.550642	0.164165	0.1003	0.583008	0.152527
0.560839	0.161139	0.101481	0.587484	0.149896
0.571036	0.152481	0.110673	0.594992	0.141854
0.581233	0.150814	0.126254	0.584195	0.138737
0.59143	0.138126	0.112777	0.604877	0.14422
0.601627	0.154657	0.109893	0.591009	0.144441

0.611824	0.138707	0.113928	0.604443	0.142922
0.622021	0.142989	0.10993	0.598192	0.148889
0.632219	0.155294	0.1042	0.592281	0.148226
0.642416	0.165613	0.100837	0.584649	0.148902
0.652613	0.150802	0.103144	0.595583	0.150471
0.66281	0.158579	0.105385	0.583929	0.152107
0.673007	0.159472	0.104794	0.585118	0.150616
0.683204	0.147751	0.103961	0.594415	0.153874
0.693401	0.128718	0.108901	0.610803	0.151578
0.703598	0.109683	0.121249	0.627917	0.141152
0.713795	0.123795	0.112039	0.613396	0.150771
0.723992	0.140055	0.102853	0.608739	0.148354
0.734189	0.139987	0.10506	0.606785	0.148169
0.744386	0.144236	0.108451	0.603692	0.143622
0.754583	0.153012	0.103434	0.600316	0.143239
0.76478	0.173968	0.102986	0.592735	0.130311
0.774978	0.172133	0.105785	0.593215	0.128868
0.785175	0.149726	0.115951	0.607021	0.127301
0.795372	0.145666	0.120012	0.61409	0.120232
0.805569	0.134163	0.127011	0.621816	0.11701
0.815766	0.11941	0.130738	0.638574	0.111278
0.825963	0.106895	0.138069	0.647892	0.107144
0.83616	0.100965	0.143365	0.652663	0.103007
0.846357	0.09493	0.144677	0.659463	0.100931
0.856554	0.090701	0.152678	0.660697	0.095925
0.866751	0.090644	0.155026	0.662379	0.091952
0.876948	0.087608	0.15925	0.66397	0.089173
0.887145	0.089997	0.159281	0.667633	0.083089
0.897342	0.084359	0.164603	0.671287	0.079751
0.907539	0.085874	0.169023	0.668231	0.076873
0.917737	0.086141	0.170929	0.670886	0.072044
0.927934	0.082954	0.179908	0.666579	0.07056
0.938131	0.081442	0.176743	0.672494	0.069322
0.948328	0.079476	0.178002	0.67567	0.066852
0.958525	0.077608	0.179086	0.677583	0.065724
0.968722	0.079573	0.179857	0.677295	0.063275
0.978919	0.080752	0.1812	0.676084	0.061964
0.989116	0.081536	0.183679	0.674418	0.060368
0.999313	0.080172	0.183837	0.677238	0.058753
1.00951	0.077143	0.188453	0.678156	0.056248
1.019707	0.074774	0.189952	0.680917	0.054357
1.029904	0.070113	0.189525	0.686157	0.054204
1.040101	0.070099	0.192666	0.684381	0.052854
1.050299	0.071219	0.189489	0.687249	0.052043
1.060496	0.071754	0.195754	0.682216	0.050276

1.070693	0.068494	0.19777	0.684091	0.049645
1.08089	0.068155	0.20137	0.681265	0.049211
1.091087	0.063593	0.200006	0.688603	0.047799
1.101284	0.062341	0.207244	0.68379	0.046625
1.111481	0.063208	0.202215	0.688727	0.04585
1.121678	0.063967	0.2	0.692278	0.043756
1.131875	0.063923	0.205205	0.686214	0.044657
1.142072	0.065255	0.200108	0.690386	0.044251
1.152269	0.06493	0.202276	0.689986	0.042809
1.162466	0.065772	0.203116	0.691266	0.039847
1.172663	0.068233	0.204162	0.68775	0.039856
1.18286	0.066041	0.207069	0.68963	0.03726
1.193058	0.067577	0.209397	0.687504	0.035522
1.203255	0.072241	0.206088	0.688985	0.032687
1.213452	0.070345	0.211667	0.684242	0.033746
1.223649	0.069026	0.203668	0.693936	0.03337

Table B.8: 18ZE-R-77A EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.0775	0.0892	0.7716	0.0617
0.019839	0.0811	0.1044	0.7767	0.0378
0.039679	0.0781	0.1122	0.778	0.0317
0.059518	0.0732	0.1183	0.7795	0.029
0.079358	0.0782	0.1184	0.7755	0.0279
0.099197	0.0852	0.1184	0.7672	0.0292
0.119037	0.0893	0.1217	0.7634	0.0256
0.138876	0.0886	0.1224	0.7618	0.0272
0.158716	0.0945	0.1175	0.762	0.026
0.178555	0.0957	0.1163	0.7612	0.0268
0.198395	0.096	0.115	0.7614	0.0276
0.218234	0.0978	0.1156	0.7585	0.0281
0.238074	0.1028	0.1154	0.753	0.0289
0.257913	0.1058	0.1101	0.753	0.0312
0.277753	0.1088	0.111	0.7474	0.0329
0.297592	0.1084	0.1124	0.7475	0.0318
0.317432	0.1085	0.1121	0.7474	0.032
0.337271	0.1125	0.1118	0.7426	0.0331
0.357111	0.111	0.1109	0.7448	0.0333
0.37695	0.1129	0.1077	0.7431	0.0363
0.39679	0.1183	0.1086	0.7332	0.0398
0.416629	0.1204	0.102	0.7352	0.0425
0.436469	0.1223	0.0972	0.7359	0.0445
0.456308	0.1298	0.0936	0.7312	0.0455

0.476148	0.137	0.0889	0.7232	0.0509
0.495987	0.1395	0.0904	0.7185	0.0517
0.515827	0.1482	0.0792	0.716	0.0566
0.535666	0.1489	0.0793	0.7151	0.0567
0.555506	0.1578	0.0762	0.7067	0.0592
0.575345	0.1545	0.0738	0.7103	0.0614
0.595185	0.1682	0.0706	0.6956	0.0656
0.615024	0.168	0.0674	0.6959	0.0686
0.634864	0.174	0.0625	0.6914	0.0721
0.654703	0.1819	0.0623	0.6809	0.0748
0.674543	0.1875	0.0626	0.6739	0.0761
0.694382	0.1893	0.0566	0.674	0.08
0.714222	0.1984	0.0511	0.6672	0.0833
0.734061	0.1947	0.0523	0.6655	0.0875
0.753901	0.2075	0.0487	0.6588	0.085
0.77374	0.2054	0.0499	0.6567	0.088
0.79358	0.2036	0.0487	0.6562	0.0915
0.813419	0.2038	0.0482	0.6574	0.0906
0.833259	0.2072	0.0459	0.6521	0.0948
0.853098	0.203	0.0478	0.652	0.0972
0.872938	0.21	0.046	0.6462	0.0978
0.892777	0.2121	0.0427	0.6462	0.099
0.912617	0.2181	0.0411	0.6388	0.102
0.932456	0.2222	0.0402	0.6344	0.1032
0.952296	0.2252	0.0379	0.6299	0.107
0.972135	0.2274	0.04	0.6228	0.1099
0.991975	0.2285	0.0355	0.6256	0.1104
1.011814	0.2285	0.0353	0.623	0.1133
1.031654	0.2353	0.0333	0.6167	0.1148
1.051493	0.2334	0.0374	0.6153	0.1139
1.071333	0.2301	0.0365	0.6192	0.1142
1.091172	0.2353	0.0341	0.6151	0.1154
1.111011	0.2349	0.0345	0.614	0.1166
1.130851	0.2324	0.0348	0.6159	0.1169
1.15069	0.2337	0.0356	0.6138	0.117
1.17053	0.2363	0.033	0.6134	0.1173
1.190369	0.2403	0.0313	0.6104	0.118
1.210209	0.2374	0.0342	0.6086	0.1199
1.230048	0.2436	0.032	0.6008	0.1236
1.249888	0.2472	0.0294	0.5992	0.1242
1.269727	0.2453	0.0304	0.5984	0.1258
1.289567	0.2456	0.0254	0.6038	0.1253
1.309406	0.2519	0.0271	0.5946	0.1265
1.329246	0.251	0.0278	0.5915	0.1297
1.349085	0.2555	0.0259	0.5893	0.1293

1.368925	0.2561	0.0249	0.5889	0.1301
1.388764	0.2575	0.0261	0.5833	0.133
1.408604	0.2612	0.0247	0.5826	0.1316
1.428443	0.2591	0.0258	0.5841	0.1311
1.448283	0.261	0.0244	0.5833	0.1313
1.468122	0.2627	0.0237	0.5817	0.1319
1.487962	0.2652	0.0236	0.5795	0.1316
1.507801	0.2655	0.0228	0.5808	0.1309
1.527641	0.2603	0.0223	0.5826	0.1348
1.54748	0.2619	0.0254	0.5804	0.1323
1.56732	0.2595	0.0239	0.5829	0.1337
1.587159	0.2623	0.0241	0.5814	0.1321
1.606999	0.2607	0.0243	0.581	0.134
1.626838	0.2623	0.0254	0.5772	0.1351
1.646678	0.2613	0.0241	0.5811	0.1335
1.666517	0.2588	0.0251	0.5817	0.1345
1.686357	0.2589	0.0231	0.5841	0.1339
1.706196	0.2582	0.0238	0.5833	0.1347
1.726036	0.2583	0.0236	0.5836	0.1345
1.745875	0.2628	0.0257	0.5774	0.134
1.765715	0.2593	0.0228	0.5835	0.1344
1.785554	0.2611	0.0217	0.5827	0.1345
1.805394	0.261	0.0232	0.5833	0.1325
1.825233	0.2618	0.0244	0.5801	0.1337
1.845073	0.2587	0.0241	0.582	0.1353
1.864912	0.2596	0.0227	0.5848	0.1329
1.884752	0.2644	0.0231	0.5805	0.132
1.904591	0.2631	0.0246	0.5817	0.1306
1.924431	0.2606	0.0265	0.5813	0.1316
1.94427	0.2642	0.0242	0.5815	0.1302
1.96411	0.2609	0.0241	0.5838	0.1312
1.983949	0.259	0.0244	0.5845	0.1321
2.003789	0.2639	0.0247	0.5816	0.1298
2.023628	0.2608	0.0243	0.5862	0.1287
2.043468	0.2602	0.0247	0.587	0.1282
2.063307	0.259	0.0254	0.5882	0.1275
2.083147	0.2616	0.0241	0.5886	0.1257
2.102986	0.2574	0.026	0.5899	0.1267
2.122826	0.2579	0.0234	0.5933	0.1253
2.142665	0.2561	0.0255	0.5949	0.1235
2.162505	0.3045	0.0242	0.5563	0.1149
2.182344	0.2591	0.0262	0.5952	0.1195
2.202183	0.2548	0.0271	0.5987	0.1193
2.222023	0.2534	0.0264	0.6011	0.1191
2.241862	0.2564	0.0247	0.601	0.1179

2.261702	0.2545	0.0271	0.6052	0.1132
2.281541	0.2546	0.0272	0.6054	0.1128
2.301381	0.2557	0.0247	0.6058	0.1137
2.32122	0.2552	0.026	0.6083	0.1105
2.34106	0.2544	0.0272	0.6118	0.1066
2.360899	0.252	0.0267	0.6144	0.107
2.380739	0.2533	0.0272	0.6138	0.1057
2.400578	0.2483	0.0286	0.6212	0.1018
2.420418	0.2494	0.0262	0.622	0.1023
2.440257	0.2498	0.0294	0.6238	0.097
2.460097	0.2472	0.0289	0.6287	0.0952
2.479936	0.2478	0.0281	0.6326	0.0915
2.499776	0.2461	0.0312	0.6325	0.0901
2.519615	0.2476	0.029	0.636	0.0874
2.539455	0.2448	0.0308	0.6417	0.0827
2.559294	0.2475	0.03	0.642	0.0804
2.579134	0.249	0.0302	0.6422	0.0786
2.598973	0.2446	0.0291	0.6491	0.0772
2.618813	0.2452	0.0303	0.649	0.0756
2.638652	0.2431	0.0316	0.6533	0.072
2.658492	0.2458	0.0304	0.656	0.0678
2.678331	0.2429	0.0317	0.6602	0.0652
2.698171	0.2384	0.0333	0.6652	0.0631
2.71801	0.2408	0.0331	0.6663	0.0598
2.73785	0.242	0.0316	0.6696	0.0567
2.757689	0.2394	0.0347	0.6732	0.0528
2.777529	0.2352	0.0348	0.679	0.0511
2.797368	0.2359	0.0343	0.6823	0.0475
2.817208	0.2343	0.035	0.6847	0.046
2.837047	0.2332	0.0352	0.6876	0.044
2.856887	0.2309	0.0354	0.6925	0.0412
2.876726	0.2292	0.0376	0.6941	0.0391
2.896566	0.2285	0.0369	0.696	0.0386
2.916405	0.2286	0.0364	0.6995	0.0355
2.936245	0.2268	0.039	0.7021	0.0321
2.956084	0.2262	0.0388	0.7042	0.0307
2.975924	0.2313	0.0396	0.7	0.029
2.995763	0.2207	0.0429	0.709	0.0275
3.015603	0.2227	0.0415	0.7115	0.0243
3.035442	0.2204	0.0416	0.7145	0.0236
3.055282	0.2179	0.043	0.7179	0.0211
3.075121	0.2132	0.0401	0.7265	0.0203
3.094961	0.2126	0.044	0.7244	0.019
3.1148	0.2131	0.0456	0.7247	0.0165
3.13464	0.2064	0.0474	0.731	0.0152

3.154479	0.207	0.0526	0.7264	0.014
3.174319	0.1979	0.0545	0.7351	0.0125
3.194158	0.1914	0.0584	0.7397	0.0105
3.213998	0.1848	0.0625	0.7433	0.0094
3.233837	0.1782	0.0652	0.747	0.0095
3.253676	0.1715	0.0688	0.7502	0.0094
3.273516	0.1714	0.0709	0.749	0.0087
3.293355	0.1611	0.0725	0.7588	0.0076
3.313195	0.1626	0.0794	0.7507	0.0073
3.333034	0.1589	0.0814	0.7521	0.0075
3.352874	0.145	0.0894	0.7591	0.0065
3.372713	0.1345	0.0922	0.7668	0.0065
3.392553	0.1343	0.0925	0.7665	0.0068
3.412392	0.1332	0.0943	0.7662	0.0063
3.432232	0.126	0.0989	0.7687	0.0064
3.452071	0.1141	0.1081	0.7716	0.0062

Table B.9: 18ZE-R-81 EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.054266	0.195294	0.722269	0.028171
0.049366	0.058589	0.208635	0.709363	0.023412
0.098733	0.062051	0.195765	0.718477	0.023707
0.148099	0.060725	0.202945	0.71422	0.02211
0.197465	0.075678	0.204119	0.702845	0.017358
0.246831	0.08434	0.202505	0.695655	0.0175
0.296198	0.09237	0.193651	0.697087	0.016892
0.345564	0.109251	0.183563	0.689861	0.017325
0.39493	0.113785	0.178922	0.688769	0.018525
0.444296	0.111494	0.173803	0.695108	0.019595
0.493663	0.11521	0.167692	0.698133	0.018965
0.543029	0.118177	0.159239	0.701697	0.020887
0.592395	0.11644	0.162397	0.699614	0.021548
0.641762	0.116891	0.165793	0.694124	0.023192
0.691128	0.119808	0.151808	0.704858	0.023527
0.740494	0.126228	0.152324	0.696887	0.024561
0.78986	0.12061	0.15074	0.703332	0.025318
0.839227	0.120305	0.147892	0.706796	0.025007
0.888593	0.118992	0.147092	0.707449	0.026467
0.937959	0.113828	0.149118	0.709073	0.027981
0.987325	0.108873	0.147694	0.715372	0.028061
1.036692	0.110059	0.151372	0.710799	0.027769
1.086058	0.111085	0.151375	0.707093	0.030447
1.135424	0.114209	0.146099	0.710531	0.029161

1.184791	0.109284	0.149446	0.710489	0.030781
1.234157	0.111544	0.149035	0.709357	0.030063
1.283523	0.106958	0.150561	0.712787	0.029694
1.332889	0.100692	0.160528	0.710131	0.028648
1.382256	0.112998	0.101116	0.743946	0.041939
1.431622	0.10392	0.158449	0.709529	0.028102
1.480988	0.113916	0.148634	0.707483	0.029967
1.530355	0.10615	0.150556	0.712867	0.030427
1.579721	0.105866	0.149144	0.714179	0.030811
1.629087	0.110234	0.144694	0.715032	0.03004
1.678453	0.118232	0.143012	0.708167	0.030589
1.72782	0.117691	0.139739	0.711137	0.031434
1.777186	0.11624	0.138323	0.713541	0.031896
1.826552	0.110476	0.139157	0.717583	0.032785
1.875918	0.113917	0.136566	0.715851	0.033667
1.925285	0.112968	0.136063	0.717394	0.033575
1.974651	0.115038	0.134715	0.715925	0.034323
2.024017	0.115409	0.135543	0.715249	0.033799
2.073384	0.112625	0.137444	0.717396	0.032534
2.12275	0.112441	0.134684	0.719841	0.033034
2.172116	0.111507	0.139954	0.716182	0.032357
2.221482	0.117317	0.129822	0.719561	0.0333
2.270849	0.109531	0.13754	0.720355	0.032574
2.320215	0.100151	0.140067	0.726021	0.033761
2.369581	0.115716	0.135349	0.716384	0.032551
2.418947	0.095955	0.177891	0.698136	0.028018
2.468314	0.115065	0.134935	0.718626	0.031374
2.51768	0.114764	0.137882	0.715406	0.031948
2.567046	0.110694	0.137173	0.721402	0.030731
2.616413	0.110116	0.139154	0.718462	0.032268
2.665779	0.112764	0.141745	0.715137	0.030354
2.715145	0.113382	0.144883	0.712824	0.028911
2.764511	0.114405	0.139469	0.71647	0.029656
2.813878	0.116426	0.147154	0.709096	0.027323
2.863244	0.113989	0.155308	0.704745	0.025959
2.91261	0.1081	0.158763	0.709303	0.023834
2.961976	0.105033	0.16956	0.704353	0.021054
3.011343	0.089651	0.178987	0.710972	0.02039
3.060709	0.082189	0.18051	0.717067	0.020234
3.110075	0.080151	0.188303	0.712608	0.018938
3.159442	0.08472	0.19144	0.704803	0.019036
3.208808	0.081496	0.187082	0.712002	0.01942
3.258174	0.087462	0.182546	0.710532	0.01946
3.30754	0.093476	0.174111	0.712286	0.020127
3.356907	0.106548	0.170421	0.703784	0.019247

3.406273	0.110324	0.168624	0.702129	0.018924
3.455639	0.113285	0.172184	0.695922	0.018609
3.505005	0.10482	0.173797	0.703002	0.01838
3.554372	0.105225	0.179185	0.697151	0.018439
3.603738	0.080463	0.190756	0.709325	0.019455
3.653104	0.080804	0.192215	0.707677	0.019304
3.702471	0.082381	0.192938	0.706711	0.01797
3.751837	0.077765	0.197229	0.707482	0.017523
3.801203	0.075145	0.200719	0.706947	0.017189
3.850569	0.072847	0.200178	0.708843	0.018131
3.899936	0.070218	0.203397	0.707771	0.018614
3.949302	0.072552	0.202401	0.706525	0.018522
3.998668	0.073883	0.199736	0.708227	0.018153
4.048034	0.073764	0.200489	0.707677	0.01807
4.097401	0.076591	0.197252	0.707192	0.018965
4.146767	0.078741	0.194648	0.707956	0.018655
4.196133	0.072412	0.206004	0.703284	0.018299
4.2455	0.073311	0.205173	0.703402	0.018114
4.294866	0.072887	0.202755	0.707159	0.017199
4.344232	0.073092	0.2012	0.707393	0.018315
4.393598	0.077097	0.199082	0.706025	0.017797
4.442965	0.07524	0.200721	0.706347	0.017691
4.492331	0.077815	0.196526	0.706677	0.018981
4.541697	0.076396	0.203016	0.702688	0.0179
4.591064	0.078063	0.205482	0.699756	0.0167
4.64043	0.076926	0.204832	0.701404	0.016839
4.689796	0.077552	0.201947	0.702836	0.017665
4.739162	0.081172	0.202452	0.698123	0.018253
4.788529	0.081802	0.197674	0.702262	0.018262
4.837895	0.095242	0.19359	0.694188	0.016981
4.887261	0.101626	0.19482	0.687584	0.01597
4.936627	0.110614	0.188592	0.683086	0.017708
4.985994	0.11055	0.190332	0.682437	0.016681
5.03536	0.098657	0.182948	0.693486	0.024908
5.084726	0.096106	0.178737	0.699309	0.025848

Table B.10: 18ZE-R-49B EPMA profile A to B

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.050742	0.105514	0.826607	0.017136
0.061197	0.047051	0.101151	0.824165	0.027634
0.122393	0.050361	0.146197	0.794086	0.009357
0.18359	0.04924	0.144576	0.795719	0.010465
0.244787	0.049136	0.145158	0.794282	0.011424

0.305983	0.046912	0.139935	0.801127	0.012026
0.36718	0.047271	0.140141	0.800614	0.011974
0.428377	0.047035	0.139198	0.799923	0.013844
0.489574	0.038466	0.137548	0.809225	0.014761
0.55077	0.035247	0.138932	0.810522	0.015299
0.611967	0.029912	0.146691	0.807249	0.016149
0.673164	0.029954	0.142248	0.812145	0.015654
0.73436	0.030874	0.140376	0.812056	0.016693
0.795557	0.028231	0.137483	0.81738	0.016906
0.856754	0.025112	0.135241	0.822522	0.017125
0.91795	0.020425	0.138063	0.823454	0.018057
0.979147	0.023127	0.140537	0.819644	0.016692
1.040344	0.033625	0.132974	0.814307	0.019094
1.10154	0.034369	0.088074	0.850102	0.027455
1.162737	0.026753	0.131705	0.821653	0.019889
1.223934	0.031026	0.134982	0.814778	0.019214
1.285131	0.02665	0.116828	0.835818	0.020704
1.346327	0.018976	0.136505	0.822938	0.02158
1.407524	0.012926	0.133659	0.832018	0.021398
1.468721	0.014486	0.137564	0.82634	0.02161
1.529917	0.014133	0.132869	0.830995	0.022004
1.591114	0.015602	0.132753	0.830253	0.021391
1.652311	0.015311	0.132881	0.828398	0.02341
1.713507	0.017095	0.122225	0.836959	0.02372
1.774704	0.023425	0.128969	0.823587	0.024019
1.835901	0.025923	0.126772	0.823486	0.023818
1.897097	0.027199	0.126384	0.821611	0.024806
1.958294	0.032963	0.123895	0.819052	0.024091
2.019491	0.037077	0.125739	0.812429	0.024755
2.080688	0.036859	0.118131	0.820224	0.024786
2.141884	0.036751	0.122744	0.815464	0.025042
2.203081	0.032694	0.121648	0.818918	0.02674
2.264278	0.02555	0.122069	0.825033	0.027348
2.325474	0.031097	0.122165	0.818949	0.027789
2.386671	0.034244	0.118737	0.820412	0.026606
2.447868	0.03638	0.118574	0.817568	0.027477
2.509064	0.033567	0.119581	0.818111	0.02874
2.570261	0.028597	0.119218	0.823395	0.02879
2.631458	0.033594	0.117203	0.820441	0.028763
2.692654	0.032885	0.120504	0.816659	0.029952
2.753851	0.034821	0.116804	0.81891	0.029464
2.815048	0.030276	0.118658	0.820235	0.030831
2.876245	0.037523	0.118877	0.812219	0.031381
2.937441	0.028984	0.093922	0.8422	0.034893
2.998638	0.030823	0.119179	0.819452	0.030545

3.059835	0.02598	0.126166	0.817324	0.03053
3.121031	0.024005	0.116973	0.827749	0.031273
3.182228	0.028659	0.120279	0.81958	0.031481
3.243425	0.028948	0.117831	0.821089	0.032132
3.304621	0.026662	0.118511	0.823515	0.031312
3.365818	0.024118	0.11601	0.827617	0.032255
3.427015	0.025756	0.117235	0.82421	0.032798
3.488211	0.02628	0.107127	0.833824	0.032768
3.549408	0.020558	0.121568	0.826226	0.031648
3.610605	0.021597	0.117684	0.828436	0.032282
3.671802	0.029746	0.109836	0.830062	0.030356
3.732998	0.023815	0.118133	0.826121	0.031931
3.794195	0.020035	0.11783	0.8305	0.031636
3.855392	0.019765	0.108699	0.839933	0.031603
3.916588	0.023953	0.118107	0.82707	0.03087
3.977785	0.022682	0.117124	0.829448	0.030745
4.038982	0.02122	0.119107	0.830245	0.029427
4.100178	0.028966	0.117187	0.825513	0.028334
4.161375	0.02899	0.123487	0.81803	0.029493
4.222572	0.026141	0.118933	0.82678	0.028145
4.283768	0.024456	0.117609	0.831078	0.026857
4.344965	0.023062	0.121252	0.826283	0.029403
4.406162	0.023602	0.119478	0.829116	0.027804
4.467359	0.024393	0.123904	0.825021	0.026682
4.528555	0.030797	0.120851	0.821746	0.026606
4.589752	0.030932	0.12308	0.819884	0.026104
4.650949	0.026227	0.122882	0.825944	0.024947
4.712145	0.029347	0.118967	0.825757	0.025929
4.773342	0.033531	0.119344	0.821651	0.025474
4.834539	0.028935	0.122234	0.823943	0.024889
4.895735	0.030198	0.118276	0.828145	0.023382
4.956932	0.028891	0.12114	0.827142	0.022827
5.018129	0.029717	0.116378	0.83028	0.023625
5.079325	0.030929	0.125214	0.821323	0.022534
5.140522	0.031185	0.122869	0.822903	0.023042
5.201719	0.026034	0.127367	0.823705	0.022893
5.262915	0.023624	0.123945	0.830122	0.02231
5.324112	0.01933	0.127765	0.832049	0.020855
5.385309	0.018981	0.128837	0.831621	0.020561
5.446506	0.020021	0.12847	0.830025	0.021485
5.507702	0.02598	0.129765	0.824608	0.019647
5.568899	0.02728	0.129749	0.822452	0.020518
5.630096	0.031201	0.1285	0.821659	0.01864
5.691292	0.0299	0.130301	0.820096	0.019703
5.752489	0.03064	0.129616	0.821754	0.017989

5.813686	0.026669	0.10342	0.850497	0.019414
5.874882	0.02406	0.130167	0.827309	0.018465
5.936079	0.02927	0.129098	0.824147	0.017484
5.997276	0.027911	0.128422	0.826747	0.01692
6.058472	0.019741	0.128854	0.833787	0.017618
6.119669	0.022446	0.133708	0.827574	0.016272
6.180866	0.021253	0.137621	0.824446	0.016679
6.242063	0.02625	0.135939	0.822091	0.01572
6.303259	0.027155	0.133281	0.824622	0.014942
6.364456	0.028153	0.130639	0.82616	0.015048
6.425653	0.031408	0.133836	0.819693	0.015063
6.486849	0.031351	0.134291	0.819765	0.014593
6.548046	0.031696	0.138913	0.815106	0.014285
6.609243	0.040583	0.098954	0.832459	0.028004
6.670439	0.050795	0.135741	0.800609	0.012855
6.731636	0.051907	0.139917	0.796635	0.011541
6.792833	0.049178	0.139407	0.800328	0.011087
6.854029	0.050849	0.133154	0.803837	0.01216
6.915226	0.050834	0.143474	0.794772	0.01092
6.976423	0.049201	0.138527	0.801441	0.010831
7.03762	0.051061	0.130583	0.807851	0.010505
7.098816	0.049109	0.095389	0.835461	0.020041
7.160013	0.048774	0.099195	0.829647	0.022384
7.22121	0.048619	0.100258	0.825822	0.0253
7.282406	0.049475	0.084004	0.827871	0.03865

Table B.11: 18ZE-R-49B EPMA profile C to D

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.051848	0.089006	0.83134	0.027806
0.005148	0.051631	0.090824	0.833417	0.024128
0.010296	0.037512	0.071242	0.848489	0.042756
0.015444	0.037436	0.076255	0.842963	0.043346
0.020592	0.049225	0.083636	0.838151	0.028987
0.02574	0.050609	0.108891	0.823938	0.016563
0.030888	0.051901	0.110466	0.823043	0.01459
0.036036	0.04992	0.112812	0.822472	0.014795
0.041184	0.049977	0.11406	0.822704	0.013259
0.046332	0.049588	0.116795	0.820611	0.013005
0.05148	0.050455	0.119508	0.817613	0.012424
0.056628	0.051277	0.12128	0.815408	0.012035
0.061776	0.050864	0.121547	0.815425	0.012164
0.066924	0.050123	0.120989	0.816415	0.012473
0.072072	0.050991	0.123408	0.814384	0.011216

0.07722	0.051649	0.127216	0.810833	0.010302
0.082368	0.04921	0.128242	0.811569	0.010979
0.087516	0.051481	0.127169	0.810783	0.010567
0.092664	0.050157	0.127893	0.811437	0.010514
0.097812	0.049581	0.129538	0.812131	0.00875
0.102959	0.049467	0.128858	0.812086	0.009589
0.108107	0.04956	0.121552	0.817055	0.011833
0.113255	0.050001	0.129655	0.811633	0.008711
0.118403	0.05125	0.10704	0.824923	0.016787
0.123551	0.04909	0.083885	0.835434	0.031591
0.128699	0.050186	0.131187	0.809319	0.009309
0.133847	0.042016	0.105447	0.833848	0.018689
0.138995	0.050495	0.107598	0.82611	0.015796
0.144143	0.049932	0.131944	0.808484	0.009639
0.149291	0.049959	0.13039	0.810483	0.009169
0.154439	0.048785	0.109594	0.832251	0.00937
0.159587	0.047462	0.071592	0.847139	0.033806
0.164735	0.04966	0.083	0.852176	0.015164
0.169883	0.050276	0.08711	0.847122	0.015492
0.175031	0.051475	0.1025	0.83667	0.009356
0.180179	0.051272	0.130301	0.811244	0.007184
0.185327	0.048681	0.13649	0.806958	0.007871
0.190475	0.049202	0.137671	0.805231	0.007897
0.195623	0.049843	0.137658	0.804063	0.008436
0.200771	0.049536	0.139102	0.803858	0.007504
0.205919	0.050594	0.13833	0.803677	0.0074
0.211067	0.050161	0.139312	0.802195	0.008332
0.216215	0.051892	0.136897	0.804103	0.007109
0.221363	0.050421	0.138654	0.80357	0.007354
0.226511	0.048976	0.138339	0.805511	0.007175
0.231659	0.051943	0.139448	0.801578	0.007031
0.236807	0.048045	0.138319	0.806091	0.007544
0.241955	0.051695	0.136755	0.804219	0.007331
0.247103	0.050427	0.139459	0.802604	0.007511
0.252251	0.048898	0.138879	0.804994	0.007229
0.257399	0.048696	0.140443	0.803063	0.007798
0.262547	0.050905	0.127925	0.812577	0.008592
0.267695	0.042198	0.089531	0.833264	0.035007
0.272843	0.050306	0.134554	0.807652	0.007487
0.277991	0.051573	0.138484	0.802771	0.007173
0.283139	0.048777	0.139516	0.804419	0.007289
0.288287	0.049456	0.140515	0.801995	0.008034
0.293435	0.049944	0.14017	0.802485	0.0074
0.298583	0.050074	0.142157	0.800557	0.007212
0.30373	0.05015	0.141539	0.800378	0.007932

0.308878	0.048893	0.138325	0.804795	0.007987
0.314026	0.051642	0.13864	0.802163	0.007554
0.319174	0.048612	0.142126	0.802035	0.007227
0.324322	0.048224	0.140438	0.803563	0.007774
0.32947	0.049897	0.14272	0.800034	0.007349
0.334618	0.044892	0.099605	0.827261	0.028242
0.339766	0.051124	0.139957	0.80085	0.00807
0.344914	0.048692	0.141881	0.801154	0.008273
0.350062	0.049092	0.141073	0.802164	0.007672
0.35521	0.050294	0.140029	0.802	0.007678
0.360358	0.05205	0.141124	0.797888	0.008938
0.365506	0.049522	0.138887	0.80343	0.00816
0.370654	0.049184	0.118026	0.823267	0.009522
0.375802	0.048256	0.073709	0.840476	0.037558
0.38095	0.048654	0.139412	0.804201	0.007734
0.386098	0.05006	0.140634	0.801285	0.008021
0.391246	0.049784	0.141993	0.799712	0.008511
0.396394	0.048923	0.139924	0.80326	0.007893
0.401542	0.046227	0.112422	0.827107	0.014244
0.40669	0.050158	0.091503	0.843412	0.014927
0.411838	0.049687	0.105231	0.833557	0.011525
0.416986	0.048637	0.088996	0.842886	0.019481
0.422134	0.049812	0.126369	0.815412	0.008407
0.427282	0.050412	0.136914	0.804504	0.00817
0.43243	0.050704	0.139666	0.801187	0.008442
0.437578	0.050705	0.140909	0.799262	0.009124
0.442726	0.049668	0.141301	0.80007	0.008962
0.447874	0.049476	0.138223	0.803852	0.00845
0.453022	0.050249	0.141509	0.799749	0.008493
0.45817	0.052015	0.140196	0.799746	0.008044
0.463318	0.048884	0.142819	0.799706	0.008591
0.468466	0.052322	0.140317	0.798529	0.008833
0.473614	0.049714	0.141668	0.800435	0.008183
0.478762	0.050536	0.138274	0.802588	0.008602
0.48391	0.049519	0.130226	0.811275	0.00898
0.489058	0.050571	0.12697	0.811754	0.010705
0.494206	0.049819	0.14082	0.801222	0.00814
0.499354	0.049532	0.141212	0.800203	0.009053
0.504501	0.052376	0.139964	0.798622	0.009038
0.509649	0.050965	0.141177	0.798874	0.008984
0.514797	0.052591	0.141775	0.795964	0.009669
0.519945	0.050194	0.14198	0.798749	0.009076
0.525093	0.05123	0.13751	0.801213	0.010047
0.530241	0.049292	0.140727	0.800796	0.009185
0.535389	0.050611	0.122964	0.81523	0.011195

0.540537	0.045888	0.084722	0.837662	0.031727
0.545685	0.051705	0.085238	0.840646	0.022411
0.550833	0.047931	0.071598	0.845444	0.035027
0.555981	0.049141	0.086645	0.835295	0.028919
0.561129	0.049764	0.117102	0.81985	0.013284
0.566277	0.05139	0.139829	0.799223	0.009557
0.571425	0.051311	0.140621	0.798423	0.009645
0.576573	0.050579	0.139945	0.799298	0.010179
0.581721	0.04989	0.139773	0.801317	0.00902
0.586869	0.05143	0.13763	0.800954	0.009986
0.592017	0.050318	0.137388	0.802846	0.009448
0.597165	0.050687	0.138083	0.80092	0.01031
0.602313	0.050769	0.139695	0.799345	0.010191
0.607461	0.051427	0.140388	0.799144	0.009041
0.612609	0.049645	0.138151	0.802262	0.009942
0.617757	0.050826	0.137877	0.80213	0.009167
0.622905	0.049892	0.138769	0.801645	0.009694
0.628053	0.050822	0.138305	0.799704	0.011168
0.633201	0.049904	0.136671	0.80353	0.009895
0.638349	0.050421	0.138716	0.801449	0.009415
0.643497	0.049974	0.138802	0.801344	0.00988
0.648645	0.050653	0.137309	0.802334	0.009704
0.653793	0.051004	0.137616	0.800656	0.010724
0.658941	0.051253	0.136728	0.801299	0.010721
0.664089	0.050111	0.139368	0.799851	0.01067
0.669237	0.049826	0.136633	0.803129	0.010412
0.674385	0.049954	0.136776	0.802966	0.010305
0.679533	0.050791	0.136773	0.801674	0.010762
0.684681	0.051148	0.137506	0.800892	0.010454
0.689829	0.04758	0.137298	0.804605	0.010517
0.694977	0.050431	0.135445	0.803978	0.010146
0.700125	0.049626	0.122633	0.815567	0.012174
0.705272	0.048347	0.111425	0.825671	0.014556
0.71042	0.049905	0.0852	0.843023	0.021872
0.715568	0.048677	0.135832	0.80379	0.011701
0.720716	0.049983	0.136262	0.803003	0.010752
0.725864	0.050346	0.13381	0.804894	0.010951
0.731012	0.049703	0.136685	0.802181	0.011431
0.73616	0.049697	0.136453	0.802779	0.011071
0.741308	0.050374	0.1347	0.803867	0.011059
0.746456	0.049896	0.133252	0.804985	0.011867
0.751604	0.049227	0.134856	0.804595	0.011323
0.756752	0.049946	0.134021	0.804496	0.011538
0.7619	0.049979	0.075892	0.852467	0.021662
0.767048	0.046596	0.08445	0.841469	0.027485

0.772196	0.049677	0.132682	0.805794	0.011846
0.777344	0.05018	0.136249	0.80204	0.011531
0.782492	0.049578	0.136823	0.801555	0.012044
0.78764	0.048958	0.133299	0.806062	0.011681
0.792788	0.048393	0.105391	0.827838	0.018378
0.797936	0.045998	0.090635	0.834005	0.029362
0.803084	0.047297	0.090825	0.835585	0.026293
0.808232	0.046954	0.133303	0.807916	0.011827
0.81338	0.049257	0.134558	0.804047	0.012138
0.818528	0.049439	0.135153	0.80374	0.011669
0.823676	0.048912	0.134321	0.805501	0.011266
0.828824	0.048962	0.134838	0.804295	0.011906
0.833972	0.047175	0.13504	0.806493	0.011292
0.83912	0.047523	0.136082	0.804651	0.011745
0.844268	0.04713	0.133615	0.808143	0.011112
0.849416	0.046614	0.133154	0.808597	0.011635
0.854564	0.047151	0.133258	0.807171	0.012419
0.859712	0.04687	0.117336	0.820284	0.01551
0.86486	0.045416	0.104273	0.829156	0.021155
0.870008	0.044711	0.132735	0.810435	0.012119
0.875156	0.044715	0.118245	0.824016	0.013025
0.880304	0.044975	0.126017	0.816341	0.012667
0.885452	0.044342	0.098943	0.834079	0.022636
0.8906	0.04389	0.127861	0.815633	0.012616
0.895748	0.043768	0.133998	0.81046	0.011774
0.900896	0.044714	0.134177	0.808773	0.012336
0.906043	0.04191	0.134797	0.810798	0.012495
0.911191	0.042536	0.13338	0.811458	0.012626
0.916339	0.042422	0.134011	0.810733	0.012833
0.921487	0.040131	0.132716	0.814232	0.012921
0.926635	0.041637	0.122298	0.823931	0.012134
0.931783	0.039709	0.126667	0.821476	0.012148
0.936931	0.038906	0.123457	0.82448	0.013157
0.942079	0.037681	0.133122	0.816182	0.013015
0.947227	0.03625	0.135869	0.816094	0.011788
0.952375	0.035355	0.135209	0.816696	0.01274
0.957523	0.035346	0.13431	0.817936	0.012408
0.962671	0.033204	0.136385	0.817093	0.013318
0.967819	0.030871	0.136111	0.819571	0.013447
0.972967	0.031239	0.136912	0.819871	0.011978
0.978115	0.029331	0.139559	0.818462	0.012648
0.983263	0.026198	0.136156	0.825518	0.012128
0.988411	0.025668	0.137251	0.82437	0.012711
0.993559	0.024086	0.137657	0.825541	0.012716
0.998707	0.023457	0.13857	0.824878	0.013095

1.003855	0.022382	0.139684	0.825623	0.012311
1.009003	0.020765	0.139509	0.826372	0.013353
1.014151	0.018268	0.143574	0.825363	0.012795
1.019299	0.014931	0.140102	0.831439	0.013527
1.024447	0.014622	0.141679	0.83004	0.013659
1.029595	0.01257	0.139623	0.834544	0.013263
1.034743	0.01258	0.139429	0.834441	0.01355
1.039891	0.011666	0.13985	0.834914	0.01357
1.045039	0.012257	0.141168	0.832928	0.013647
1.050187	0.013293	0.140774	0.832152	0.013781
1.055335	0.013023	0.139502	0.833269	0.014206
1.060483	0.01394	0.140435	0.832152	0.013473
1.065631	0.014494	0.140125	0.832162	0.013218
1.070779	0.01559	0.138283	0.832208	0.013918
1.075927	0.014087	0.138842	0.832861	0.01421
1.081075	0.013656	0.142859	0.829684	0.0138
1.086223	0.013423	0.139119	0.834892	0.012565
1.091371	0.012542	0.140801	0.832722	0.013935
1.096519	0.011749	0.138091	0.836584	0.013575
1.101667	0.01238	0.139974	0.833499	0.014147
1.106814	0.012581	0.141613	0.831676	0.01413
1.111962	0.012807	0.139453	0.834047	0.013694
1.11711	0.01342	0.139238	0.833663	0.013679
1.122258	0.013647	0.140065	0.833049	0.013239
1.127406	0.014679	0.138949	0.83226	0.014112
1.132554	0.01568	0.138713	0.831577	0.01403
1.137702	0.014968	0.139282	0.832205	0.013544
1.14285	0.017271	0.138572	0.830495	0.013662
1.147998	0.016866	0.136753	0.832451	0.01393
1.153146	0.016681	0.137248	0.832567	0.013504
1.158294	0.016935	0.137981	0.831028	0.014056
1.163442	0.018179	0.137432	0.829663	0.014727
1.16859	0.019287	0.135883	0.830496	0.014334
1.173738	0.018384	0.139425	0.8285	0.01369
1.178886	0.019156	0.137555	0.829951	0.013337
1.184034	0.020152	0.139864	0.825953	0.01403
1.189182	0.019231	0.136569	0.830131	0.014069
1.19433	0.018459	0.132837	0.834173	0.014531
1.199478	0.01857	0.132033	0.835267	0.014129
1.204626	0.01842	0.131341	0.835767	0.014471
1.209774	0.018643	0.137739	0.829345	0.014273
1.214922	0.018928	0.136109	0.830832	0.014131
1.22007	0.018299	0.136767	0.829663	0.015271
1.225218	0.017232	0.131036	0.83653	0.015202
1.230366	0.0194	0.118953	0.841472	0.020175

1.235514	0.01757	0.127397	0.841029	0.014004
1.240662	0.019093	0.134877	0.832591	0.013439
1.24581	0.018115	0.137618	0.829844	0.014423
1.250958	0.018186	0.137474	0.829563	0.014777
1.256106	0.018414	0.139354	0.827282	0.014949
1.261254	0.018096	0.137705	0.830529	0.013669
1.266402	0.018655	0.136065	0.830132	0.015147
1.27155	0.018408	0.137787	0.828908	0.014897
1.276698	0.018045	0.13776	0.830285	0.01391
1.281846	0.018385	0.137214	0.829469	0.014932

Table B.12: 18ZE-R-71 EPMA profile

x (mm)	X_{Ca}	X_{Mg}	X_{Fe}	X_{Mn}
0	0.133393	0.060725	0.769698	0.036184
0.039897	0.124702	0.083025	0.76516	0.027112
0.079794	0.116842	0.082863	0.77172	0.028576
0.119692	0.11177	0.084774	0.773638	0.029818
0.159589	0.114806	0.067314	0.785114	0.032767
0.199486	0.114559	0.047616	0.784783	0.053041
0.239383	0.103479	0.042728	0.798349	0.055444
0.27928	0.112739	0.045633	0.786833	0.054795
0.319178	0.061282	0.055184	0.823438	0.060096
0.359075	0.110633	0.046058	0.788691	0.054617
0.398972	0.114951	0.052127	0.790306	0.042616
0.438869	0.121041	0.066221	0.780493	0.032245
0.478766	0.123471	0.061539	0.78124	0.03375
0.518664	0.118746	0.040303	0.784806	0.056145
0.558561	0.11917	0.05947	0.787654	0.033707
0.598458	0.12167	0.05866	0.787045	0.032625
0.638355	0.117657	0.042122	0.786541	0.05368
0.678252	0.121152	0.048463	0.786045	0.044341
0.71815	0.115621	0.046863	0.788978	0.048538
0.758047	0.120674	0.049923	0.785748	0.043655
0.797944	0.107412	0.042822	0.79908	0.050686
0.837841	0.120759	0.049486	0.789944	0.039811
0.877738	0.118095	0.052502	0.789326	0.040076
0.917635	0.120413	0.056014	0.789673	0.033901
0.957533	0.120462	0.056891	0.787366	0.035282
0.99743	0.122381	0.051735	0.791408	0.034476
1.037327	0.121213	0.053192	0.788345	0.03725
1.077224	0.120986	0.047081	0.787749	0.044184
1.117121	0.120973	0.05476	0.788038	0.03623
1.157019	0.123039	0.053212	0.786485	0.037265

1.196916	0.121892	0.048589	0.787078	0.042442
1.236813	0.125109	0.044412	0.785228	0.045251
1.27671	0.123777	0.050566	0.78392	0.041737
1.316607	0.075864	0.042294	0.830874	0.050969
1.356505	0.082246	0.040784	0.825701	0.051269
1.396402	0.126003	0.048367	0.781136	0.044494
1.436299	0.132791	0.054161	0.771148	0.041899
1.476196	0.126284	0.054071	0.775077	0.044568
1.516093	0.126746	0.053544	0.772594	0.047117
1.555991	0.123418	0.055437	0.773985	0.04716
1.595888	0.120674	0.054449	0.775368	0.04951
1.635785	0.118881	0.051482	0.781169	0.048469
1.675682	0.122603	0.049646	0.778515	0.049237
1.715579	0.116244	0.03625	0.796428	0.051079
1.755477	0.120289	0.048391	0.780076	0.051245
1.795374	0.11895	0.051321	0.777109	0.05262
1.835271	0.121422	0.04736	0.777545	0.053673
1.875168	0.119865	0.051749	0.773452	0.054934
1.915065	0.122604	0.048619	0.773603	0.055174
1.954963	0.11945	0.051124	0.774333	0.055093
1.99486	0.116543	0.049256	0.778402	0.055799
2.034757	0.122273	0.050148	0.773568	0.054012
2.074654	0.122831	0.04707	0.779055	0.051044
2.114551	0.118913	0.042883	0.785828	0.052376
2.154449	0.120039	0.047466	0.778081	0.054414
2.194346	0.115983	0.0507	0.776819	0.056498
2.234243	0.116584	0.049917	0.776408	0.057091
2.27414	0.120972	0.046853	0.774811	0.057364
2.314037	0.115163	0.048601	0.780746	0.055491
2.353934	0.114582	0.050854	0.780116	0.054447
2.393832	0.110148	0.046908	0.787285	0.05566
2.433729	0.114555	0.048869	0.780407	0.056169
2.473626	0.113324	0.050594	0.778024	0.058058
2.513523	0.112598	0.050309	0.777702	0.059392
2.55342	0.111845	0.050497	0.779906	0.057753
2.593318	0.111626	0.049844	0.78065	0.05788
2.633215	0.110075	0.053355	0.779395	0.057175
2.673112	0.111112	0.048059	0.785205	0.055624
2.713009	0.10271	0.045281	0.795589	0.05642
2.752906	0.096937	0.04653	0.800337	0.056196
2.792804	0.098408	0.043382	0.802582	0.055628
2.832701	0.074543	0.041508	0.825482	0.058468
2.872598	0.077924	0.042536	0.823104	0.056437
2.912495	0.086908	0.042544	0.813246	0.057302
2.952392	0.110526	0.045793	0.789273	0.054408

2.99229	0.086252	0.039032	0.816135	0.058582
3.032187	0.073975	0.035615	0.831586	0.058824
3.072084	0.07548	0.034741	0.829128	0.060651
3.111981	0.111752	0.040896	0.79364	0.053713
3.151878	0.094559	0.042312	0.805155	0.057974
3.191776	0.106927	0.044593	0.794286	0.054194
3.231673	0.131051	0.04409	0.772015	0.052845
3.27157	0.113592	0.046733	0.784602	0.055074
3.311467	0.109982	0.045618	0.789932	0.054468
3.351364	0.112336	0.048828	0.783502	0.055334
3.391262	0.112942	0.048913	0.781865	0.056279
3.431159	0.113253	0.04219	0.790402	0.054156
3.471056	0.107177	0.042653	0.793779	0.056391
3.510953	0.115765	0.041958	0.788196	0.05408
3.55085	0.113324	0.04191	0.790239	0.054528
3.590748	0.117531	0.045683	0.782163	0.054623
3.630645	0.114987	0.04615	0.783519	0.055344
3.670542	0.116212	0.053097	0.773766	0.056925
3.710439	0.116466	0.049857	0.775823	0.057855
3.750336	0.117186	0.048175	0.777572	0.057067
3.790233	0.120257	0.046729	0.776923	0.056091
3.830131	0.120869	0.047141	0.775749	0.056241
3.870028	0.119598	0.050588	0.77481	0.055005
3.909925	0.120022	0.048235	0.778173	0.053571
3.949822	0.117292	0.049402	0.779399	0.053908
3.989719	0.117665	0.050291	0.77951	0.052534
4.029617	0.117496	0.048096	0.783045	0.051363
4.069514	0.117224	0.051372	0.781363	0.050041
4.109411	0.11687	0.048817	0.783604	0.050709
4.149308	0.117978	0.05109	0.782058	0.048875
4.189205	0.115054	0.049954	0.785795	0.049197
4.229103	0.122488	0.044879	0.784961	0.047673
4.269	0.121975	0.047151	0.784159	0.046716
4.308897	0.123199	0.050842	0.780927	0.045032
4.348794	0.121639	0.049769	0.783921	0.044672
4.388691	0.121699	0.053589	0.780969	0.043743
4.428589	0.118708	0.050718	0.789783	0.040791
4.468486	0.120083	0.051387	0.787787	0.040743
4.508383	0.121561	0.05148	0.787695	0.039264
4.54828	0.122562	0.050869	0.786956	0.039613
4.588177	0.121199	0.039642	0.785444	0.053715
4.628075	0.119433	0.04575	0.788781	0.046035
4.667972	0.12106	0.053374	0.78893	0.036637
4.707869	0.119742	0.053986	0.790558	0.035714
4.747766	0.121834	0.056782	0.786628	0.034756

4.787663	0.120323	0.055775	0.790169	0.033733
4.827561	0.118456	0.05394	0.794418	0.033186
4.867458	0.120295	0.053347	0.793777	0.032581
4.907355	0.120813	0.057356	0.789011	0.032819
4.947252	0.120037	0.057889	0.787062	0.035013
4.987149	0.118881	0.046459	0.787804	0.046856
5.027047	0.12237	0.046809	0.783937	0.046883
5.066944	0.117825	0.050116	0.788067	0.043992
5.106841	0.119498	0.058688	0.787564	0.03425
5.146738	0.121631	0.047053	0.787278	0.044038
5.186635	0.119655	0.060347	0.787673	0.032325
5.226533	0.121614	0.06007	0.787306	0.031011
5.26643	0.116383	0.062073	0.789783	0.031761
5.306327	0.114938	0.064935	0.78854	0.031587
5.346224	0.114876	0.065431	0.787764	0.031929
5.386121	0.11517	0.06686	0.786739	0.031232
5.426018	0.1154	0.066949	0.786737	0.030915
5.465916	0.115603	0.071698	0.781509	0.03119
5.505813	0.114187	0.073611	0.782931	0.02927
5.54571	0.115626	0.063387	0.78323	0.037757

C. Additional LA-ICPMS Maps

C.1 18ZE-R-14B

Figure C.1: Li, C, Na, Mg, and Al LA-ICPMS maps of 18ZE-R-14B

Figure C.2: Si, P, S, K, and Ca LA-ICPMS maps of 18ZE-R-14B

Figure C.3: Sc, Ti, V, Cr, and Mn LA-ICPMS maps of 18ZE-R-14B

Figure C.4: Fe, Co, Zn, Ga, and Rb LA-ICPMS maps of 18ZE-R-14B

Figure C.5: Sr, Y, Zr, Nb, and Ba LA-ICPMS maps of 18ZE-R-14B

Figure C.6: Nd, Sm, Eu, Gd, and Tb LA-ICPMS maps of 18ZE-R-14B

Figure C.7: Dy, Ho, Er, Tm, and Yb LA-ICPMS maps of 18ZE-R-14B

Figure C.8: Lu, Hf, and Pb LA-ICPMS maps of 18ZE-R-14B

Figure C.9: Pb, Th, U, and total integrated composition (TIC) LA-ICPMS maps of 18ZE-R-14B

C.2 18ZE-R-73C-L

Figure C.10: Li, C, Na, Mg, and Al LA-ICPMS maps of 18ZE-R-73C-L

Figure C.11: Si, P, S, K, and Ca LA-ICPMS maps of 18ZE-R-73C-L

Figure C.12: Sc, Ti, V, Cr, and Mn LA-ICPMS maps of 18ZE-R-73C-L

Figure C.13: Fe, Co, Zn, Ga, and Rb LA-ICPMS maps of 18ZE-R-73C-L

Figure C.14: Sr, Y, Zr, Nb, and Ba LA-ICPMS maps of 18ZE-R-73C-L

Figure C.15: Nd, Sm, Eu, Gd, and Tb LA-ICPMS maps of 18ZE-R-73C-L

Figure C.16: Dy, Ho, Er, Tm, and Yb LA-ICPMS maps of 18ZE-R-73C-L

Figure C.17: Lu, Hf, and Pb LA-ICPMS maps of 18ZE-R-73C-L

Figure C.19: Li, C, Na, Mg, and Al LA-ICPMS maps of 18ZE-R-73C-S

Figure C.20: Si, P, S, K, and Ca LA-ICPMS maps of 18ZE-R-73C-S

Figure C.21: Sc, Ti, V, Cr, and Mn LA-ICPMS maps of 18ZE-R-73C-S

Figure C.22: Fe, Co, Zn, Ga, and Rb LA-ICPMS maps of 18ZE-R-73C-S

Figure C.23: Sr, Y, Zr, Nb, and Ba LA-ICPMS maps of 18ZE-R-73C-S

Figure C.24: Nd, Sm, Eu, Gd, and Tb LA-ICPMS maps of 18ZE-R-73C-S

Figure C.25: Dy, Ho, Er, Tm, and Yb LA-ICPMS maps of 18ZE-R-73C-S

Figure C.26: Lu, Hf, and Pb LA-ICPMS maps of 18ZE-R-73C-S

Figure C.27: Pb, Th, U, and total integrated composition (TIC) LA-ICPMS maps of 18ZE-R-73C-S

C.4 18ZE-R-77A

Figure C.28: Li, C, Na, Mg, and Al LA-ICPMS maps of 18ZE-R-77A

Figure C.29: Si, P, S, K, and Ca LA-ICPMS maps of 18ZE-R-77A

Figure C.30: Sc, Ti, V, Cr, and Mn LA-ICPMS maps of 18ZE-R-77A

Figure C.31: Fe, Co, Zn, Ga, and Rb LA-ICPMS maps of 18ZE-R-77A

Figure C.32: Sr, Y, Zr, Nb, and Ba LA-ICPMS maps of 18ZE-R-77A

Figure C.33: Nd, Sm, Eu, Gd, and Tb LA-ICPMS maps of 18ZE-R-77A

Figure C.34: Dy, Ho, Er, Tm, and Yb LA-ICPMS maps of 18ZE-R-77A

Figure C.35: Lu, Hf, and Pb LA-ICPMS maps of 18ZE-R-77A

Figure C.36: Pb, Th, U, and total integrated composition (TIC) LA-ICPMS maps of 18ZE-R-77A

C.5 18ZE-R-49B

Figure C.37: Li, C, Na, Mg, and Al LA-ICPMS maps of 18ZE-R-49B

Figure C.38: Si, P, S, K, and Ca LA-ICPMS maps of 18ZE-R-49B

Figure C.39: Sc, Ti, V, Cr, and Mn LA-ICPMS maps of 18ZE-R-49B

Figure C.40: Fe, Co, Zn, Ga, and Rb LA-ICPMS maps of 18ZE-R-49B

Figure C.41: Sr, Y, Zr, Nb, and Ba LA-ICPMS maps of 18ZE-R-49B

Figure C.42: Nd, Sm, Eu, Gd, and Tb LA-ICPMS maps of 18ZE-R-49B

Figure C.43: Dy, Ho, Er, Tm, and Yb LA-ICPMS maps of 18ZE-R-49B

Figure C.44: Lu, Hf, and Pb LA-ICPMS maps of 18ZE-R-49B

Figure C.45: Pb, Th, U, and total integrated composition (TIC) LA-ICPMS maps of 18ZE-R-49B

C.6 18ZE-R-71

Figure C.46: Li, C, Na, Mg, and Al LA-ICPMS maps of 18ZE-R-71

Figure C.47: Si, P, S, K, and Ca LA-ICPMS maps of 18ZE-R-71

Figure C.48: Sc, Ti, V, Cr, and Mn LA-ICPMS maps of 18ZE-R-71

Figure C.49: Fe, Co, Zn, Ga, and Rb LA-ICPMS maps of 18ZE-R-71

Figure C.50: Sr, Y, Zr, Nb, and Ba LA-ICPMS maps of 18ZE-R-71

Figure C.51: Nd, Sm, Eu, Gd, and Tb LA-ICPMS maps of 18ZE-R-71

Figure C.52: Dy, Ho, Er, Tm, and Yb LA-ICPMS maps of 18ZE-R-71

Figure C.53: Lu, Hf, and Pb LA-ICPMS maps of 18ZE-R-71

Figure C.54: Pb, Th, U, and total integrated composition (TIC) LA-ICPMS maps of 18ZE-R-71

D. G_FRAC source code

main.py

```
1 from Garnet import Garnet
2 from GarnetCSD import GarnetCSD, NUM_SHELLS
3 from Sphere import Sphere
4 from Ellipsoid import Ellipsoid
5 from GeochemConst import *
6 from ComponentMol import *
7 from GarnetComponentMol import GarnetComponentMol
8 from Traverse import Traverse
9 from CompoProfile import CompoProfile
10 from SampleComp import SampleComp
11
12 import easygui
13 import os
14 import matplotlib.pyplot as plt
15 import pandas as pd
16 import re
17 import sys
18
19 isDebug = False
20
21 sys.setrecursionlimit(NUM_SHELLS*3)
22 #print(sys.getrecursionlimit())
23 SAMPLE_COL = "Name"
24 #Begin the actual program
25 #Start by getting the traverse data:
26
27 print('Choose the csv file for the traverse')
28 #travIn = input('Enter the name and directory of the csv file for the
    traverse: ')
29 if isDebug:
30     #travIn = "./TestData/TestTrav.csv"
31     travIn = easygui.fileopenbox('Choose the csv file for the traverse',
        default="/home/sabastien/Documents/Carleton/Probe/Central sections/
        Garnet_CSVs/*.csv")
32 else:
33     travIn = easygui.fileopenbox('Choose the csv file for the traverse',
```

```

    default="*.csv")
34
35 if travIn != None:
36     travIn = travIn.strip()
37     travIn = travIn.strip('\"')
38
39
40
41 #gen = int(input("Enter the garnet generation to plot: "))
42 plt.rcParams['font.size'] = 18
43 plt.rcParams['axes.linewidth'] = 2
44 #Make and plot the traverses
45 trav = Traverse(travIn)
46 travFig = plt.figure(figsize = (12,8))
47 travAx = travFig.add_subplot()
48
49 trav.plotAll(travAx)
50 print("Please click on the plot where you want to split it in half, if
    you are satisfied with the plot as is, exit the window")
51 plt.show()
52
53 #I am going to try to make this program take a geochemical csv file like
    THERIN_Generator, then allow the user to select from list
54 if isDebug:
55     fileIn = "./TestData/TestGeochem.csv"
56 else:
57     fileIn = easygui.fileopenbox('Select the csv file where the
    geochemical data is stored',default="*.csv")
58
59 geochemDF = pd.read_csv(fileIn)
60
61 samples = list(geochemDF[SAMPLE_COL])
62
63 msg = "Select the sample to use"
64 title = "Sample selection"
65 chosenSample = easygui.choicebox(msg,title,samples)
66
67 presentCmpnts = []
68 wtCompo = []
69 #Now should know which row to use
70 selectedRow = geochemDF[geochemDF["Name"] == chosenSample]#Not sure if
    there is a better way
71
72 for i in range(len(COMPONENTS)):
73     if not(COMPONENTS[i].element == C.element or COMPONENTS[i].element ==
    H.element):
74
75         try:
76             wtCompo.append(float(selectedRow[COMPONENTS[i].oxName]))
77             presentCmpnts.append(COMPONENTS[i])
78         except:
79             print("Component " + COMPONENTS[i].oxName + " not present in file"
    )
80

```



```

81
82
83 # #Ask if user wishes to bin the sample
84 # msg = "Do you wish to bin the CSD?"
85 # title = ""
86 # choices = ["Yes","No"]
87 # isBinned = easygui.ynbox(msg,title,choices)
88 isBinned = False
89 #Okay now we can have a thing for user input
90 if isDebug:
91     volume = 0.075
92     density = 4.19
93     database = "tcdb"
94     radInterval = 0.3
95 else:
96     title = "User Input"
97     msg = "Please provide the following information"
98     if isBinned:
99         lastField = "Number of bins"
100     else:
101         lastField = "Radius Interval (mm)"
102     fieldNames = ["Scanned Volume (cm^3)","Density (g/cm^3)","Database
Filename",lastField]
103
104     fieldValues = easygui.multenterbox(msg,title, fieldNames)
105     # make sure that none of the fields was left blank
106     # Gotta make things a little bit idiot proof
107     while 1:
108         if fieldValues == None: break
109         errmsg = ""
110         for i in range(len(fieldNames)):
111             if fieldValues[i].strip() == "":
112                 errmsg = errmsg + ('"%s" is a required field.\n\n' % fieldNames[
i])
113         if errmsg == "": break # no problems found
114         fieldValues = multenterbox(errmsg, title, fieldNames, fieldValues)
115
116
117
118     volume = float(fieldValues[0].strip())
119     density = float(fieldValues[1].strip())
120     database = fieldValues[2].strip()
121
122     radInterval = float(fieldValues[3].strip())
123
124     name = chosenSample
125
126
127     mass = density*volume
128
129     sampleCompo = SampleComp(name,wtCompo,presentCmpnts,mass)
130
131     redCo2 = True
132     h2o = 100

```



```

133 co2 = 100
134
135 sampleCompo.calcO2(redCo2,co2,h2o)
136 composition = sampleCompo.molArray
137
138
139
140
141 #Code for selecting the blob file
142 if isDebug:
143     #blobIn = "./TestData/TestBlob.xlsx"
144     blobIn = easygui.fileopenbox("Choose the xlsx file that the blob data
is stored in",default="/home/sabastien/Documents/Carleton/Blob Output/
XLSX files/*.xlsx")
145     outputDir = "./TestData/TestOutputC"
146 else:
147     blobIn = easygui.fileopenbox("Choose the xlsx file that the blob data
is stored in",default="*.xlsx")
148     outputDir = easygui.diropenbox("Select the directory to save output")
149 if os.name == 'nt':#PC
150     outputDir += "\\\"
151
152 else:#Mac or linux
153     outputDir += "/"
154
155 if blobIn != None:
156
157
158
159     #now make the csd
160     scannedCSD = GarnetCSD(blobIn,trav.selectedTrav,composition,volume,
name)
161     msg = "Do you wish to save memory by not plotting the individual
garnet compositions? WARNING: Selecting No will cause the program to
use a lot of RAM for samples with a lot of garnets"
162     title = ""
163     choices = ["Yes","No"]
164     saveMem = easygui.ynbox(msg,title,choices)
165     #saveMem = True
166     interpFig = plt.figure(figsize = (12,8))
167     interpAx = interpFig.add_subplot()
168
169     trav.selectedTrav.plotInterpolants(interpAx,radInterval)
170
171     plt.show()
172     check = easygui.ynbox("Continue?",title,choices)
173     if check:
174         scannedCSD.fractionateGarnet(outputDir, database,radInterval,
saveMem)
175
176         interpFig.savefig(outputDir + "OriginalTrav.svg")
177         plt.show()
178 else:
179     print("No blob file chosen, ending program...")

```

```

180 else:
181     print("No csv file chosen, ending program...")
182

```

Component.py

```

1 #A simple class to define elemental components of a rock
2 class Component:
3
4     def __init__(self, name, M, ox, cNum, oName):
5
6         self.element = name
7         self.weight = M
8         self.ox2cat = ox #ratio of O to cation if in an oxide
9         self.catNum = cNum # Num of cations in an oxide
10        self.oxName = oName

```

ComponentMol.py

```

1 #This is a simple class for monitoring concentration of a component in a
  rock or mineral composition
2 from Component import Component
3 import copy
4
5 class ComponentMol(Component):
6
7     def __init__(self, componentIn, molIn=0):
8         #Initialize the super using the parameters of componentIn
9         componentCopy = copy.deepcopy(componentIn)
10        super().__init__(componentCopy.element, componentCopy.weight,
        componentCopy.ox2cat, componentCopy.catNum, componentCopy.oxName)
11
12        self.mol = molIn
13
14    def sumComponents(self, otherComp):
15        #Returns a new component that is a sum of the two
16        #Checks if it is the same type of component
17
18        if(self.element == otherComp.element):
19            summedMol = self.mol + otherComp.mol
20
21            return ComponentMol(self, summedMol)
22        #returns nothing if they dont match
23
24    def subtractComponent(self, otherComp):
25        #Returns a new component that is self - otherComp
26        if(self.element == otherComp.element):
27            diffMol = self.mol - otherComp.mol
28
29            return ComponentMol(self, diffMol)
30        #returns nothing if they dont match
31
32
33

```

```

34 def addComponentList(cList1, cList2):
35     #This is a function to add together the composition of cList1 and cList2
36     #Returns another list of componentmols
37     summedList = []
38     matchIndex2 = []
39     for i in range(len(cList1)):
40         #cycle through cList1 and try to add every component from cList2
41         didMatch = False
42         for j in range(len(cList2)):
43             molSum = cList1[i].sumComponents(cList2[j])
44             #Check to see if molSum was calculated
45             if molSum != None:
46
47                 summedList.append(molSum)
48                 #If molSum calculated then keep track of the index in list 2
49                 #print("They match")
50                 didMatch = True
51                 matchIndex2.append(j)
52
53             if not didMatch:
54                 summedList.append(cList1[i])
55
56     #Only append the components that didnt have a match in the second list
57     for i in range(len(cList2)):
58         #Saves if it has a match in matchIndex2
59         noMatch = True
60         for j in range(len(matchIndex2)):
61             if i == matchIndex2[j]:
62                 noMatch = False
63         if noMatch:
64             summedList.append(cList2[i])
65
66     return summedList
67
68 def subComponentList(cList1, cList2):
69     #The same as the add but it subtracts cList2 from cList1
70     diffList = []
71     matchIndex2 = []
72     for i in range(len(cList1)):
73         #cycle through cList1 and try to add every component from cList2
74         didMatch = False
75         for j in range(len(cList2)):
76             molDiff = cList1[i].subtractComponent(cList2[j])
77             #Check to see if molSum was calculated
78             if molDiff != None:
79
80                 diffList.append(molDiff)
81                 #If molSum calculated then keep track of the index in list 2
82                 #print("They match")
83                 didMatch = True
84                 matchIndex2.append(j)
85
86             if not didMatch:
87                 #Returns the same value if the component isnt present in cList2

```

```

88     diffList.append(cList1[i])
89
90     #Only append the components that didnt have a match in the second list
91     for i in range(len(cList2)):
92         #Saves if it has a match in matchIndex2
93         noMatch = True
94         for j in range(len(matchIndex2)):
95             if i == matchIndex2[j]:
96                 noMatch = False
97         if noMatch:
98             molDiff = cList2[i].subtractComponent(ComponentMol(cList2[i],0))
99             #Returns a negative value if the component isnt in the first list
100             diffList.append(molDiff)
101
102     return diffList

```

GarnetComponent.py

```

1  #Class for defining garnet components
2  from ComponentMol import ComponentMol
3
4  class GarnetComponent:
5
6      def __init__(self, catName, endMemName, formulaList):
7          #A garnet component is an endmember, it has a cation assuming form
7          X3Al2Si3O12 where X is the cation
8          #It also has an endmember name like spss, py, etc
9          #The formula is a list of components where the amount of mol is equal
9          to the amount in the formula
10         self.cation = catName
11         self.endMember = endMemName #This should be the same as the endmember
11         code in theriak-domino
12         self.formula = formulaList #This is a list of ComponentMols
13
14         self.weight = 0
15         #Calculate molar weight based on the formula
16         for i in range(len(self.formula)):
17             component = self.formula[i]
18             compWeight = component.weight*component.mol
19             self.weight += compWeight

```

GarnetComponentMol.py

```

1  #This is like ComponentMol but instead its for the GarnetComponents
2  #There is probably a more polymorphic way to implement these but this
2  works for now
3  #By for now I mean forever
4  from GarnetComponent import GarnetComponent
5  from ComponentMol import *
6  import copy
7
8  class GarnetComponentMol(GarnetComponent):
9
10     def __init__(self, grtIn, xIn=0, molIn=0):

```

```

11     #Takes all properties from grtIn and assigns an amount of mols and a
    mol fraction
12     grtCopy = copy.deepcopy(grtIn)
13     super().__init__(grtCopy.cation,grtCopy.endMember,grtCopy.formula)
14     self.molFrac = xIn #This should add to 1 with the other garnet
    components
15     self.mol = molIn
16
17 def getComponentMols(self):
18     #Method that returns a list of ComponentMols which make up the
    GarnetComponentMol
19     componentList = []
20
21     for i in range(len(self.formula)):
22         #For each component in the formula, multiply it by the mol of the
    garnetComponent
23         mol = self.formula[i].mol*self.mol
24         componentList.append(ComponentMol(self.formula[i],mol))
25
26     return componentList

```

GeochemConst.py

```

1 #GeochemConst.py
2 #Contains definitions of the different components
3
4 from Component import Component
5 from GarnetComponent import GarnetComponent
6 from ComponentMol import ComponentMol
7
8 #Making the components: Input values are name, molar weight, oxide ratio,
    cation number, Cation name
9 Si = Component("Si", 28.086, 2, 1, "SiO2")
10 Al = Component("Al", 26.982, 3/2, 2, "Al2O3")
11 Fe = Component("Fe", 55.933, 1, 1, "FeO")
12 Fe3 = Component("Fe3", 55.933, 3/2, 2, "Fe2O3")
13 Mn = Component("Mn", 54.938, 1, 1, "MnO")
14 Mg = Component("Mg", 24.305, 1, 1, "MgO")
15 Ca = Component("Ca", 40.078, 1, 1, "CaO")
16 Na = Component("Na", 22.990, 1/2, 2, "Na2O")
17 K = Component("K", 39.098, 1/2, 2, "K2O")
18 Ti = Component("Ti", 47.88, 2, 1, "TiO2")
19 P = Component("P", 30.974, 5/2, 2, "P2O5")
20 H = Component("H", 1.008, 1/2, 2, "H2O")
21 C = Component("C", 12.011, 2, 1, "CO2")
22 O = Component("O", 15.999, 1, 1, "O2") #Oxide is O2 1:1 ratio
23
24 COMPONENTS = [Si, Al, Fe, Fe3, Mn, Mg, Ca, Na, K, Ti, H, C, O, P] #No P2O5
    because unreliable data, add if desired
25 GRT_DENSITY = 4.19 #Density in g/cm^3
26
27
28 SPSS = GarnetComponent("Mn", "spss", [ComponentMol(Mn, 3), ComponentMol(Al, 2),
    ComponentMol(Si, 3), ComponentMol(O, 12)])

```



```

29 PY = GarnetComponent("Mg","py",[ComponentMol(Mg,3),ComponentMol(Al,2),
    ComponentMol(Si,3),ComponentMol(0,12)])
30 GR = GarnetComponent("Ca","gr",[ComponentMol(Ca,3),ComponentMol(Al,2),
    ComponentMol(Si,3),ComponentMol(0,12)])
31 ALM = GarnetComponent("Fe","alm",[ComponentMol(Fe,3),ComponentMol(Al,2),
    ComponentMol(Si,3),ComponentMol(0,12)])
32
33 GRT_CMPNT = [SPSS,PY,GR,ALM]

```

Composition.py

```

1 #This class is essentially just a list of componentMols
2 #Allow for straightforward operations when adding compositions and stuff
3 #Class isnt done yet
4
5 from ComponentMol import ComponentMol
6 import copy
7
8 class Composition:
9
10     def __init__(self, molList):
11
12         self.componentList = molList
13
14
15     def addComposition(self, compoIn):
16         #This is a function to add together the composition of cList1 and cList2
17         #Returns another list of componentmols
18         summedList = []
19         matchIndex2 = []
20         for i in range(len(cList1)):
21             #cycle through cList1 and try to add every component from cList2
22             didMatch = False
23             for j in range(len(cList2)):
24                 molSum = cList1[i].sumComponents(cList2[j])
25                 #Check to see if molSum was calculated
26                 if molSum != None:
27
28                     summedList.append(molSum)
29                     #If molSum calculated then keep track of the index in list 2
30                     #print("They match")
31                     didMatch = True
32                     matchIndex2.append(j)
33
34             if not didMatch:
35                 summedList.append(cList1[i])
36
37         #Only append the components that didnt have a match in the second list
38         for i in range(len(cList2)):
39             #Saves if it has a match in matchIndex2
40             noMatch = True
41             for j in range(len(matchIndex2)):
42                 if i == matchIndex2[j]:
43                     noMatch = False

```

```

44     if noMatch:
45         summedList.append(cList2[i])
46
47     return summedList
48
49     def subComposition(self, compoIn):
50         #The same as the add but it subtracts cList2 from cList1
51         diffList = []
52         matchIndex2 = []
53         for i in range(len(cList1)):
54             #cycle through cList1 and try to add every component from cList2
55             didMatch = False
56             for j in range(len(cList2)):
57                 molDiff = cList1[i].subtractComponent(cList2[j])
58                 #Check to see if molSum was calculated
59                 if molDiff != None:
60
61                     diffList.append(molDiff)
62                     #If molSum calculated then keep track of the index in list 2
63                     #print("They match")
64                     didMatch = True
65                     matchIndex2.append(j)
66
67             if not didMatch:
68                 #Returns the same value if the component isnt present in cList2
69                 diffList.append(cList1[i])
70
71         #Only append the components that didnt have a match in the second list
72         for i in range(len(cList2)):
73             #Saves if it has a match in matchIndex2
74             noMatch = True
75             for j in range(len(matchIndex2)):
76                 if i == matchIndex2[j]:
77                     noMatch = False
78             if noMatch:
79                 molDiff = cList2[i].subtractComponent(ComponentMol(cList2[i],0))
80                 #Returns a negative value if the component isnt in the first list
81                 diffList.append(molDiff)
82
83     return diffList

```

SampleComp.py

```

1  from Component import Component
2  from ComponentMol import *
3  from GeochemConst import *
4
5  import easygui
6  REMOVE_AP = False#Temporary constant, set as true if you want to remove Ca
   as apatite
7  #A class for handling each record in a table of compositions
8  class SampleComp:
9
10     def __init__(self, nameIn, wtArrayIn, componentsIn, sampleMass):

```

```

11     self.name = nameIn
12     self.wtArray = wtArrayIn
13     self.components = componentsIn #The components that correspond to
each weight
14     self.mass = sampleMass #Mass in g
15     self.convertMol()
16
17
18     def convertMol(self):
19         #Convert wt% to mols as cations!
20         msg = "Do you want to remove Phosphorous as Apatite?"
21         title = ""
22         choices = ["Yes", "No"]
23         removeAp = easygui.ynbox(msg, title, choices)
24         self.molArray = []
25         fe0Pos = -1
26         fe203Pos = -1
27         Ca0Pos = -1
28         PPos = -1
29         for i in range(len(self.wtArray)):
30
31             oxideWeight = self.components[i].weight*self.components[i].
catNum + self.components[i].catNum*self.components[i].ox2cat*0.weight #
Oxide M = M component * cations in oxide + M O * #O in oxide
32             weightComponent = (self.wtArray[i]/100)*self.mass
33
34
35
36             mol = self.components[i].catNum*weightComponent/oxideWeight #
CatNum * Wt / M gives number of mols of that cation
37             thisComponent = ComponentMol(self.components[i], mol)
38             self.molArray.append(thisComponent)
39
40             if self.components[i].oxName== "Fe0":
41                 fe0Pos = i
42             elif self.components[i].oxName == "Fe203":
43                 fe203Pos = i
44
45             if self.components[i].oxName == "Ca0":
46                 Ca0Pos = i
47             if self.components[i].oxName == "P205":
48                 PPos = i
49
50             #Basically if there is both Fe0 and Fe203 in the sample
composition then
51             #add them together and put the total in the Fe0 column and bring
the Fe203 column with 0
52             if fe0Pos >= 0 and fe203Pos >= 0:
53                 self.molArray[fe0Pos].mol += self.molArray[fe203Pos].mol
54                 self.molArray.pop(fe203Pos)
55                 self.components.pop(fe203Pos)#This makes the wtArray not match
with the components, shouldnt be an issue because wtArray isnt used
again
56             elif fe203Pos >=0:
57                 #Convert to Fe0

```

```

57         self.molArray[fe203Pos] = ComponentMol(Fe, self.molArray[
fe203Pos].mol)
58
59     #This is used if removing Ca with apatite
60     #Calculates the proportion based on a formula Ca5(P04)3(OH,F,Cl)
61     if CaOPos >= 0 and PPos >= 0 and removeAp:
62         CaRemoval = self.molArray[PPos].mol*5/3
63         self.molArray[CaOPos].mol -= CaRemoval
64         self.molArray.pop(PPos)
65     elif PPos >= 0 and not removeAp:
66         self.molArray.pop(PPos)
67
68
69
70     def calcO2(self, redCO2, CO2, H2O):
71         #Adds to the molArray the amount of O2 that works with the amount
of CO2 and H2O
72         hComponent = ComponentMol(H, H2O*2)
73         cComponent = ComponentMol(C, CO2)
74         oComponent = ComponentMol(O, 0)
75
76         #Add up the proportionate amount of mols of O for each component
77         self.molArray.append(hComponent)
78         for i in range(len(self.molArray)):
79             oComponent.mol += self.molArray[i].mol* self.molArray[i].
ox2cat
80         if not redCO2:
81             oComponent.mol += cComponent.mol* cComponent.ox2cat
82
83         self.molArray.append(cComponent)
84         self.molArray.append(oComponent)
85
86
87
88
89     # def convertMolCent(self):
90     #     #Convert mol to mol %
91     #     #Note this is not molar oxides, just %Mol of Cations
92     #     #Shouldnt be hard to alter this to do mol% oxides though
93
94     #     self.molCent = []
95     #     totMol = sum(self.molArray)
96
97     #     for elem in self.molArray:
98     #         percent = 100*elem/totMol
99     #         self.molCent.append(round(percent, 5))
100
101     # def writeTHERINcompo(self, redCO2, CO2, H2O):
102     #     #Makes the composition line for the THERIN file
103     #     mol_O = 0
104     #     therin = ""
105     #     for i in range(len(self.molArray)):
106     #         #IF block, writes to the file and calculates Oxygen
107     #         #If a CO2 or H2O value is given, they will ignore the values

```

```

that might be in the data tables
108 #           #If CO2 is reduced, it will ignore the value for the Oxygen
calculation
109 #           currComp = self.components[i]
110 #           if self.molArray[i] > 0:
111
112 #               if redCO2 or CO2 >= 0:
113 #                   if H2O >= 0:
114 #                       if currComp.formula!= "H2O" and currComp.formula
!= "CO2" :
115 #                           mol_0 += self.molArray[i]*currComp.ox2cat
116 #                           therin += currComp.cation.upper() + "(" +
str(self.molArray[i]) + ")"
117 #                       elif currComp.formula!= "CO2":#Ignore the CO2 column
for adding up mols of stuff
118 #                           mol_0 += self.molArray[i]*currComp.ox2cat
119 #                           therin += currComp.cation.upper() + "(" + str(
self.molArray[i]) + ")"
120 #                       else:
121 #                           if H2O >= 0:
122 #                               if currComp.formula!= "H2O":
123 #                                   mol_0 += self.molArray[i]*currComp.ox2cat
124 #                                   therin += currComp.cation.upper() + "(" +
str(self.molArray[i]) + ")"
125 #                               else:
126 #                                   mol_0 += self.molArray[i]*currComp.ox2cat
127 #                                   therin += currComp.cation.upper() + "(" +
str(self.molArray[i]) + ")"
128
129 #               if not redCO2 and CO2 < 0:#This is to catch if CO2 is
reduced but you still have a value provided in the data table
130 #                   if currComp.formula== "CO2":
131 #                       mol_0 += self.molArray[i]*currComp.ox2cat
132 #                       therin += currComp.cation.upper() + "(" +
str(self.molArray[i]) + ")"
133 #                   elif redCO2 and CO2 <0:
134 #                       if currComp.formula== "CO2":
135 #                           therin += currComp.cation.upper() + "(" + str(
self.molArray[i]) + ")"
136
137 #           #Write preset C and H into file
138 #           if CO2 >= 0 and not redCO2:
139 #               mol_0 += CO2*2
140 #               therin += "C(" + str(CO2) + ")"
141 #           elif CO2 >= 0:
142 #               therin += "C(" + str(CO2) + ")"
143
144
145 #           if H2O >= 0:
146 #               mol_0 += H2O
147 #               therin += "H(" + str(H2O*2) + ")"
148
149 #           therin += "O(" + str(round(mol_0,6)) + ")*"
150 #           return therin

```


Shape.py

```
1 #Abstract class definition of a shape
2 #Garnets can have a shape (sphere or ellipsoid)
3 #All shapes have volume and surface area but I am excluding SA for now
4
5 from abc import ABC, abstractmethod
6
7 class Shape(ABC):
8
9     def getVolume(self):
10         pass
11
12     def calcVol(self):
13         pass
14
15     def getDim(self):
16         #method for getting a defining dimension
17         pass
18
19     def growByDim(self, dim):
20         #Method to grow the shape by incrementing the defining dimension by
        dim
21         #This will maintain all aspect ratios
22         pass
23
24     def growByVol(self, vol):
25         #Method to grow shape by incrementing the volume by vol
26         #This will maintain all aspect ratios
27         pass
```

Ellipsoid.py

```
1 #Its an ellipsoid
2 #A possible shape for a garnet
3 #Has a,b, and c axis
4 from Shape import Shape
5 import math
6
7 class Ellipsoid(Shape):
8
9     def __init__(self,a,b,c):
10         #A,B,C are the semi-axes that define the ellipsoid
11         #For garnets, aAx will be the one used for shell thickness
12         self.aAx = a
13         self.bAx = b
14         self.cAx = c
15         self.calcVol()
16
17     def calcVol(self):
18         #Calculate volume of ellipsoid
19         vol = 4/3*math.pi*self.aAx*self.bAx*self.cAx
20         self.volume = vol
21
22     def getVolume(self):
```

```

23     return self.volume
24
25     def getDim(self):
26         return self.aAx
27
28     def calcABC(self):
29         #Going backwards from volume but assuming aspect ratio is the same
30         ba = self.bAx/self.aAx
31         ca = self.cAx/self.aAx
32         newA = (self.volume*3/(4*math.pi*ba*ca))**(1./3)
33         self.aAx = newA
34         self.bAx = newA*ba
35         self.cAx = newA*ca
36
37     def growByDim(self,dim):
38
39         #Gotta define ratios first
40         ba = self.bAx/self.aAx
41         ca = self.cAx/self.aAx
42
43         #Maintain the aspect ratio of the ellipsoid
44         self.aAx += dim
45         self.bAx += dim*ba
46         self.cAx += dim*ca
47         self.calcVol()
48
49     def growByVol(self, vol):
50         #Increment volume by vol
51         self.volume += vol
52         self.calcABC()
53
54     def getRescale(self, factor):
55         #Returns a new ellipsoid that is the same as this one but rescaled by
56         "factor"
57         ba = self.bAx/self.aAx
58         ca = self.cAx/self.aAx
59         newA = self.aAx/factor
60         newB = newA*ba
61         newC = newA*ca
62         newEllipsoid = Ellipsoid(newA, newB, newC)
63
64     return newEllipsoid

```

Sphere.py

```

1 #Its a sphere
2 #A possible shape for a garnet
3 #Has a volume and a radius
4 from Ellipsoid import Ellipsoid
5 import math
6
7 class Sphere(Ellipsoid):
8     #Special case of ellipsoid where a,b,c = rad
9     def __init__(self,rad):

```

```

10     self.radius = rad
11     super().__init__(rad,rad,rad)
12
13 #Everything below removed since sphere extends ellipsoid now
14     #self.calcVol()
15
16     #def calcVol(self):
17         #Calculates the volume of the sphere
18         #vol = 4/3*math.pi*self.radius**3
19         #self.volume = vol
20
21     # def getVolume(self):
22     #     return self.volume
23
24     # def getDim(self):
25     #     return self.radius
26
27     # def growByDim(self, dim):
28     #     #Increment radius by dim
29     #     self.radius += dim
30     #     self.calcVol()
31
32     def calcRad(self):
33         #working backwards to get radius from volume
34         super().calcABC()
35         self.radius = self.aAx
36
37
38     # def growByVol(self, vol):
39     #     #Increment volume by vol
40     #     self.volume += vol
41     #     self.calcRad()

```

CompoProfile.py

```

1 #General class to be extended by the Traverse class and the Model class
2 #Defines methods that can be used by any garnet composition profile
3 #Extended by Model and Traverse
4 import matplotlib.pyplot as plt
5 import matplotlib as mpl
6 import os
7 import numpy as np
8 import pandas as pd
9 from GeochemConst import GRT_CMPNT, ALM
10 from scipy.interpolate import interp1d
11
12 class CompoProfile:
13
14     def __init__(self):
15
16         #Empty initialization, defines the variables all CompoProfiles should
17         #have
18
19         self.x = [] #distance in mm

```

```

19     #mol fraction
20     self.pltColour = 'black'
21     self.pltLine = 'None'
22     self.pltMark = 'None'
23     self.cmpnts = [[],[],[],[]]#Array for mn,mg,ca,fe, each corresponds to
    a value in CMPNT
24
25
26
27     def plotCompo(self, key, pltIn, mrkSize):
28         #Plots the composition of a specific component in pltIn
29         #input key should be one of the CMPNT
30         #mrkSize input used for convenience when plotting things on different
    sized plots
31         for i in range(len(GRT_CMPNT)):
32             if(key==GRT_CMPNT[i].cation):
33                 yComp = self.cmpnts[i]
34
35
36         pltIn.plot(self.x, yComp, color = self.pltColour, marker = self.
    pltMark, linestyle = self.pltLine, markersize = mrkSize, linewidth = 2,
    label = key)
37
38     def getCmpnt(self, key):
39         #Returns the array of whatever component was input to key
40         #This is for user probing
41         val = []
42         for i in range(len(GRT_CMPNT)):
43             if(key==GRT_CMPNT[i].cation):
44                 val = self.cmpnts[i]
45         return val
46
47     def compareProfile(self, compare, wFile, name):
48         #Comparison must be another CompoProfile object
49         #This method returns multiple values of S (standard error) for each
    component in the form of Root Mean Squared Error, plus an average value
    of S.
50         #The unit of S is mol fraction,
51         #Assumes that these are two non-identical arrays CompoProfiles (e.g. a
    model and a traverse, or two different models)
52         #Also assumes that both arrays start from core and go to the rims,
    does not perform any translations
53         #Will take each x value of comparison and find what the composition
    should be at that x in "this"
54         #Does this by interpolating between the closest two points at each x
    in compare
55         #The intention is to compare a model profile to a half traverse, so it
    will interpolate values between points on the model for a least square
    regression
56
57         self.rmse= [] #Standard Error as root mean square error
58         self.nrmse = [] #Normalized RMSE
59
60         for i in range(len(GRT_CMPNT)):

```

```

61     thisCmpnt = []
62     thatCmpnt = []
63
64
65     for j in range(len(compare.x)):
66         compoAtX = self.interpCompoAtX(compare.x[j], GRT_CMPNT[i].cation)
67         if compoAtX >= 0:
68             thisCmpnt.append(compoAtX)
69             thatCmpnt.append(compare.cmpnts[i][j])
70
71     thisCmpnt = np.array(thisCmpnt)
72     thatCmpnt = np.array(thatCmpnt)
73     rmse = np.sqrt(((thisCmpnt - thatCmpnt)**2).mean()) #calculate root
mean square error
74
75     nrmse = rmse/(thatCmpnt.mean()) #Normalize to mean of the measured
profile, NOTE: Can also use the range -> try both?
76
77     self.rmse.append(rmse)
78     self.nrmse.append(nrmse)
79
80     #Build next line to write to file in the order of RMSE(CMPNT1),RMSE(
CMPNT2)...,RMSE(Average),NRMSE(CMPNT1),NRMSE(CMPNT2)..NRMSE(Average)
81     nextLine = name + ","
82     for i in range(len(self.rmse)):
83         nextLine += str(self.rmse[i]) + ","
84     nextLine += str(sum(self.rmse)/len(self.rmse)) + ','
85
86     for i in range(len(self.nrmse)):
87         nextLine += str(self.nrmse[i]) + ","
88     nrmseAvg = sum(self.nrmse)/len(self.nrmse)
89     nextLine += str(nrmseAvg) + '\n'
90
91
92
93     wFile.write(nextLine)
94
95     return nrmseAvg
96
97
98 def interpCompoAtX(self, xVal, key):
99     #Linearly interpolate the composition between to points on the model
to get the exact value at an x position
100     #
101     count = 0
102     while count < len(self.x) and self.x[count] < xVal:
103         count += 1
104
105     compoAtX = -1
106     if count >= 0 and count < len(self.x):
107         for i in range(len(GRT_CMPNT)):
108
109             if GRT_CMPNT[i].cation == key:
110                 rightX = self.x[count]

```



```

111         leftX = self.x[count-1]
112
113         rightCmpnt = self.cmpnts[i][count]
114         leftCmpnt = self.cmpnts[i][count-1]
115
116
117         #linearly interpolate between two points and get the value at
xVal
118         slope = (rightCmpnt-leftCmpnt)/(rightX-leftX)
119         midX = xVal - leftX
120         compoAtX = midX*slope + leftCmpnt
121
122         return compoAtX #Returns -1 if the first cell was to the right of the
input xVal or if it is attempting to interpolate past the model size
123
124
125 def scipyInterp(self, kindIn='linear'):
126     #Function that initializes numpy arrays for each component and
interpolates the values to create continuous functions
127
128     npCmpnts = np.array([np.array(cmpnt) for cmpnt in self.cmpnts]) #Make
numpy arrays for each component
129     npX = np.array(self.x)
130     self.interpComp = []
131     #Interpolate each component with npX and store new function in
interpComp
132     for i in range(len(npCmpnts)):
133         thisInterp = interp1d(npX, npCmpnts[i], kind=kindIn)
134         self.interpComp.append(thisInterp)
135
136
137 def plotInterpolants(self, pltIn, interval=0):
138     #Plot the interpolated profile as lines
139     #Very similar to the function plotAll in Traverse.py
140     #Doing this here because I can see utility in all CompoProfiles
141     #Will display lines at each interval or non if interval is 0 or less
142
143     colours = ['green', 'blue', 'orange', 'red']
144     #pltIn.set_xlim(min(self.x), max(self.x))
145     pltAlm = pltIn.twinx()
146
147     pltIn.set_xlabel("Distance (mm)", fontsize = 24)
148     pltIn.set_ylabel("X (Ca,Mn,Mg)", fontsize = 24)
149
150     #Uncomment these lines if you want everything on the same scale
151
152
153     pltAlm.set_ylabel("X (Fe)", fontsize = 24, rotation = -90)
154
155
156     #Plot each interpolated profile
157     maxY = 0
158     for i in range(len(GRT_CMPNT)):
159         pltColour = colours[i]

```

```

160     yComp = self.interpComp[i]
161     xComp = np.array(self.x)
162     if(GRT_CMPNT[i] == ALM):
163         pltAlm.plot(xComp, yComp(xComp), color = pltColour, marker = 'None'
164 , linestyle = "-", markersize = 7, linewidth = 2, label = GRT_CMPNT[i]
165 ].cation)
166     else:
167         if max(self.cmpnts[i]) > maxY:
168             maxY = max(self.cmpnts[i])
169             pltIn.plot(xComp, yComp(xComp), color = pltColour, marker = 'None'
170 , linestyle = "-", markersize = 7, linewidth = 2, label = GRT_CMPNT[i]
171 .cation)
172     pltIn.legend(loc = 'upper left')
173     pltAlm.legend(loc = 'upper right')
174     pltIn.xaxis.set_tick_params(which='major', size=10, width=2, direction
175 = 'in', top='on')
176     pltIn.xaxis.set_tick_params(which='minor', size=7, width=2, direction=
177 'in', top='on')
178     pltIn.yaxis.set_tick_params(which='major', size=10, width=2, direction
179 = 'in', right=False)
180     pltIn.yaxis.set_tick_params(which='minor', size=7, width=2, direction=
181 'in', right=False)
182     pltAlm.xaxis.set_tick_params(which='major', size=10, width=2,
183 direction='in', top='on')
184     pltAlm.xaxis.set_tick_params(which='minor', size=7, width=2, direction
185 = 'in', top='on')
186     pltAlm.yaxis.set_tick_params(which='major', size=10, width=2,
187 direction='in', right=True)
188     pltAlm.yaxis.set_tick_params(which='minor', size=7, width=2, direction
189 = 'in', right=True)
190
191     pltIn.xaxis.set_major_locator(mpl.ticker.MultipleLocator(0.5))
192     pltIn.xaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.1))
193     pltIn.yaxis.set_major_locator(mpl.ticker.MultipleLocator(0.1))
194     pltIn.yaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.02))
195
196     pltAlm.xaxis.set_major_locator(mpl.ticker.MultipleLocator(0.5))
197     pltAlm.xaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.1))
198     pltAlm.yaxis.set_major_locator(mpl.ticker.MultipleLocator(0.1))
199     pltAlm.yaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.02))
200
201     pltIn.set_ylim(0,0.4)
202     pltAlm.set_ylim(0.55,0.85)
203
204     #Plot the vertical lines at each interval
205     if(interval >= 0):
206         numIntervals = int(max(self.x)/interval)
207         thisInterval = interval
208         #Plot horizontal line at every interval :)
209         for i in range(numIntervals):
210
211             pltIn.plot([thisInterval,thisInterval],[-100,100],color = 'black',

```

```

202     linestyle = "--")
203     thisInterval += interval
204     #Last plot is usually smaller than the interval
205     #So plotting htat line as well
206     if(numIntervals*interval < max(self.x)):
207         pltIn.plot([max(self.x),max(self.x)],[-100,100],color = 'black',
208             linestyle = "--")
209
210 def extrapCore(self, avgInterval, distance):
211     #This method assumes the left side of a CompoProfile is the core of a
212     #mineral
213     #It then averages the values across avgInterval where avgInterval is a
214     #number of cells
215     #It then extends that average to the left by distance in mm
216     #This only needs to add one cell at the beginning of each array and
217     #move all others to the right
218     #Trying this out to see if extrapolating the core is better than
219     #stretching the whole profile
220     avgCore = [0,0,0,0]
221
222     for i in range(avgInterval):
223
224         for j in range(len(GRT_CMPNT)):
225             avgCore[j] += self.cmpnts[j][i]
226
227     newCmpnt = [[],[],[],[ ]]
228     for i in range(len(GRT_CMPNT)):
229         avgCore[i] /= avgInterval
230         newCmpnt[i].append(avgCore[i])
231
232     newX = [0]
233
234     #Need to move every cell over to the right
235     #Setting the first cell as 0 always
236     for i in range(len(self.x)):
237         newX.append(self.x[i]+distance)
238         for j in range(len(GRT_CMPNT)):
239             newCmpnt[j].append(self.cmpnts[j][i])
240
241     self.x = newX
242     self.cmpnts = newCmpnt

```

Traverse.py

```

1 #Class to open and manage the measured garnet traverse
2 #Must be in a csv file with the following header:
3 #x (mm),Ca,Mg,Fe,Mn
4 #The unit for components should be mol fraction
5 #This class is an extension of CompoProfile
6 import matplotlib.pyplot as plt
7 import matplotlib as mpl
8 import os
9 import numpy as np

```

```

10 import pandas as pd
11 import easygui
12
13 from CompoProfile import CompoProfile
14 from GeochemConst import GRT_CMPNT, ALM
15
16 class Traverse(CompoProfile):
17
18     def __init__(self, fileName):
19         #Read the file containg probe data and store it in this object
20
21         CompoProfile.__init__(self)
22         self.pltMark = 'o'
23
24         #open the csv file
25         try:
26             grtFile = open(fileName, 'r')
27         except:
28             print("No csv file found at location:")
29             print(fileName)
30             return
31
32         grtdf = pd.read_csv(fileName)
33         self.x = list(grtdf['x (mm)'])
34         for i in range(len(GRT_CMPNT)):
35             self.cmpnts[i] = list(grtdf[GRT_CMPNT[i].cation])
36
37
38
39     def plotAll(self, pltIn):
40         #Method to plot all components on one plot
41         #Assumes that the Fe component is much higher than the rest, plots it
42         #on seperate axis
43         colours = ['green','blue','orange','red']
44         symbols = ['o','^','s','p']
45         pltAlm = pltIn.twinx()
46
47         self.travPlot = pltIn #Saves the plot to the object
48
49         #Loop for plotting
50         for i in range(len(GRT_CMPNT)):
51             self.pltColour = colours[i]
52             self.pltMark = symbols[i]
53             if(GRT_CMPNT[i] == ALM):
54                 CompoProfile.plotCompo(self, GRT_CMPNT[i].cation, pltAlm, 7)
55             else:
56                 CompoProfile.plotCompo(self, GRT_CMPNT[i].cation, pltIn, 7)
57
58         pltIn.set_xlabel("Distance (mm)", fontsize = 24)
59         pltIn.set_ylabel("X (Ca,Mn,Mg)", fontsize = 24)
60
61         #Uncomment these lines if you want everything on the same scale
62         pltIn.set_ylim(0,0.4)
63         pltAlm.set_ylim(0.45,0.85)

```

```

63     pltAlm.set_ylabel("X (Fe)", fontsize = 24, rotation = -90)
64     pltIn.legend(loc = 'upper left')
65     pltAlm.legend(loc = 'upper right')
66     pltIn.xaxis.set_tick_params(which='major', size=10, width=2, direction
67     ='in', top='on')
68     pltIn.xaxis.set_tick_params(which='minor', size=7, width=2, direction=
69     'in', top='on')
70     pltIn.yaxis.set_tick_params(which='major', size=10, width=2, direction
71     ='in', right=False)
72     pltIn.yaxis.set_tick_params(which='minor', size=7, width=2, direction=
73     'in', right=False)
74
75     pltAlm.xaxis.set_tick_params(which='major', size=10, width=2,
76     direction='in', top='on')
77     pltAlm.xaxis.set_tick_params(which='minor', size=7, width=2, direction
78     ='in', top='on')
79     pltAlm.yaxis.set_tick_params(which='major', size=10, width=2,
80     direction='in', right=True)
81     pltAlm.yaxis.set_tick_params(which='minor', size=7, width=2, direction
82     ='in', right=True)
83
84     pltIn.xaxis.set_major_locator(mpl.ticker.MultipleLocator(1))
85     pltIn.xaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.2))
86     pltIn.yaxis.set_major_locator(mpl.ticker.MultipleLocator(0.1))
87     pltIn.yaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.02))
88
89     pltAlm.xaxis.set_major_locator(mpl.ticker.MultipleLocator(1))
90     pltAlm.xaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.2))
91     pltAlm.yaxis.set_major_locator(mpl.ticker.MultipleLocator(0.1))
92     pltAlm.yaxis.set_minor_locator(mpl.ticker.MultipleLocator(0.02))
93
94     #This is to set up the stuff for splitting the plot in half, assuming
95     that you input a full traverse instead of a half traverse
96     self.cid = pltIn.figure.canvas.mpl_connect('button_press_event',self.
97     travClick)
98     self.splitLine = pltIn.plot([0],[0]) #create an empty line
99     self.selectedTrav = self.splitTrav(self.x[0] - 1,False)#Sets the
100     baseline to leftTrav is empty and rightTrav = this. This is basically
101     if you want to input just a half traverse, however it assumes that it
102     is the right half
103
104     def travClick(self, event):
105         #When the plot is clicked, draw a vertical line where clicked and
106         store that value as the new 0 for splitting the traverse
107         #Will ask for confirmation before drawing and storing the location.
108         #It can be changed as many times as desired
109         self.splitLine.pop(0).remove()
110         newZero = event.xdata
111         self.travPlot.autoscale(False)
112         self.splitLine = self.travPlot.plot([newZero,newZero],[-100,100],color
113         = 'black',linestyle = '--')
114
115     title = ""

```



```

102 msg = "Split traverse at x = " + str(newZero) + "?"
103 answer = easygui.boolbox(msg,title,["Yes","No"])
104 #answer = input('Split traverse at x = ' + str(newZero) +'? (y/n)')
105 if answer:
106     msg = "Take the left or right side?"
107     selLeft = easygui.boolbox(msg,title,["Left","Right"])
108     self.selectedTrav = self.splitTrav(newZero,selLeft)
109     plt.draw()
110     print("Done, you may now exit this plot or choose a different x
location to split the traverse.")
111
112
113
114 def splitTrav(self,xPos, selectLeft):
115     #Method for splitting the traverse into two halves at the inputted
xPos
116     #Assumes xpos will never exactly equal to an x position on the
traverse
117     #The two halves are CompoProfile objects with the same data of their
respective halves of this Traverse object
118     #They will be stored in the travSplit array so that they can be
ambiguously referenced.
119     #They will contain a little less info but maintain most of the core
stuff
120
121     count = 0
122     #Finds the index of the datapoint to the right of the selected x
123     while(self.x[count] < xPos):
124         count+=1
125
126
127     xRightIndex = count
128
129     xLeftIndex = count - 1
130
131     #initialize travSplit array to hold the two halves and the two sides
of the traverse
132     self.travSplit= []
133     rightTrav = CompoProfile()
134     leftTrav = CompoProfile()
135     rightTrav.pltMark = 'o'
136     leftTrav.pltMark = 'o'
137     leftTrav.pltColour = 'blue' #So it can be differentiated on the plot
138
139     #Build the contained arrays
140     #First calculate the value at 0 using linear interpolation
141     #This allows for modelling from 0
142     rightTrav.x.append(0)
143     leftTrav.x.append(0)
144     for i in range(len(GRT_CMPNT)):
145         #Append the composition at 0 to both left and right traverse since
they should be the same
146         zeroVal = self.interpCompoAtX(xPos,GRT_CMPNT[i].cation)
147         rightTrav.cmpnts[i].append(zeroVal)

```

```

148     leftTrav.cmpnts[i].append(zeroVal)
149     for i in range(xRightIndex, len(self.x)):
150
151         rightTrav.x.append(self.x[i] - xPos)
152         for j in range(len(GRT_CMPNT)):
153             rightTrav.cmpnts[j].append(self.cmpnts[j][i])
154
155
156     #Flips the left Traverse
157     for i in range(xLeftIndex, -1, -1):
158         leftTrav.x.append(xPos - self.x[i])
159         for j in range(len(GRT_CMPNT)):
160             leftTrav.cmpnts[j].append(self.cmpnts[j][i])
161
162
163     #Add the two traverses to travSplit
164     if len(rightTrav.x) > 0:
165         self.travSplit.append(rightTrav)
166         if not selectLeft:
167             return rightTrav
168     if len(leftTrav.x) > 0:
169         self.travSplit.append(leftTrav)
170         if selectLeft:
171             return leftTrav
172

```

Garnet.py

```

1  #This is a garnet
2  #I am going to attempt to define it recursively
3  #God help me
4
5  #Garnets have a shape, composition, and density
6  from Shape import Shape
7  from GeochemConst import *
8  from Component import Component
9  from ComponentMol import *
10 from GarnetComponent import GarnetComponent
11 from GarnetComponentMol import GarnetComponentMol
12 import copy
13
14
15 class Garnet:
16
17     #Base case, the base shape should have the same dimensions of the shell
18     #thickness
19     #E.g if shell thickness is 0.002 then the radius of the basecase sphere
20     #should be 0.002
21     #I guess for ellipsoids since shell thickness varies depending on the
22     #axis we will define shell thickness as the one used for the a axis
23     def __init__(self, crystalShape, grtCompo, nextGarnet=None, numGrt = 1):
24         self.grtShape = crystalShape
25
26         self.composition = copy.deepcopy(grtCompo) #This should be an array of

```

```

    GarnetComponentMol, this is the composition of this shell
24
25     self.density = GRT_DENSITY/1000#Assumes same density for all (just for
    now I guess) convert it to g/mm^3 because blob uses mm
26
27     self.nextShell = nextGarnet #base case is None, the next garnet can
    have its own composition and density
28
29
30     self.bigAx = self.grtShape.getDim()
31     #Only need to define number of garnets upoon nucleation
32     if nextGarnet == None:
33         self.numGrT = numGrT #number of garnets of this size class (base
    number is 1 which would look at every garnet individually)
34     else:
35         self.numGrT = nextGarnet.numGrT
36
37     self.totVol = self.grtShape.getVolume() #Total volume is same as shape
    volume
38     if(nextGarnet != None):
39         self.shellVol = self.totVol - self.nextShell.totVol #Shell volume is
    the total volume less total volume of the next smallest shell
40         #self.shellThick = self.grtShape.getDim() - self.nextShell.grtShape.
    getDim()
41     else:
42         self.shellVol = self.totVol #Base case tot and shell vol are same
43         #self.shellThick = self.grtShape.getDim()#Gets radius for sphere and
    aAx for ellipsoid
44         #Get the mols of the shell and the mols of the garnet
45
46
47
48     self.calcShellMol()
49     self.calcTotMol()
50
51     #Can add a thing to delete the inner garnet to speed things up but
    will be unable to monitor the garnet composition
52
53
54
55 def calcShellMol(self):
56     #This will calculate the mols of components in a single shell in this
    garnet
57     #Assumes that the form of garnet is X3Al2Si3O12 where X is anything in
    CMPNT
58     #Will also renormalize composition to 1 in case there are minor
    discrepancies
59     mass = self.shellVol*self.density #Calculated mass of garnet
60     molGrT = []
61
62     for i in range(len(self.composition)):
63         #Calculate mols of garnet for each component
64         massSum = 0
65         for j in range(len(self.composition)):

```

```

66         #Sum up the masses of each component based on mol fraction
67         massSum += self.composition[j].weight*self.composition[j].molFrac
68
69         cmpntMol = self.composition[i].molFrac*mass/massSum #Convert the mol
fraction to mols
70         self.composition[i].mol = cmpntMol
71
72
73
74     def calcTotMol(self):
75         #Not a truly recursive function but close enough
76         #Trying to limit our coputation time and ram usage
77         #totComposition is another list of garnet endmembers which dont have a
mol fraction but a mol total which
78         #Is equal to the sum of mols for every shell in all garnets of this
size class
79         if(self.nextShell == None):
80             #Define the basecase where only one shell so total mol is shellMol
81             self.totComposition = copy.deepcopy(self.composition) #The only case
where totMol can also have a mol fraction
82         else:
83             self.totComposition = []
84             for i in range(len(self.composition)):
85                 totMol = self.nextShell.totComposition[i].mol + self.composition[i
].mol*self.numGrt #calculate the total mol for this component will
multiply each shell by the number of garnets in this size class
86                 thisComposition = GarnetComponentMol(self.composition[i],molIn=
totMol) #Mol fraction will be zero
87                 self.totComposition.append(thisComposition)#Takes total from the
next shell and adds it to current shell
88
89     def growGarnet(self, compo, growDim):
90         #Grows the garnet by growDim with composition of compo
91         newShape = copy.deepcopy(self.grtShape)
92
93         #print("Old radius: " + str(newShape.getDim()))
94
95         newShape.growByDim(growDim)
96
97         #print("New radius: " + str(newShape.getDim()))
98
99         newShell = Garnet(newShape,compo,nextGarnet = self)
100         return newShell
101
102     def getCompoAsComponentMol(self):
103         #Gets the composition of the garnet as a list of ComponentMol
104         molList = self.totComposition[0].getComponentMols()
105
106         #print(molList[0].element + ": " + str(molList[0].mol))
107
108         for i in range(1,len(self.composition)):
109             #Cycles through every garnet component converts to a list of
ComponentMols and sums it with molList
110             thisMolList = self.totComposition[i].getComponentMols()

```

```

111     molList = addComponentList(molList,thisMolList)
112     return molList
113
114
115
116 def getProfileComp(self):
117     #This will return the compositional profile of the garnet as a 2D list
    of GarnetComponentMol
118     if(self.nextShell == None):
119         #Define basecase
120         compProfile = []
121
122     else:
123         compProfile = self.nextShell.getProfileComp()
124
125     compProfile.append(self.composition)
126     return compProfile
127
128 def getProfileX(self):
129     #Returns a list of x-values for plotting the profile
130     if(self.nextShell == None):
131         #Define basecase
132         xProfile = []
133
134     else:
135         xProfile = self.nextShell.getProfileX()
136
137     xProfile.append(self.bigAx)
138     return xProfile
139
140 def getProfileVol(self):
141     #Does the same as the ones above but returns the shell volume as an
    array
142     if(self.nextShell == None):
143         #Define basecase
144         volProfile = []
145
146     else:
147         volProfile = self.nextShell.getProfileVol()
148
149     volProfile.append(self.shellVol)
150     return volProfile

```

GarnetCSD.py

```

1 #This is a class for reading and modelling garnet CSDs
2 #It can read a blob output file and use Garnet.py to model garnet growth
3 #Maybe it will do more in the far future but this is the goal for now
4
5 from Garnet import Garnet
6 from GeochemConst import *
7 from Shape import Shape
8 from Sphere import Sphere
9 from Ellipsoid import Ellipsoid

```

```

10 from CompoProfile import CompoProfile
11 from ComponentMol import *
12 from GarnetComponentMol import GarnetComponentMol
13 from SCRIPT_Generator import *
14
15 import matplotlib.pyplot as plt
16 import os
17 import numpy as np
18 import pandas as pd
19 import easygui
20 import math
21 import copy
22 import sys
23 import pdb
24
25 NUM_SHELLS = 4000 #This is the number of garnet shells the biggest garnet
    will have
26 #DATABASE = "tcdb55c2_COHmelt.txt"
27
28 EQ_PARAM = 0.00000001
29
30 CORE_AVG_INDEX = 3 #Number of cells to average for the core composition
31 class GarnetCSD:
32
33     def __init__(self, blobFileName, garnetProfile, rockCompo, rockVolume,
        sampleName, numBins = 0):
34
35         self.composition = rockCompo #This is a list of ComponentMol objects
        that define the rock composition
36         self.grtProfile = garnetProfile #This is the CompoProfile object that
        is a half profile that defines the zoning in the garnet
37         self.rockVol = rockVolume
38         #Now need to open up the blob file to build the crystal list
39         blobDF = pd.read_excel(blobFileName) #Assumes that formatting has not
        changed from default blob output
40         self.name = sampleName
41         self.crystalList = [] #Empty list to fill with Shape entries
42
43         blobDF = blobDF.dropna() #Sometimes empty rows at the end mess up
        calculations
44
45         #Choose temperature and pressure range:
46         title = "PT range"
47         msg = "Please provide min and max temperature and pressure"
48
49         fieldNames = ["Tmin", "Tmax", "Pmin", "Pmax"]
50
51         fieldValues = easygui.multenterbox(msg, title, fieldNames)
52         # make sure that none of the fields was left blank
53         # Gotta make things a little bit idiot proof
54         while 1:
55             if fieldValues == None: break
56             errmsg = ""
57             for i in range(len(fieldNames)):

```



```

58         if fieldValues[i].strip() == "":
59             errmsg = errmsg + ("%s" is a required field.\n\n' % fieldNames[
i])
60         if errmsg == "": break # no problems found
61         fieldValues = multenterbox(errmsg, title, fieldNames, fieldValues)
62
63
64
65         self.T1 = int(fieldValues[0].strip())
66         self.T2 = int(fieldValues[1].strip())
67         self.P1 = int(fieldValues[2].strip())
68         self.P2 = int(fieldValues[3].strip())
69
70
71
72         #Ask user to choose if using spheres or ellipsoids
73         msg = "Are garnets spheres or ellipsoids?"
74         title = ""
75         choices = ["Sphere","Ellipsoid"]
76         reply = "Sphere" #Ellipsoid doesnt do much atm
77         # reply = easygui.buttonbox(msg,title,choices)
78         #reply = "Sphere" #Only works for Spheres right now, need to think
about size independent growth of ellipsoids
79         if(reply==choices[0]):
80             volume = list(blobDF['Volume (mm^3)'])
81
82             for i in range(len(volume)):
83                 #If spheres, it will recalculate the radius from the volume
84                 #if not math.isnan(volume[i]):
85                 thisRad = (volume[i]*3/(4*math.pi))**(1./3)
86                 self.crystalList.append(Sphere(thisRad))
87
88             elif(reply == choices[1]):
89                 #If ellipsoid it uses the PEllipsoid data
90                 # #It should be that rad1 > rad2 > rad3
91                 # rad1 = list(blobDF['PEllipsoid Rad1 (mm)'])
92                 # rad2 = list(blobDF['PEllipsoid Rad2 (mm)'])
93                 # rad3 = list(blobDF['PEllipsoid Rad3 (mm)'])
94
95                 # for i in range(len(rad1)):
96                 #     if not math.isnan(rad1[i]):
97                 #         self.crystalList.append(Ellipsoid(rad1[i],rad2[i],rad3[i]))
98
99                 #Average out the ratios so all ellipsoids are the same shape and
grow with the same dimensions
100                 avgEllipsoid = self.getAvgEllipsoid(blobDF)
101                 volume = list(blobDF['Volume (mm^3)'])
102
103                 for i in range(len(volume)):
104                     #Need to rescale the avg ellipsoid to fit the volume of each
garnet
105                     #if not math.isnan(volume[i]):
106                     ratioAB = avgEllipsoid.aAx/avgEllipsoid.bAx
107                     ratioBC = avgEllipsoid.bAx/avgEllipsoid.cAx

```

```

108         thisA = ((3*ratioAB**2*ratioBC*volume[i])/(math.pi*4))**(1/3)
109         thisB = thisA/ratioAB
110         thisC = thisB/ratioBC
111
112         self.crystalList.append(Ellipsoid(thisA,thisB,thisC))
113     else:
114         print("Error: No option chosen")
115         return
116
117     #Okay now we need to stretch the garnet profile to fit with the long
118     dimension of the ellipsoid or the radius of the sphere
119     #This is so the profile matches up with the biggest garnet
120
121     self.quickSortCrystals(0,len(self.crystalList)-1)
122     self.numCrystals = []
123
124     #Added support for binning but I dont think its needed
125     #Still the code is here
126     if(numBins > 0):
127         #Break things up into seperate bins
128         binSize = (self.crystalList[0].getDim() - self.crystalList[len(self.
129 crystalList)-1].getDim())/numBins
130         newCrystalList = []
131
132         hiBin = self.crystalList[0].getDim()
133         #make new crystalList with a crystalSize equal to he highest radius
134         in that bin interval
135         for i in range(numBins):
136             thisInterval = hiBin-i*binSize #each value in bins represent the
137             upperbounds of that bin
138             nextInterval = hiBin-(i+1)*binSize
139             numInBin = 0
140             biggestInBin = Sphere(0)
141             for crystal in self.crystalList:
142                 if crystal.getDim() <= thisInterval and crystal.getDim() >
143                 nextInterval:
144                     numInBin += 1
145                     if crystal.getDim() > biggestInBin.getDim():
146                         biggestInBin = crystal
147                         #the biggest in the bin is the crystal that gets put in the
148                         new crystalList
149                     if numInBin > 0:
150                         newCrystalList.append(biggestInBin)
151                         self.numCrystals.append(numInBin)
152
153         self.crystalList = newCrystalList
154
155     travRad = max(self.grtProfile.x) #Radius of the garnet measured in the
156     microprobe profile
157
158     minDiff = sys.float_info.max
159     # for i in range (len(self.crystalList) - 1):
160     #     radDiff = self.crystalList[i].getDim()-self.crystalList[i+1].

```

```

getDim()
155     # if radDiff > 0:
156     #     minDiff = min(radDiff,minDiff)
157     #This makes sure that a shell is not bigger than the difference in
radius between any two garnets
158     self.shellThick = min(minDiff, self.crystalList[0].getDim()/NUM_SHELLS
)

159
160     #Instead of stretching, lets try extrapolating the core inwards:
161     radAdd = self.crystalList[0].getDim() - travRad
162     msg = "Extrapolate to core or stretch profile?"
163     title = ""
164     choices = ["Extrapolate","Stretch"]
165     reply = easygui.buttonbox(msg,title,choices)
166     if radAdd > 0 and reply == choices[0]: #In case the biggest garnet has
a radius smaller than traverse length
167         self.grtProfile.extrapCore(CORE_AVG_INDEX, radAdd)
168     else:
169         scaleFactor = self.crystalList[0].getDim()/travRad #The scaling
factor to convert the x values in grtProfile to be the same size as the
radius or a axis of ellipsoid

170
171         for i in range(len(self.grtProfile.x)):
172             #Rescale x
173             self.grtProfile.x[i] = scaleFactor*self.grtProfile.x[i]
174
175         self.grtProfile.scipyInterp() #Initialize the interpolated numpy
arrays

176
177         self.garnetList = [] #This is what we will be working with for the
most part, it is where all the garnets will grow and be stored

178
179
180 def quickSortCrystals(self, low, high):
181     #Function to sort the garnets by volume
182     #Lets do a quick sort because thats fun
183     #better to sort biggest to smallest
184     if low < high:
185
186         i = low - 1
187         pivot = self.crystalList[high].getVolume() #Compare every element in
list to the pivot

188
189         for j in range(low,high):
190
191             if(self.crystalList[j].getVolume() >= pivot):
192                 #Increment i by 1 if j is bigger than pivot
193                 #Then swap element at i and j
194
195                 i = i + 1
196                 self.crystalList[i], self.crystalList[j] = self.crystalList[j],
self.crystalList[i]
197
198             #Swap element at high and element at i + 1

```

```

199     #Putting all elements bigger in volume to left of the element at
high
200     self.crystalList[i+1], self.crystalList[high] = self.crystalList[
high], self.crystalList[i+1]
201
202     pi = i + 1
203
204     self.quickSortCrystals(low, pi-1)
205     self.quickSortCrystals(pi+1, high)
206
207 def fractionateGarnet(self, outputDir, database, radInterval=0,
memorySave = False):
208     #A method to fractionate garnet and output the composition at each
radInterval
209     #Set memorySave to True if you want it to run faster but it wont plot
the individual garnets
210     writeFile = outputDir + "Output.txt"
211     try:
212         outFile = open(writeFile, 'w')
213     except:
214         print('Problem creating new file')
215         exit(0)
216
217     currComposition = self.composition
218     therein = ""
219     for i in range(len(currComposition)):
220         if currComposition[i].mol < 0:
221             currComposition[i].mol = 0
222             therein += currComposition[i].element.upper() + "({:7.6f})".format(
currComposition[i].mol)
223
224     stream = "Initial composition: " + therein
225     print(stream)
226     outFile.write(stream + "\n")
227     self.writeScriptFiles(outputDir, 0, database)
228
229     count = 1
230     self.growGarnetShell(memorySave)
231     garnetPlotList = [0]
232     while(self.garnetList[0].bigAx < self.crystalList[0].getDim()-self.
shellThick):
233         #Grow garnet until the biggest garnet is one shell away from its max
size (or just over one shell away)
234         self.growGarnetShell(memorySave)
235
236         if(abs(self.garnetList[0].bigAx-radInterval*count)<self.shellThick):
237
238
239             #print("Biggest Radius = " + str(self.garnetList[0].bigAx))
240             #print(self.garnetList[0].composition[0].endMember + ": " + str(
self.garnetList[0].composition[0].molFrac))
241             #print("Number of garnets: " + str(len(self.garnetList)))
242
243     self.calcTotalGarnetMol()

```

```

244
245
246
247     self.writeScriptFiles(outputDir, count, database)
248
249     stream = "Stage" + str(count) + ":"
250     print(stream)
251     outFile.write(stream+"\n")
252     stream = str(len(self.garnetList)) + " garnets grown"
253     print(stream)
254     outFile.write(stream+"\n")
255     stream = "Largest radius: " + str(self.garnetList[0].bigAx) + "mm"
256     print(stream)
257     outFile.write(stream+"\n")
258     stream = "Total garnet volume: " + str(self.calcTotVol()) + "mm^3"
259     print(stream)
260     outFile.write(stream+"\n")
261
262     if garnetPlotList[len(garnetPlotList)-1] != len(self.garnetList) -
1:
263         grtIndex = len(self.garnetList)-1
264
265         garnetPlotList.append(grtIndex) #To plot these guys later
266
267         # for num in garnetPlotList:
268         #     self.plotGarnet(num)
269         # plt.show()
270         # print("Volumes are:")
271         # for garn in self.garnetList:
272         #     print(garn.totVol)
273         # print("Outer Shell:")
274         # for garn in self.garnetList:
275         #     print(str(garn.composition[0].molFrac) + "," + str(garn.
composition[1].molFrac) + "," + str(garn.composition[2].molFrac) + ","
+ str(garn.composition[3].molFrac))
276
277         # print("Radius:")
278         # for garn in self.garnetList:
279         #     print(garn.bigAx)
280         # print("Mol Sum:")
281         # for garn in self.garnetList:
282         #     thisCompo = garn.getCompoAsComponentMol()
283         #     compoString = ""
284         #     for cmpnt in thisCompo:
285         #         compoString += cmpnt.element + ": " + str(cmpnt.mol) + ", "
286         #     print(compoString)
287
288         # for i in range(len(self.totGarnetMol)):
289         #     print("Total mol of " + self.totGarnetMol[i].element + " = " +
str(self.totGarnetMol[i].mol))
290
291         count += 1
292
293     self.calcTotalGarnetMol()

```

```

294 self.writeScriptFiles(outputDir, count, database)
295 stream = "Stage" + str(count) + ":"
296 print(stream)
297 outFile.write(stream+"\n")
298 stream = str(len(self.garnetList)) + " garnets grown"
299 print(stream)
300 outFile.write(stream+"\n")
301 stream = "Largest radius: " + str(self.garnetList[0].bigAx) + "mm"
302 print(stream)
303 outFile.write(stream+"\n")
304 stream = "Total garnet volume: " + str(self.calcTotVol()) + "mm^3"
305 print(stream)
306 outFile.write(stream+"\n")
307
308 # print("Volumes are:")
309 # for garn in self.garnetList:
310 #     print(garn.totVol)
311 # print("Outer Shell:")
312 # for garn in self.garnetList:
313 #     print(str(garn.composition[0].molFrac) + "," + str(garn.
composition[1].molFrac) + "," + str(garn.composition[2].molFrac) + ","
+ str(garn.composition[3].molFrac))
314
315 # print("Radius:")
316 # for garn in self.garnetList:
317 #     print(garn.bigAx)
318 # print("Mol Sum:")
319 # for garn in self.garnetList:
320 #     thisCompo = garn.getCompoAsComponentMol()
321 #     compoString = ""
322 #     for cmpnt in thisCompo:
323 #         compoString += cmpnt.element + ": " + str(cmpnt.mol) + ", "
324 #     print(compoString)
325 # for i in range(len(self.totGarnetMol)):
326 #     print("Total mol of " + self.totGarnetMol[i].element + " = " +
str(self.totGarnetMol[i].mol))
327
328
329 stream = "Done growing garnets"
330 print(stream)
331 outFile.write(stream)
332 outFile.close()
333 if not memorySave:
334     for num in garnetPlotList:
335         self.plotGarnet(num, outputDir)
336
337 # print("\n\n\n")
338 # print("Verifying garnet sizes:")
339 # for i in range(len(self.crystalList)):
340 #     finalSize = self.garnetList[i].bigAx #+ self.shellThick
341 #     finalVol = (finalSize**3)*(4/3)*math.pi
342
343 #     if finalSize - self.crystalList[i].getDim() > EQ_PARAM:
344 #         print("Garnet " + str(i+1) + " is too big")

```



```

345     #     print("Rad diff = " + str(finalSize- self.crystalList[i].getDim
346         ()))
347     #     print("Vol diff = " + str(finalVol-self.crystalList[i].getVolume
348         ()))
349     #     elif finalSize - self.crystalList[i].getDim() < EQ_PARAM:
350     #         print("Garnet " + str(i + 1) + " is too small")
351     #         print("Rad diff = " + str(self.crystalList[i].getDim()-finalSize
352         ))
353     #         print("Vol diff = " + str(self.crystalList[i].getVolume() -
354         finalVol))
355     #     print("\n")
356
357
358 def growGarnetShell(self, memorySave):
359     #Function to grow an additional shell of garnet
360     #Will add a new garnet once the radius difference between the last
361     garnet and the next one is sufficient
362
363
364     if len(self.garnetList) == 0: #Initialize first garnet
365         firstShellCompo = self.getShellCompo(self.shellThick,0)
366         self.shellCount = 0 #Number of shells in the biggest garnet
367         if len(self.numCrystals) == 0:
368             binNum = 1
369         else:
370             binNum = self.numCrystals[0]
371             self.nucleateGarnet(self.crystalList[0],firstShellCompo,self.
372             shellThick,binNum)
373         # print("Shell Thickness = " + str(self.shellThick))
374         print("First garnet nucleated")
375
376     else:
377         #First calculate the next composition interval
378         biggestRad = self.garnetList[0].bigAx
379
380         #This condition is part of the nucleation parameter
381         #Ensures to only add shellExcess when about to nucleate
382         #This way we can add shellThick to the nucleus and all the crystals
383         and maintain the appropriate
384         #size ratios
385         if(self.shellCount != self.shellsAtNextGr):
386             nextShellRad = biggestRad + self.shellThick
387             thisShellThick = self.shellThick
388         else:
389             nextShellRad = biggestRad + self.shellExcess
390             thisShellThick = self.shellExcess
391
392         nextShellCompo = self.getShellCompo(nextShellRad,biggestRad)
393         #Grow each garnet with composition nextShellCompo and thickness of
394         thisShellThick
395         for i in range(len(self.garnetList)):
396             self.garnetList[i] = self.garnetList[i].growGarnet(nextShellCompo,
397             thisShellThick)
398         if memorySave and self.garnetList[i].nextShell != None:

```

```

390         del self.garnetList[i].nextShell
391
392
393         #This nucleates new garnet when needed:
394         if(self.shellCount > self.shellsAtNextGrt): #This difference
shouldnt be greater than 2
395
396         if len(self.numCrystals) == 0:
397             binNum = 1
398         else:
399             binNum = self.numCrystals[0]
400             self.nucleateGarnet(self.crystalList[len(self.garnetList)],
nextShellCompo, self.shellThick, binNum)
401         if self.shellCount == self.shellsAtNextGrt:
402             # print("self.shellCount == self.shellsAtNextGrt")
403             self.growGarnetShell(memorySave)
404
405
406         self.shellCount +=1
407
408
409     def getShellCompo(self,xHi,xLo):
410         #Gets the average composition of the profile between xHi and xLo and
returns it
411         #As a list of GarnetComponentMols
412         shellCompo = []
413
414         for i in range(len(self.grtProfile.interpComp)):
415             thisProfile = self.grtProfile.interpComp[i]
416             if(xHi <= self.crystalList[0].getDim()):
417                 shellX = (thisProfile(xHi) + thisProfile(xLo))/2
418             else:
419                 shellX = (thisProfile(self.crystalList[0].getDim()) + thisProfile(
xLo))/2
420             shellCompo.append(GarnetComponentMol(GRT_CMPNT[i],shellX))
421         return shellCompo
422
423
424
425     def nucleateGarnet(self, garnetShape,garnetCompo,firstThick,grtsInBin):
426         #Function to nucleate a new garnet with the same aspect ratio of
garnet shape
427
428         rescaleFactor = garnetShape.getDim()/firstThick #Determines the
scaling factor required to maintain the aspect ratio of a garnet with
dimension of shell thickness
429         nucleusShape = garnetShape.getRescale(rescaleFactor)
430
431         nucleus = Garnet(nucleusShape, garnetCompo,numGrt = grtsInBin)
432         if(len(self.garnetList) > 0):
433             lastGrt = len(self.garnetList)-1
434             verifyDiff = self.crystalList[lastGrt].getDim()-self.crystalList[
lastGrt+1].getDim()
435             actualDiff = self.garnetList[lastGrt].bigAx - nucleus.bigAx

```

```

436     # print("Difference should be " + str(verifyDiff) + " is actually "
+ str(actualDiff))
437     #Determine nucleation parameters for NEXT garnet
438     if(len(self.crystalList) > len(self.garnetList)+1):
439         thisGrt = len(self.garnetList)
440
441         nextGrt = thisGrt + 1
442         radDiff = self.crystalList[thisGrt].getDim()-self.crystalList[
nextGrt].getDim()
443         if radDiff >= self.shellThick:
444             self.shellsAtNextGrt= int(radDiff/self.shellThick) + self.
shellCount #This is the number of shells the biggest garnet when the
next garnet nucleates (minus 1)
445             self.shellExcess = radDiff%self.shellThick #This is the thickness
of that extra shell
446         else:
447             while abs(radDiff) <= EQ_PARAM:
448                 #Nucleates all garnets that have the same size
449                 # print("Same radius")
450                 self.garnetList.append(nucleus)
451                 garnetShape = self.crystalList[len(self.garnetList)]
452                 rescaleFactor = garnetShape.getDim()/firstThick #Determines the
scaling factor required to maintain the aspect ratio of a garnet with
dimension of shell thickness
453                 nucleusShape = garnetShape.getRescale(rescaleFactor)
454                 nucleus = Garnet(nucleusShape, garnetCompo,numGrt = grtsInBin)
455
456                 lastGrt = len(self.garnetList)-1
457                 verifyDiff = self.crystalList[lastGrt].getDim()-self.crystalList
[lastGrt+1].getDim()
458                 actualDiff = self.garnetList[lastGrt].bigAx - nucleus.bigAx
459                 # print("Difference should be " + str(verifyDiff) + " is
actually " + str(actualDiff))
460
461                 if(len(self.crystalList) > len(self.garnetList)+1):
462                     thisGrt = len(self.garnetList)
463                     nextGrt = thisGrt + 1
464                     radDiff = self.crystalList[thisGrt].getDim()-self.crystalList[
nextGrt].getDim()
465
466                     self.shellsAtNextGrt= int(radDiff/self.shellThick) + self.
shellCount #This is the number of shells the biggest garnet when the
next garnet nucleates (minus 1)
467                     self.shellExcess = radDiff%self.shellThick #This is the
thickness of that extra shell
468                 else:
469                     self.shellsAtNextGrt = NUM_SHELLS + len(self.garnetList) + 1 #
Makes sure no more nucleation occurs
470                     self.shellExcess = 0
471                     radDiff = sys.float_info.max
472                 while radDiff < nucleus.bigAx:
473                     #For instances when the difference between this garnet and the
next is smaller than the thickness of the shell
474                     #Nucleates the next garnet with a smaller initial shell size

```

```

475         #pdb.set_trace()
476         # print("Nucleus radius = " + str(nucleus.bigAx))
477         # print("Next garnet radius difference = " + str(radDiff))
478
479         self.garnetList.append(nucleus)
480         firstThick = nucleus.bigAx - radDiff
481         # print("Nucleus radius = " + str(firstThick))
482         garnetShape = self.crystalList[len(self.garnetList)]
483         rescaleFactor = garnetShape.getDim()/firstThick #Determines the
scaling factor required to maintain the aspect ratio of a garnet with
dimension of shell thickness
484         nucleusShape = garnetShape.getRescale(rescaleFactor)
485         nucleus = Garnet(nucleusShape, garnetCompo,numGrt = grtsInBin)
486
487         lastGrt = len(self.garnetList)-1
488         verifyDiff = self.crystalList[lastGrt].getDim()-self.crystalList
[lastGrt+1].getDim()
489         actualDiff = self.garnetList[lastGrt].bigAx - nucleus.bigAx
490         # print("Difference should be " + str(verifyDiff) + " is
actually " + str(actualDiff))
491
492         if(len(self.crystalList) > len(self.garnetList)+1):
493             thisGrt = len(self.garnetList)
494             nextGrt = thisGrt + 1
495             radDiff = self.crystalList[thisGrt].getDim()-self.crystalList[
nextGrt].getDim()
496             # print("Next garnet radius difference = " + str(radDiff))
497             self.shellsAtNextGrt= int((radDiff-firstThick)/self.shellThick
) + self.shellCount + 1#This is the number of shells the biggest garnet
when the next garnet nucleates (minus 1)
498             self.shellExcess = (radDiff-firstThick)%self.shellThick #This
is the thickness of that extra shell
499         else:
500             self.shellsAtNextGrt = NUM_SHELLS + len(self.garnetList) + 1 #
Makes sure no more nucleation occurs
501             self.shellExcess = 0
502             radDiff = sys.float_info.max
503             # print("ShellCount = " + str(self.shellCount))
504             # print("ShellsAtNextGrt = " + str(self.shellsAtNextGrt))
505             # print("\n")
506         else:
507             self.shellsAtNextGrt = NUM_SHELLS + len(self.garnetList) + 1 #Makes
sure no more nucleation occurs
508             self.shellExcess = 0
509
510
511         self.garnetList.append(nucleus)
512
513
514
515     def calcTotalGarnetMol(self):
516         #Calculate total mols of all garnet components
517         #This will return an array of ComponentMol not GarnetComponentMol
518         self.totGarnetMol = copy.deepcopy(self.garnetList[0]).

```

```

getCompoAsComponentMol()) #Get the composition of the first garnet
519
520
521     for i in range(1,len(self.garnetList)):
522         #Add each garnet composition to totGarnetMol
523
524         thisGarnetCompo = self.garnetList[i].getCompoAsComponentMol()
525         self.totGarnetMol = addComponentList(self.totGarnetMol,
thisGarnetCompo)
526
527
528
529
530 def writeScriptFiles(self, thisDir, fracStep, database):
531     #Write script files for the current composition
532     #For isopleths, it uses the composition of the next biggest shell
533
534     #First get the composition of the next shell, this is what will be
written into the script file
535     if len(self.garnetList) == 0:
536         biggestRad = 0
537         currComposition = self.composition
538     else:
539         biggestRad = self.garnetList[0].bigAx
540         currComposition = subComponentList(self.composition, self.
totGarnetMol)
541         nextShellRad = biggestRad + self.shellThick
542         if nextShellRad > self.crystalList[0].getDim():
543             nextShellRad = self.crystalList[0].getDim()
544         nextShellCompo = self.getShellCompo(nextShellRad,biggestRad)
545
546
547         # print("Total Composition:")
548         # compoString = ""
549         # for cmpnt in self.composition:
550         #     compoString += cmpnt.element + ": " + str(cmpnt.mol) + ", "
551         # print(compoString)
552         # compoString = ""
553         # print("After removal of garnet:")
554         # for cmpnt in currComposition:
555         #     compoString += cmpnt.element + ": " + str(cmpnt.mol) + ", "
556         # print(compoString)
557
558         iterName = self.name + '_Stage{:02d}'.format(fracStep)
559         #Generate the therin composition string
560         therin = ""
561         for i in range(len(currComposition)):
562             if currComposition[i].mol < 0:
563                 currComposition[i].mol = 0
564             therin += currComposition[i].element.upper() + "({:7.6f})".format(
currComposition[i].mol)
565
566         phaseScript(therin,self.P1,self.P2,self.T1,self.T2,iterName,thisDir,
database)

```

```

567
568 #Now generate the isopleth script files
569 for i in range(len(nextShellCompo)):
570     componentName = nextShellCompo[i].endMember
571     targetCompo = nextShellCompo[i].molFrac
572     #Calculate range of mol fraction +/- 10% of the target composition
573     compoStep = round_sig(targetCompo*0.05)
574     compoStart = round_sig(targetCompo - 2*compoStep)
575     compoEnd = round_sig(targetCompo + 2*compoStep)
576     isoScript(therin, self.P1, self.P2, self.T1, self.T2, iterName,
thisDir, database, "GARNET", componentName, compoStart, compoEnd,
compoStep)
577
578 def getAvgEllipsoid(self, blobIn):
579     #Takes the blobIn as a pandas table
580     #Average the aspect ratios of all the ellipsoids and returns the
average ellipsoid
581     #This way we can work with a "standardized" ellipsoid that grows the
same way for every garnet
582     rad1 = blobIn['PEllipsoid Rad1 (mm)'].to_numpy()
583     rad2 = blobIn['PEllipsoid Rad2 (mm)'].to_numpy()
584     rad3 = blobIn['PEllipsoid Rad3 (mm)'].to_numpy()
585
586     #ratio12 = rad1/rad2 ratio23 = rad2/rad3 ratio12*ratio23 = rad1/rad3
587     ratio12 = rad1/rad2
588     ratio23 = rad2/rad3
589
590     avgR12 = np.average(ratio12)
591     avgR23 = np.average(ratio23)
592
593     #Volume of ellipsoid doesnt matter so set rad3 = 1
594     modelR2 = avgR23
595     modelR1 = avgR12*modelR2
596     modelEllip = Ellipsoid(modelR1,modelR2,1)
597
598     return modelEllip
599
600
601 def plotGarnet(self, grtNum, saveDir):
602     #Plots an individual garnet composition
603     #Will plot mol fraction (fracAx), mols (molAx), and volume (volAx)
604     #Wont show the plot right away so that multiple garnets can be shown
at the same time
605
606     thisGrt = self.garnetList[grtNum]
607     thisCompo = thisGrt.getProfileComp()
608     thisX = thisGrt.getProfileX()
609     thisVol = thisGrt.getProfileVol()
610
611     if len(thisX) == len(thisCompo): #verify these operations were
performed correctly when retrieving the values
612         fracList = []
613         molList = []
614         for elem in GRT_CMPNT:

```



```

615         fracList.append([])
616         molList.append([])
617     for i in range (len(thisCompo)):
618
619
620         for j in range(len(thisCompo[i])):
621
622             fracList[j].append(thisCompo[i][j].molFrac)
623             molList[j].append(thisCompo[i][j].mol)
624
625     thisFig =plt.figure(figsize =(16,10))
626     figName = "Garnet" + str(grtNum+1)
627
628     thisFig.suptitle(figName, fontsize=16)
629
630     fracAx = thisFig.add_subplot(311)
631     colours = ['green','blue','orange','red']
632
633     #Set xlimit of every plot to the size of the biggest garnet, so it
is easier to compare
634     biggestRad = self.garnetList[0].bigAx
635     fracAx.set_xlim(0,biggestRad)
636
637     fracAlm = fracAx.twinx()
638
639     fracAx.set_xlabel("x (mm)")
640     fracAx.set_ylabel("X (Ca,Mn,Mg)")
641
642     fracAlm.set_ylabel("X (Fe)")
643
644     molAx = thisFig.add_subplot(312)
645     molAx.set_xlim(0,biggestRad)
646     molAlm = molAx.twinx()
647
648     molAx.set_xlabel("x (mm)")
649     molAx.set_ylabel("mol (Ca,Mn,Mg)")
650     molAlm.set_ylabel("mol (Fe)")
651
652     volAx = thisFig.add_subplot(313)
653     volAx.set_xlim(0,biggestRad)
654     volAx.set_xlabel("x (mm)")
655     volAx.set_ylabel("Shell Volume (mm$^3$)")
656
657
658     #Plot each interpolated profile
659     for i in range(len(GRT_CMPNT)):
660         pltColour = colours[i]
661         yFrac = fracList[i]
662         yMol = molList[i]
663         xComp = thisX
664         if(GRT_CMPNT[i] == ALM):
665             fracAlm.plot(xComp, yFrac, color = pltColour, marker = 'None',
linestyle = "-", markersize = 7, linewidth = 1, label = GRT_CMPNT[i].
cation)

```

```

666         molAlm.plot(xComp, yMol, color = pltColour, marker = 'None',
        linestyle = "-", markersize = 7, linewidth = 1, label = GRT_CMPNT[i].
        cation)
667     else:
668         fracAx.plot(xComp, yFrac, color = pltColour, marker = 'None',
        linestyle = "-", markersize = 7, linewidth = 1, label = GRT_CMPNT[i].
        cation)
669         molAx.plot(xComp, yMol, color = pltColour, marker = 'None',
        linestyle = "-", markersize = 7, linewidth = 1, label = GRT_CMPNT[i].
        cation)
670
671     volAx.plot(thisX, thisVol, color = 'black', marker = 'None',
        linestyle = '-', markersize = 7, linewidth = 1, label = "Volume")
672
673     fracAx.legend(fontsize = 14, loc = 'upper left')
674     fracAlm.legend(fontsize = 14, loc = 'upper right')
675     molAx.legend(fontsize = 14, loc = 'upper left')
676     molAlm.legend(fontsize = 14, loc = 'upper right')
677
678     figName += ".svg"
679     thisFig.show()
680     thisFig.savefig(saveDir + figName)
681 else:
682     print("Error with plotting garnet compositions")
683
684 def calcTotVol(self):
685     #Returns the total volume of garnet so far
686
687     totVolCSD = 0
688     for grt in self.garnetList:
689         totVolCSD += grt.totVol*grt.numGrt
690
691     return totVolCSD
692
693
694
695 def round_sig(x, sig=3):
696     return round(x, sig-int(math.floor(math.log10(abs(x))))-1)

```

Script_Generator.py

```

1 #SCRIPT_Generator.py
2 #Possible future direction, copy a script file as a template?
3 #For now, more methods can be added or these ones can be changed to fit
  with what you need
4 #Note that \n makes a newline, this set up works for me but I dont know
  what
5 #THERIN_Generator.py has these two methods implemented to automatically
  generate these files
6 #from a csv file of wt% compositions.
7
8 #This method creates a script file that will calculate the phase
  assemblages
9 def phaseScript(compoLine, P1, P2, T1, T2, sample, fileLoc, database):

```

```

10  fileName = sample + "_Phase"
11  writeFile = fileLoc + fileName + ".txt"#Full filepath
12  #This portion just ensures that the file can be made
13  try:
14      writeFile = open(writeFile, 'w')
15  except:
16      print('Problem creating new file')
17      exit(0)
18
19  writeFile.write("script." + fileName + ".txt\n")
20  writeFile.write(fileName + ".plt\n" + database + "\n")
21  writeFile.write("    1.0000    300    0.010000    0.1000000E-08
0.1000000E-08    0.1000000E+01 0.1000000E-03    400    400    500\n")#
22  These values are used instead of those of theriak.ini compare to that
23  to see what each one is
24  writeFile.write("0      " + compoLine + "          *\n\n\n\n\n\n\n")
25  writeFile.write("TC  " + str(T1) + "    " + str(T2) + "\n")
26  writeFile.write("P   " + str(P1) + "    " + str(P2) + "\n\n1\n 0.0000000
E+00    0.0000000E+00\n")
27  writeFile.write("_"+ fileName + "_pix")
28  writeFile.close()
29  domjob(fileName, fileLoc)
30  scriptList(fileName, fileLoc)
31
32  #This method will create a script file that will calculate the phase
33  isopleths for
34  #whichever endmember entered in to the field endMem.
35  #Note to self: Edit this in future to use any mineral
36  def isoScript(compoLine, P1, P2, T1, T2, sample, fileLoc, database, phase,
endMem, minVal, maxVal, interval):
37      fileName = sample + "_" + endMem
38      writeFile = fileLoc + fileName + ".txt"
39      try:
40          writeFile = open(writeFile, 'w')
41      except:
42          print('Problem creating new file')
43          exit(0)
44
45      writeFile.write("script." + fileName + ".txt\n")
46      writeFile.write(fileName + ".plt\n" + database + "\n")
47      writeFile.write("    1.0000    300    0.010000    0.1000000E-08
0.1000000E-08    0.1000000E+01 0.1000000E-03    400    400    500\n")#
48  Not sure what these numbers mean
49  writeFile.write("0      " + compoLine + "          *\n\n\n\n\n\n\n")
50  writeFile.write("TC  " + str(T1) + "    " + str(T2) + "\n")
51  writeFile.write("P   " + str(P1) + "    " + str(P2) + "\n")
52  writeFile.write(phase + "    " + endMem + "    1" + "    " + str(minVal) + "
" + str(maxVal) + "    " + str(interval) + "\n\n1\n 0.0000000E+00
0.0000000E+00\n")
53  writeFile.write("_"+ fileName + "_pix")
54  writeFile.close()
55  domjob(fileName, fileLoc)
56  scriptList(fileName, fileLoc)

```

```

54 #Generate a script for volume% of a specific phase
55 def volScript(compoLine, P1, P2, T1, T2, sample, fileLoc, database, phase,
    minVal, maxVal, interval):
56     fileName = sample + "_vol"
57     writeFile = fileLoc + fileName + ".txt"
58     try:
59         writeFile = open(writeFile, 'w')
60     except:
61         print('Problem creating new file')
62         exit(0)
63
64     writeFile.write("script." + fileName + ".txt\n")
65     writeFile.write(fileName + ".plt\n" + database + "\n")
66     writeFile.write("    1.0000    300    0.010000    0.1000000E-08
0.1000000E-08    0.1000000E+01 0.1000000E-03    400    400    500\n")#
    Not sure what these numbers mean
67     writeFile.write("0      " + compoLine + "      *\n\n\n\n\n\n\n")
68     writeFile.write("TC      " + str(T1) + "      " + str(T2) + "\n")
69     writeFile.write("P      " + str(P1) + "      " + str(P2) + "\n")
70     writeFile.write(phase + "    vol%" + "    1" + "      " + str(minVal) + "      " +
    str(maxVal) + "      " + str(interval) + "\n1\n 0.0000000E+00    0.0000000E
+00\n")
71     writeFile.write("_" + fileName + "_pix")
72     writeFile.close()
73     domjob(fileName, fileLoc)
74     scriptList(fileName, fileLoc)
75
76
77 #Method to write to domjob file
78 #Probably need to edit a domino made domjob file but whatever
79 def domjob(fileName, filepath):
80     writeFile = filepath + "domjob.txt"
81     try:
82         writeFile = open(writeFile, 'a')
83     except:
84         print('Problem creating new file')
85         exit(0)
86     writeFile.write("domino      " + fileName + ".txt\n")
87     writeFile.write("guzzler      " + fileName + ".plt      " + fileName + ".cln      "
    + fileName + ".rxn\n")
88     writeFile.write("exploit      " + fileName + ".cln      " + fileName + ".ps\n")
89     writeFile.close()
90
91 def scriptList(fileName, filepath):
92     #Method for writing a list of the scripts, for use with bash scripts
93     writeFile = filepath + "scriptList.txt"
94     try:
95         writeFile = open(writeFile, 'a')
96     except:
97         print('Problem creating new file')
98         exit(0)
99     writeFile.write(fileName + "\n")
100    writeFile.close()

```

E. EBRC calculated with G_FFRAC

Table E.1: 18ZE-R-11A G.FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	1.3679	0.5166	0.1690	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	0
1	1.3679	0.5166	0.1690	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	7.163E-03
2	1.3679	0.5166	0.1690	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	6.600E-02
3	1.3678	0.5166	0.1690	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	2.696E-01
4	1.3678	0.5166	0.1690	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	8.070E-01
5	1.3678	0.5166	0.1690	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	2.004E+00
6	1.3677	0.5165	0.1689	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	4.542E+00
7	1.3676	0.5165	0.1689	0.0035	0.1052	0.0269	0.0434	0.0668	0.0189	9.758E+00
8	1.3673	0.5163	0.1689	0.0034	0.1052	0.0268	0.0434	0.0668	0.0189	1.953E+01
9	1.3669	0.5160	0.1684	0.0034	0.1052	0.0267	0.0434	0.0668	0.0189	3.642E+01
10	1.3662	0.5155	0.1680	0.0033	0.1051	0.0266	0.0434	0.0668	0.0189	6.384E+01
11	1.3651	0.5148	0.1672	0.0032	0.1051	0.0263	0.0434	0.0668	0.0189	1.056E+02
12	1.3635	0.5137	0.1662	0.0031	0.1050	0.0260	0.0434	0.0668	0.0189	1.670E+02
13	1.3613	0.5122	0.1646	0.0030	0.1049	0.0256	0.0434	0.0668	0.0189	2.532E+02
14	1.3582	0.5102	0.1624	0.0029	0.1047	0.0251	0.0434	0.0668	0.0189	3.704E+02
15	1.3542	0.5075	0.1595	0.0028	0.1044	0.0243	0.0434	0.0668	0.0189	5.251E+02
16	1.3490	0.5041	0.1558	0.0026	0.1041	0.0233	0.0434	0.0668	0.0189	7.240E+02
17	1.3425	0.4997	0.1511	0.0025	0.1037	0.0219	0.0434	0.0668	0.0189	9.755E+02
18	1.3344	0.4943	0.1454	0.0022	0.1033	0.0203	0.0434	0.0668	0.0189	1.286E+03
19	1.3245	0.4877	0.1385	0.0019	0.1027	0.0183	0.0434	0.0668	0.0189	1.666E+03
20	1.3134	0.4803	0.1305	0.0016	0.1019	0.0163	0.0434	0.0668	0.0189	2.091E+03

Table E.2: 18ZE-R-14A G_FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	1.34315	0.56023	0.22918	0.00347	0.07789	0.04678	0.22542	0.03786	0.02454	0
1	1.34315	0.56023	0.22918	0.00347	0.07788	0.04678	0.22542	0.03786	0.02454	3.987E-02
2	1.34314	0.56023	0.22917	0.00347	0.07788	0.04678	0.22542	0.03786	0.02454	5.048E-01
3	1.34308	0.56019	0.22915	0.00346	0.07788	0.04676	0.22542	0.03786	0.02454	2.526E+00
4	1.34290	0.56007	0.22904	0.00342	0.07788	0.04671	0.22542	0.03786	0.02454	9.586E+00
5	1.34236	0.55971	0.22870	0.00337	0.07787	0.04658	0.22542	0.03786	0.02454	3.050E+01
6	1.34092	0.55875	0.22769	0.00328	0.07783	0.04628	0.22542	0.03786	0.02454	8.599E+01
7	1.33739	0.55639	0.22504	0.00318	0.07771	0.04563	0.22542	0.03786	0.02454	2.224E+02
8	1.32966	0.55124	0.21900	0.00310	0.07736	0.04436	0.22542	0.03786	0.02454	5.212E+02
9	1.31472	0.54128	0.20710	0.00305	0.07661	0.04213	0.22542	0.03786	0.02454	1.099E+03
10	1.28878	0.52399	0.18656	0.00299	0.07521	0.03819	0.22542	0.03786	0.02454	2.101E+03
11	1.24900	0.49747	0.15544	0.00291	0.07295	0.03186	0.22542	0.03786	0.02454	3.636E+03

Table E.3: 18ZE-R-14B G-FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	0.59709	0.19326	0.05928	0.00160	0.03660	0.02301	0.06964	0.01314	0.00558	0
1	0.59709	0.19326	0.05928	0.00160	0.03660	0.02301	0.06964	0.01314	0.00558	4.166E-03
2	0.59709	0.19326	0.05928	0.00160	0.03660	0.02301	0.06964	0.01314	0.00558	3.856E-02
3	0.59709	0.19326	0.05928	0.00160	0.03660	0.02301	0.06964	0.01314	0.00558	1.717E-01
4	0.59708	0.19325	0.05927	0.00160	0.03660	0.02300	0.06964	0.01314	0.00558	5.600E-01
5	0.59705	0.19324	0.05926	0.00159	0.03660	0.02300	0.06964	0.01314	0.00558	1.520E+00
6	0.59699	0.19320	0.05922	0.00159	0.03660	0.02298	0.06964	0.01314	0.00558	3.898E+00
7	0.59684	0.19310	0.05912	0.00158	0.03659	0.02295	0.06964	0.01314	0.00558	9.567E+00
8	0.59650	0.19287	0.05889	0.00156	0.03657	0.02287	0.06964	0.01314	0.00558	2.292E+01
9	0.59573	0.19236	0.05838	0.00152	0.03653	0.02270	0.06964	0.01314	0.00558	5.213E+01
10	0.59423	0.19136	0.05735	0.00145	0.03644	0.02239	0.06964	0.01314	0.00558	1.097E+02
11	0.59157	0.18958	0.05551	0.00135	0.03627	0.02183	0.06964	0.01314	0.00558	2.118E+02
12	0.58732	0.18675	0.05257	0.00123	0.03600	0.02092	0.06964	0.01314	0.00558	3.747E+02

Table E.4: 18ZE-R-14C G_FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	0.5736	0.43059	0.12899	0.00186	0.02574	0.03262	0.0621	0.0654	0.02013	0
1	0.57359	0.43059	0.12899	0.00186	0.02574	0.03262	0.0621	0.0654	0.02013	1.140E-01
2	0.57357	0.43057	0.12898	0.00186	0.02574	0.03261	0.0621	0.0654	0.02013	1.194E+00
3	0.57344	0.43049	0.12889	0.00185	0.02574	0.03259	0.0621	0.0654	0.02013	6.073E+00
4	0.57301	0.4302	0.12861	0.00181	0.02573	0.03249	0.0621	0.0654	0.02013	2.256E+01
5	0.57195	0.42949	0.12788	0.00174	0.02571	0.03225	0.0621	0.0654	0.02013	6.355E+01
6	0.56974	0.42802	0.12632	0.00164	0.02565	0.03176	0.0621	0.0654	0.02013	1.488E+02
7	0.56559	0.42526	0.1233	0.00152	0.02554	0.03086	0.0621	0.0654	0.02013	3.088E+02
8	0.55842	0.42047	0.11794	0.0014	0.02532	0.02938	0.0621	0.0654	0.02013	5.858E+02
9	0.54685	0.41276	0.10925	0.00132	0.02494	0.02697	0.0621	0.0654	0.02013	1.032E+03
10	0.52927	0.40104	0.096	0.00128	0.02426	0.02336	0.0621	0.0654	0.02013	1.710E+03
11	0.50408	0.38425	0.07708	0.00123	0.02314	0.01826	0.0621	0.0654	0.02013	2.680E+03
12	0.47468	0.36465	0.05505	0.00117	0.02151	0.01258	0.0621	0.0654	0.02013	3.811E+03

Table E.5: 18ZE-R-16 G_FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	0.83752	0.38104	0.11669	0.00259	0.08746	0.04332	0.07286	0.09325	0.01073	0
1	0.83752	0.38104	0.11669	0.00259	0.08746	0.04332	0.07286	0.09325	0.01073	5.608E-02
2	0.8375	0.38103	0.11668	0.00259	0.08746	0.04332	0.07286	0.09325	0.01073	6.255E-01
3	0.83744	0.38098	0.11665	0.00257	0.08746	0.0433	0.07286	0.09325	0.01073	3.230E+00
4	0.83723	0.38084	0.11655	0.00252	0.08745	0.04325	0.07286	0.09325	0.01073	1.128E+01
5	0.83674	0.38052	0.11631	0.00242	0.08743	0.04312	0.07286	0.09325	0.01073	2.980E+01
6	0.83581	0.3799	0.11583	0.00224	0.0874	0.04288	0.07286	0.09325	0.01073	6.550E+01
7	0.83422	0.37884	0.11496	0.00199	0.08734	0.04247	0.07286	0.09325	0.01073	1.265E+02
8	0.83172	0.37717	0.11354	0.00169	0.08722	0.04181	0.07286	0.09325	0.01073	2.219E+02
9	0.82806	0.37473	0.11128	0.00135	0.08699	0.04098	0.07286	0.09325	0.01073	3.620E+02
10	0.82454	0.37239	0.10905	0.00109	0.08675	0.04019	0.07286	0.09325	0.01073	4.965E+02

Table E.6: 18ZE-R-77A G_FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	1.45726	0.444	0.2043	0.00246	0.08421	0.02963	0.08156	0.10673	0.01422	0
1	1.45726	0.44399	0.2043	0.00246	0.08421	0.02963	0.08156	0.10673	0.01422	7.474E-02
2	1.45724	0.44398	0.20429	0.00246	0.08421	0.02962	0.08156	0.10673	0.01422	9.292E-01
3	1.45714	0.44391	0.20423	0.00245	0.0842	0.0296	0.08156	0.10673	0.01422	4.705E+00
4	1.45684	0.44371	0.20405	0.00241	0.0842	0.02952	0.08156	0.10673	0.01422	1.629E+01
5	1.45606	0.44319	0.20356	0.00234	0.08417	0.02932	0.08156	0.10673	0.01422	4.634E+01
6	1.45424	0.44198	0.20239	0.00219	0.08412	0.02888	0.08156	0.10673	0.01422	1.161E+02
7	1.45046	0.43946	0.19985	0.00198	0.08399	0.02797	0.08156	0.10673	0.01422	2.615E+02
8	1.44332	0.4347	0.19487	0.00173	0.08373	0.02634	0.08156	0.10673	0.01422	5.361E+02
9	1.43105	0.42652	0.18603	0.00147	0.0832	0.02368	0.08156	0.10673	0.01422	1.008E+03
10	1.4114	0.41342	0.17142	0.00127	0.08195	0.0201	0.08156	0.10673	0.01422	1.764E+03
11	1.3838	0.39502	0.15037	0.00108	0.07943	0.01625	0.08156	0.10673	0.01422	2.823E+03

Table E.7: 18ZE-R-81 G_FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	0.89603	0.34442	0.1204	0.00177	0.08904	0.06416	0.09412	0.04359	0.01189	0
1	0.89603	0.34442	0.1204	0.00177	0.08904	0.06416	0.09412	0.04359	0.01189	3.321E-02
2	0.89602	0.34441	0.12039	0.00177	0.08904	0.06416	0.09412	0.04359	0.01189	2.669E-01
3	0.896	0.3444	0.12038	0.00177	0.08903	0.06416	0.09412	0.04359	0.01189	9.297E-01
4	0.89596	0.34438	0.12035	0.00177	0.08903	0.06416	0.09412	0.04359	0.01189	2.448E+00
5	0.89588	0.34432	0.12029	0.00177	0.08901	0.06415	0.09412	0.04359	0.01189	5.630E+00
6	0.89571	0.34421	0.12017	0.00176	0.08899	0.06413	0.09412	0.04359	0.01189	1.202E+01
7	0.89538	0.34399	0.11994	0.00175	0.08894	0.06409	0.09412	0.04359	0.01189	2.454E+01
8	0.89472	0.34355	0.11947	0.00174	0.08884	0.06402	0.09412	0.04359	0.01189	4.984E+01
9	0.89319	0.34253	0.1184	0.0017	0.08861	0.06383	0.09412	0.04359	0.01189	1.078E+02
10	0.8893	0.33993	0.11568	0.00162	0.08796	0.06339	0.09412	0.04359	0.01189	2.554E+02
11	0.87911	0.33314	0.10861	0.00144	0.086	0.0624	0.09412	0.04359	0.01189	6.405E+02
12	0.85405	0.31643	0.09075	0.00088	0.08093	0.06083	0.09412	0.04359	0.01189	1.589E+03
13	0.85084	0.3143	0.08845	0.00079	0.0803	0.06065	0.09412	0.04359	0.01189	1.711E+03

Table E.8: 18ZE-R-49B G-FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	0.85093	0.47616	0.13958	0.00065	0.06025	0.00424	0.02056	0.12594	0.01333	0
1	0.85093	0.47616	0.13958	0.00065	0.06025	0.00424	0.02056	0.12594	0.01333	7.277E-03
2	0.85093	0.47616	0.13958	0.00065	0.06025	0.00424	0.02056	0.12594	0.01333	7.540E-02
3	0.85092	0.47615	0.13958	0.00065	0.06025	0.00424	0.02056	0.12594	0.01333	3.335E-01
4	0.8509	0.47614	0.13956	0.00065	0.06025	0.00424	0.02056	0.12594	0.01333	9.650E-01
5	0.85087	0.47612	0.13954	0.00064	0.06025	0.00424	0.02056	0.12594	0.01333	2.207E+00
6	0.85082	0.47608	0.13949	0.00064	0.06024	0.00424	0.02056	0.12594	0.01333	4.350E+00
7	0.85073	0.47602	0.13942	0.00064	0.06023	0.00423	0.02056	0.12594	0.01333	7.713E+00
8	0.8506	0.47594	0.13931	0.00064	0.06021	0.00423	0.02056	0.12594	0.01333	1.267E+01
9	0.85042	0.47582	0.13916	0.00063	0.06019	0.00422	0.02056	0.12594	0.01333	1.973E+01
10	0.85016	0.47565	0.13895	0.00063	0.06016	0.00422	0.02056	0.12594	0.01333	2.950E+01
11	0.84982	0.47542	0.13867	0.00062	0.06012	0.00421	0.02056	0.12594	0.01333	4.264E+01
12	0.84938	0.47512	0.1383	0.00061	0.06006	0.0042	0.02056	0.12594	0.01333	5.995E+01
13	0.84879	0.47473	0.13782	0.0006	0.05999	0.00418	0.02056	0.12594	0.01333	8.232E+01
14	0.84806	0.47425	0.13722	0.00058	0.05989	0.00416	0.02056	0.12594	0.01333	1.106E+02
15	0.84714	0.47363	0.13646	0.00057	0.05977	0.00414	0.02056	0.12594	0.01333	1.459E+02
16	0.84602	0.47288	0.13553	0.00055	0.05963	0.00411	0.02056	0.12594	0.01333	1.893E+02
17	0.84465	0.47197	0.1344	0.00053	0.05944	0.00408	0.02056	0.12594	0.01333	2.419E+02
18	0.84301	0.47088	0.13305	0.0005	0.05922	0.00403	0.02056	0.12594	0.01333	3.050E+02
19	0.84107	0.46958	0.13147	0.00047	0.05896	0.00397	0.02056	0.12594	0.01333	3.797E+02
20	0.83879	0.46806	0.12964	0.00045	0.05864	0.00385	0.02056	0.12594	0.01333	4.674E+02
21	0.83613	0.46629	0.12751	0.00042	0.05828	0.00372	0.02056	0.12594	0.01333	5.693E+02
22	0.83308	0.46425	0.12504	0.00038	0.05789	0.00357	0.02056	0.12594	0.01333	6.869E+02
23	0.8296	0.46194	0.12216	0.00029	0.05755	0.0034	0.02056	0.12594	0.01333	8.214E+02
24	0.82917	0.46165	0.1218	0.00028	0.05751	0.00338	0.02056	0.12594	0.01333	8.381E+02

Table E.9: 18ZE-R-71 G_FRAC output

G_FRAC Stage	Si	Al	Fe	Mn	Mg	Ca	Na	K	Ti	Garnet removed (mm ³)
0	1.97313	0.41788	0.19245	0.0038	0.06339	0.02671	0.02729	0.23346	0.01008	0
1	1.97312	0.41788	0.19245	0.0038	0.06339	0.02671	0.02729	0.23346	0.01008	1.87E-01
2	1.97306	0.41784	0.1924	0.0038	0.06339	0.0267	0.02729	0.23346	0.01008	2.45E+00
3	1.97282	0.41767	0.19221	0.00378	0.06338	0.02667	0.02729	0.23346	0.01008	1.19E+01
4	1.97209	0.41719	0.19165	0.00375	0.06334	0.02659	0.02729	0.23346	0.01008	4.02E+01
5	1.97016	0.41591	0.19015	0.00365	0.06324	0.02635	0.02729	0.23346	0.01008	1.15E+02
6	1.96555	0.41283	0.18653	0.00346	0.06301	0.02578	0.02729	0.23346	0.01008	2.94E+02
7	1.9556	0.40619	0.17868	0.00311	0.06247	0.02457	0.02729	0.23346	0.01008	6.79E+02
8	1.9365	0.39346	0.16364	0.00248	0.06135	0.02226	0.02729	0.23346	0.01008	1.42E+03
9	1.90362	0.37154	0.13791	0.0014	0.0592	0.01833	0.02729	0.23346	0.01008	2.69E+03
10	1.86688	0.34705	0.10944	0.00027	0.05642	0.01398	0.02729	0.23346	0.01008	4.11E+03