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# Equilibrium thermodynamics of the Lyell Highway eclogites

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*Abstract*

One sample of the Lyell Highway eclogite and one sample of the enclosing aluminous schist have been studied using equilibrium thermodynamics (Powell and Holland 1988). The resultant average P-T estimate of both cores and rims in the eclogite is very well constrained at 15.2 ± 1.05 kb and 698 ± 28°C. However, only one rim assemblage of the enclosing schist was in equilibrium and gave a pressure estimate of 16.4 ± 1.3 kb (at 700°C). These estimates are consistent with those of Kamperman (1984) derived by traditional geothermometers and geobarometers. Close correlation between P estimates in eclogite and the enclosing schist suggests their juxtaposition prior to the peak of metamorphism. Rim assemblages equilibrated at only slightly higher temperatures than cores (difference of 11–21°C). In contrast to Kamperman (1984), a small decrease in P from core to rim is recorded, but this is not considered a significant P-T vector indicator.

## INTRODUCTION

Eclogites occur on the Lyell Highway at approximately 145° 52', 042° 08', as metre scale elongate pods (boudins?) enclosed by Precambrian aluminous schists. The petrology of both the eclogite and enclosing schist is described in detail by Kamperman (1984). In summary, the eclogite is basaltic with chemical affinities to island arc basalt and is thought to have origionally been lava flows (Kamperman, 1984). No igneous textures are preserved; the rocks now have a granoblastic texture of:

garnet - omphacitic clinopyroxene - amphibole -
phengite - quartz ± K-feldspar

Minor phases include; rutile and zoisite. Secondary phases include; biotite, amphibole, chlorite, albite and pyrrhotite-pyrite. Aluminous schists have meta-sedimentary origins and consist of;

garnet - phengite - quartz - biotite ±
albite ± kyanite ± tourmaline

Accessories include zircon, apatite and graphite. Secondary phases include biotite and chlorite. Only one eclogite sample (67644) and one aluminous schist sample (67662) sufficiently preserve their equilibrium mineral compositions to derive P-T estimates by equilibrium thermodynamics.

## EQUILIBRIUM THERMODYNAMICS: METHOD

Average P-T calculations from assemblages in chemical equilibrium are derived by the method outlined by Powell and Holland (1988). For the background theory on equilibrium thermodynamics refer to Powell (1978) and Powell and Holland (1985). For a chosen chemical system, the P-T calculations involve identifying all balanced independent reactions which can be drawn between the specified mineral end-members in the rock studied (i.e. Table 5). These reactions are localised in P-T space by satisfying the equilibrium relationship:

$$\Delta G^\circ + RT \ln K = 0$$

For each reaction, $\Delta G^\circ$ is calculated for different P-T estimates using the thermodynamic properties of each end-member. This method employs the internally consistent thermodynamic data set developed by Holland and Powell (1985). A much expanded version of this thermodynamic data set (Holland and Powell, 1990) has been used in this study. All calculations were performed using the 1990 version of the program THERMOCALC v1.2 (Powell and Holland, pers. comm. 1990). The uncertainties on activities used in this study are as recommended by Powell and Holland (1988).

Mineral analyses used in this report are those presented by Kamperman (1984) (Table 1) and recalculated using the program RECALC (Powell, pers. comm., 1990). Methods of calculation of mineral end-member activities are contained in Appendix 2. All eclogite assemblages and the schist assemblage used in this study had sufficient end-members (11–12) within the $CaO$-$K_2O$-$Na_2O$-$FeO$-$MgO$-$Al_2O_3$-$SiO_2$-$H_2O$ system to define 3 to 4 independent reactions (Table 5). The intersection of these independent reactions (with an error of ± 2 kb) define a band of average P estimates in P-T space (Table 2). Similarly a band of average T estimates in P-T space is defined, using an error of 40°C for each independent reaction (Table 3). The average P and average T bands are plotted in Figure 1. Intersection of average P and average T bands give rise to the average P-T loci (Table 4 and fig. 1). Only samples that satisfy the chi squared test (where no outliers are used in the average, i.e. $f<1.6$) are presented in this report.

## RESULTS

The independent reactions used to define the average pressure and average temperature bands in eclogite assemblages are listed in Table 5. Results of calculations defining the $P_{ave}$ and $T_{ave}$ bands are contained in Tables 2 and 3 and plotted in Figure 1. The average of all core and rim pressure estimates at 700°C in the eclogite sample is 15.2 ± 1.05 kb. Pressure estimates from rim analyses are up to 0.6 kb lower than core pressures. The average of all core and rim T estimates (at 15 kb) is 698 ± 28°C. Average P-T loci are contained in Table 4 and plotted in Figure 1. Average P-T loci for all cores is 15.6 ± 1.5 kb, 704 ± 39°C and for all rims is 15.2 ± 1.4 kb, 710 ± 34°C.

Only the average P could be calculated from one rim assemblage in the enclosing schists (Table 2). The average P (at 700°C) from assemblage 67662 rim#3 (16.4 ± 1.3 kb) is consistent with the P of equilibration in the eclogite.

## DISCUSSION and CONCLUSIONS

Average T's and P's of equilibration of the eclogite sample are generally consistent with, but slightly lower (by 5–38°C and 0.1–2.0 kb) than the earlier estimates by Kamperman (1984) (715–730°C, 15.6–17.0 kb).

Rim pressures are slightly lower than cores (by $\leq 0.6$ kb) and rim temperatures are slightly higher than the cores (by 8–21°C). This is inconsistent with the pressure increase of 1.4 kb from core to rim reported by Kamperman (1984). Kamperman reports far more significant increases in T from core to rim (up to 110°C) than found by this study. In both studies the difference in P estimates between cores and rims are below the range in error. Consequently neither the up P vector of Kamperman (1984) nor the down P vector of this study can be considered real. Constraints on the P-T path experienced by these eclogites would be more reliably pursued by phase stability constraints based on mineral reaction textures.

The P estimate from the aluminous schist (67662 rim#3) is consistent with estimates from the eclogite sample. Pressure estimates by Kamperman (1984) for this schist, based on $Si^{4+}$ in phengite, are 3–5 kb lower than his P estimates in the eclogite. This difference is not considered real, but is a result of the phengite geobarometer being calibrated at much lower temperatures than those at which the eclogite was equilibrated (Kamperman, 1984). The close correlation in P estimates, presented in this report, between the aluminous schist and the eclogite sample further supports the conclusion of Kamperman (1984) that the eclogite and schist were in juxtaposition prior to the peak of metamorphism.

## REFERENCES

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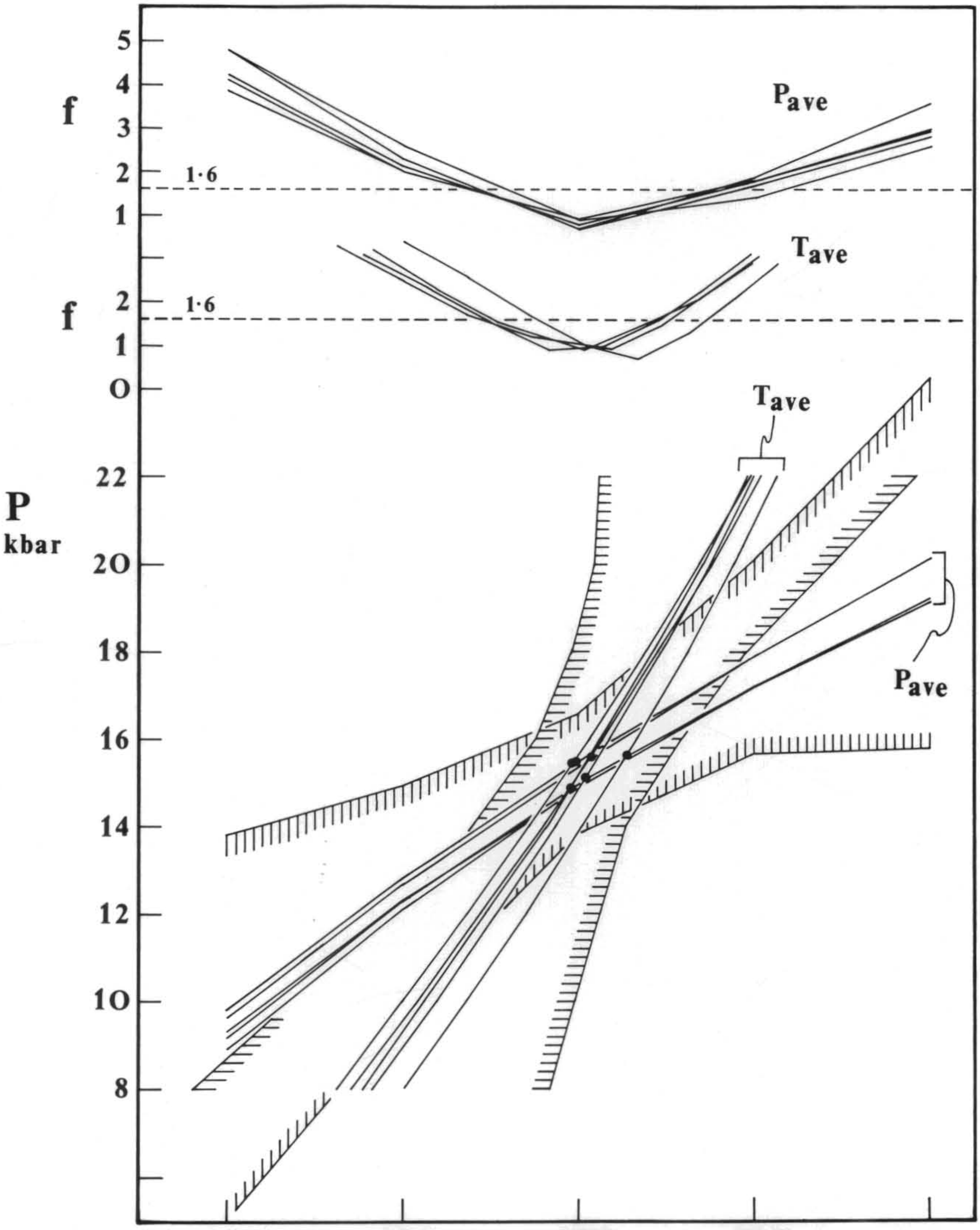

**Figure 1.** *All average P and average T results from eclogite sample (67644) plotted in P-T space. Error bands encompass all errors for all average P estimates (vertical shading) and all average T estimates (horizontal shading). Chi squared test for average P and average T plotted at top of figure. Dots are P-T loci without errors (see Figure 2).*

5 cm

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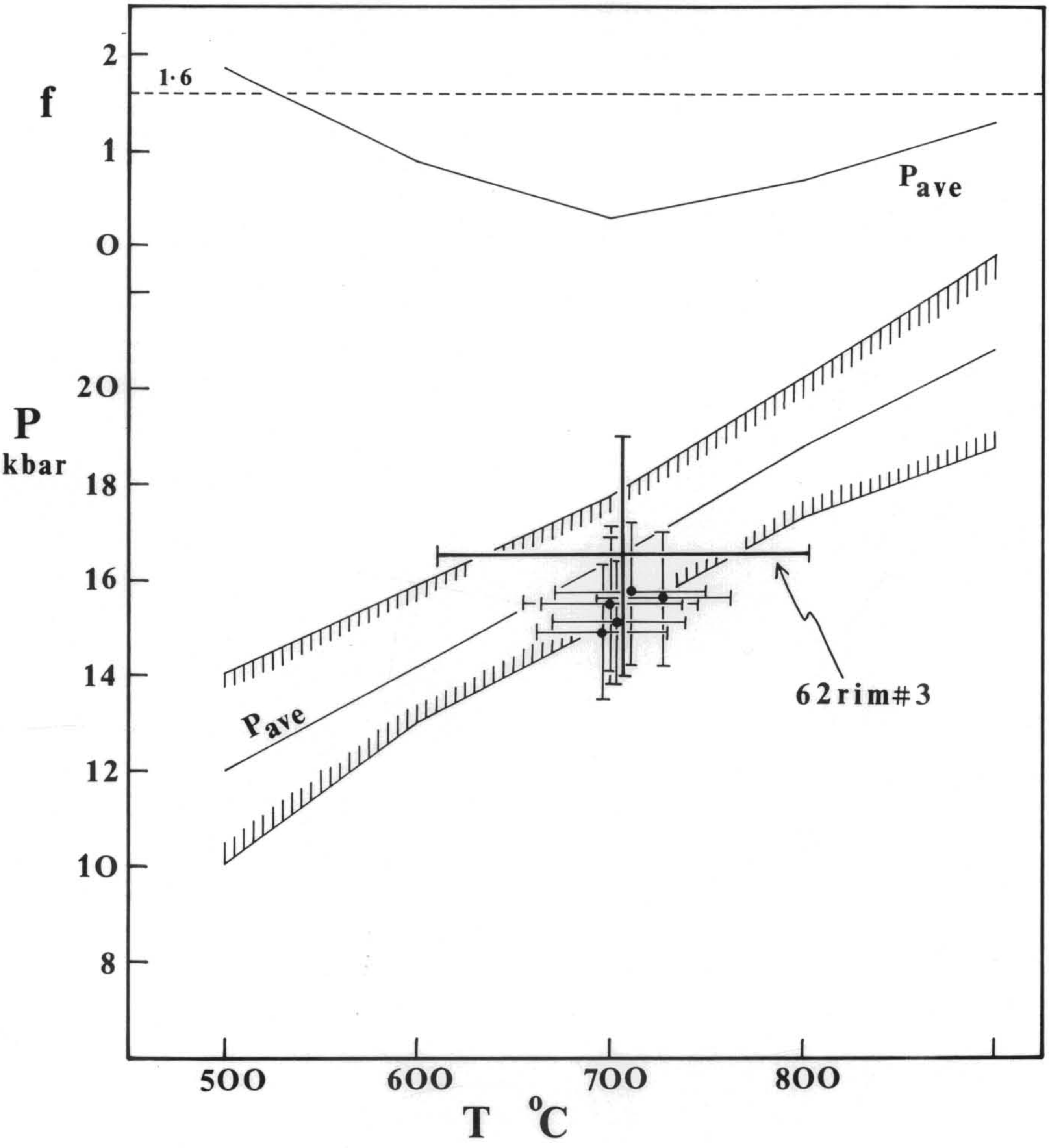

**Figure 2.** *Average P band in aluminous schist rim assemblage (67662 rim# 3). Average P-T loci and error bars of this same sample are plotted as labelled. All other P-T loci are core and rim estimates from the eclogite sample (67644) for comparison.*

5 cm

**Table 1.** *Mineral analyses used in calculations. Sourced from Kamperman (1984) and recalculated using RECALC (Powell pers. comm. 1990).*

| GARNET | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 67644 # 1 | | 67644 # 2 | | 67644 # 3 | | 67662 # 1 | | 67662 # 2 | | 67662 # 3 | |
| | Core | Rim | Core | Rim | Core | Rim | Core | Rim | Core | Rim | Core | Rim |
| $SiO_2$ | 38.85 | 38.70 | 38.94 | 39.05 | 38.83 | 39.45 | 36.66 | 36.90 | 37.10 | 37.19 | 37.53 | 37.54 |
| $TiO_2$ | - | - | - | - | - | - | - | - | - | - | - | - |
| $Al_2O_3$ | 22.22 | 22.46 | 22.32 | 22.38 | 22.29 | 22.66 | 21.75 | 21.76 | 21.60 | 21.65 | 22.04 | 21.87 |
| FeO | 21.88 | 22.91 | 20.36 | 20.62 | 21.20 | 19.31 | 36.64 | 35.84 | 35.62 | 34.81 | 31.99 | 31.70 |
| MnO | 0.33 | 0.41 | 0.40 | - | 0.32 | 0.34 | 0.89 | 0.62 | 0.93 | 0.82 | - | - |
| MgO | 7.33 | 8.49 | 7.20 | 8.47 | 7.89 | 9.97 | 3.18 | 3.94 | 4.01 | 4.53 | 5.69 | 5.27 |
| CaO | 9.39 | 7.03 | 10.78 | 9.48 | 9.47 | 8.27 | 0.88 | 0.93 | 0.74 | 1.00 | 2.75 | 3.35 |
| $Na_2O$ | - | - | - | - | - | - | - | - | - | - | - | 0.27 |
| $K_2O$ | - | - | - | - | - | - | - | - | - | - | - | - |
| $\Sigma$ | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| | | | | | | | | | | | | |
| X(Si,T1) | 0.993 | 0.987 | 0.992 | 0.996 | 0.989 | 0.992 | 0.985 | 0.986 | 0.991 | 0.990 | 0.986 | 0.988 |
| X(Al,M1) | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| X(Ca,M2) | 0.257 | 0.192 | 0.294 | 0.258 | 0.259 | 0.223 | 0.025 | 0.027 | 0.021 | 0.029 | 0.077 | 0.094 |
| X($Fe_2$,M2) | 0.468 | 0.489 | 0.434 | 0.437 | 0.452 | 0.406 | 0.823 | 0.801 | 0.796 | 0.775 | 0.703 | 0.698 |
| X(Mg,M2) | 0.279 | 0.323 | 0.273 | 0.320 | 0.300 | 0.373 | 0.127 | 0.157 | 0.160 | 0.180 | 0.223 | 0.207 |
| $d_{gr}$ | - | - | - | - | - | - | - | - | - | 0.000039 | - | 0.00137 |
| $d_{alm}$ | 0.123 | 0.134 | 0.1004 | 0.103 | 0.109 | 0.083 | - | - | - | 0.458 | - | 0.347 |
| $d_{py}$ | 0.036 | 0.047 | 0.037 | 0.052 | 0.044 | 0.075 | - | - | - | 0.0061 | - | 0.0106 |

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**Table 1.** *(continued)*

| CLINOPYROXENE | | | PHENGITE | | | | | AMPHIBOLE | | | FELDSPAR | | | BIOTITE | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 67644 | | | 67644 | | 67662 | | | 67644 | | | 67644 | 67662 | | 67644 |
| | Core | Rim | | Core | Rim | Core | Rim | | Core | Rim | | Core | Rim | | |
| $SiO_2$ | 55.69 | 54.81 | | 49.40 | 47.73 | 51.27 | 52.12 | | 49.38 | 48.35 | | 65.78 | 67.80 | | 36.42 |
| $TiO_2$ | - | - | | 0.68 | 0.77 | 1.13 | 0.67 | | 0.40 | 0.35 | | - | - | | 1.98 |
| $Al_2O_3$ | 10.33 | 11.75 | | 27.01 | 26.04 | 33.81 | 32.87 | | 13.12 | 13.40 | | 18.38 | 20.90 | | 18.74 |
| FeO | 3.37 | 4.15 | | 1.17 | 1.55 | 1.41 | 1.71 | | - | - | | - | - | | 24.45 |
| MnO | - | - | | - | - | - | - | | 6.77 | 6.83 | | - | - | | - |
| MgO | 9.84 | 9.62 | | 3.94 | 3.66 | 2.24 | 2.41 | | 16.36 | 16.43 | | - | - | | 8.70 |
| CaO | 15.25 | 14.79 | | - | - | - | - | | 10.35 | 10.38 | | - | 1.03 | | - |
| $Na_2O$ | 5.53 | 4.47 | | 0.31 | 0.25 | 0.98 | 0.87 | | 3.01 | 2.88 | | - | 10.26 | | - |
| $K_2O$ | - | 0.41 | | 9.58 | 9.48 | 9.16 | 9.36 | | 0.67 | 0.53 | | 15.84 | - | | 9.71 |
| Σ | 100.00 | 100.00 | | 92.09 | 89.48 | 100.00 | 100.00 | | 100.07 | 99.14 | | 100.00 | 100.00 | | 100.00 |
| | | | | | | | | | | | | | | | |
| X(Si,T1) | 0.990 | 0.975 | X(Si,T1) | 0.686 | 0.682 | 0.605 | 0.632 | X(Si,T1) | 0.699 | 0.680 | X(Si,T1) | 0.755 | 0.739 | X(Si,T1) | 0.335 |
| X(Al,T1) | 0.010 | 0.025 | X(Al,T1) | 0.314 | 0.318 | 0.395 | 0.368 | X(Al,T1) | 0.301 | 0.320 | X(Al,T1) | 0.245 | 0.261 | X(Al,T1) | 0.665 |
| X(Al,T1) | 0.412 | 0.443 | X(Si,T2) | 1.000 | 1.000 | 1.000 | 1.000 | X(Si,T2) | 1.000 | 1.000 | X(K,A) | 0.928 | - | X(Si,T2) | 1.000 |
| X(Fe$_2$,M1) | 0.095 | 0.109 | X(Al,M1) | 0.773 | 0.763 | 0.853 | 0.846 | (X(Al,M1) | 0.462 | 0.459 | X(Na,A) | - | 0.867 | X(Al,M1) | 0.144 |
| X(Mg,M1) | 0.493 | 0.449 | X(Mg,M1) | 0.190 | 0.189 | 0.098 | 0.112 | X(Mg,M1) | 0.178 | 0.202 | X(Ca,A) | - | 0.048 | X(Fe$_2$,M1) | 0.395 |
| X(Ca,M2) | 0.581 | 0.564 | X(FE$_3$,M1) | 0.020 | 0.027 | 0.022 | 0.027 | X(Ca,M2) | 0.763 | 0.773 | X(an) | - | 0.053 | X(Mg,M1) | 0.294 |
| X(Na,M2) | 0.381 | 0.308 | X(FE$_2$,M2) | - | 0.037 | - | 0.036 | X(Na,M2) | 0.237 | 0.227 | X(ab) | - | 0.947 | X(FE$_3$,M1) | 0.112 |
| X(FE$_2$,M2) | 0.005 | 0.015 | X(Mg,M2) | 0.022 | 0.007 | 0.012 | 0.001 | X(Mg,M3) | 1.000 | 1.000 | $a_{an}$ | - | 0.069 | X(FE$_2$,M2) | 0.485 |
| X(Mg,M2) | 0.028 | 0.061 | X(V,M2) | 0.978 | 0.957 | 0.988 | 0.963 | X(Na,A) | 0.330 | 0.322 | | | | X(Mg,M2) | 0.361 |
| X(di) | 0.493 | 0.449 | X(Na,A) | 0.041 | 0.034 | 0.119 | 0.106 | X(V,A) | 0.553 | 0.584 | | | | X(V,M2) | 0.154 |
| X(hed) | 0.0948 | 0.109 | X(K,A) | 0.834 | 0.852 | 0.732 | 0.748 | X(hb) | 0.103 | 0.123 | | | | X(K,A) | 0.908 |
| X(cats) | 0.239 | 0.250 | X(mu) | 0.420 | 0.412 | 0.502 | 0.479 | X(parg) | 0.045 | 0.0541 | | | | X(phl) | 0.0253 |
| | | | X(cel) | 0.225 | 0.218 | 0.089 | 0.109 | X(ed) | 0.006 | 0.008 | | | | X(ann) | 0.0610 |
| | | | | | | | | | | | | | | X(east) | 0.0247 |

**Table 2.** *Average pressure calculations, data defining band in P-T space. Sd(P) is standard deviation on P estimate at the given T, f is chi squared test.*

| Sample | End-members used | | 500 | 600 | 700 | 800 | 900 °C |
|---|---|---|---|---|---|---|---|
| 67644 | py-alm-cel-di-cats- | $P_{ave}$ | 9.8 | 12.8 | 15.5 | 17.9 | 20.1 |
| core # 1 | hed-hb-parg-ed- | Sd(P) | 4.00 | 2.15 | 1.05 | 2.21 | 4.20 |
| | san-q-$H_2O$ | f | 4.8 | 2.3 | 0.7 | 1.9 | 3.3 |
| 67644 | As above | $P_{ave}$ | 9.3 | 12.3 | 15.0 | 17.2 | 19.1 |
| rim # 1 | | Sd(P) | 3.33 | 1.85 | 1.05 | 2.09 | 3.78 |
| | | f | 4.1 | 2.0 | 0.9 | 1.8 | 3.0 |
| 67644 | As above | $P_{ave}$ | 9.8 | 12.8 | 15.5 | 17.9 | 20.1 |
| core # 2 | | Sd(P) | 3.31 | 1.87 | 1.05 | 1.98 | 3.55 |
| | | f | 3.9 | 2.0 | 0.9 | 1.7 | 2.8 |
| 67644 | As above | $P_{ave}$ | 9.2 | 12.3 | 14.9 | 17.2 | 19.2 |
| rim # 2 | | Sd(P) | 3.46 | 1.94 | 1.05 | 1.94 | 3.66 |
| | | f | 4.2 | 2.1 | 0.8 | 1.7 | 2.9 |
| 67644 | As above | $P_{ave}$ | 9.6 | 12.7 | 15.4 | 17.9 | 20.1 |
| core # 3 | | Sd(P) | 3.50 | 2.03 | 1.05 | 1.84 | 3.43 |
| | | f | 4.2 | 2.1 | 0.9 | 1.6 | 2.7 |
| 67644 | As above | $P_{ave}$ | 8.9 | 12.1 | 14.9 | 17.2 | 19.2 |
| rim # 3 | | Sd(P) | 3.92 | 2.37 | 1.05 | 1.57 | 3.33 |
| | | f | 4.8 | 2.6 | 0.9 | 1.4 | 2.6 |
| 67662 | py-alm-gr-mu- | $P_{ave}$ | 12.0 | 14.2 | 16.4 | 18.6 | 20.8 |
| rim # 3 | phl-east-ab-an | Sd(P) | 1.98 | 1.17 | 1.31 | 1.45 | 2.03 |
| | q-ky-$H_2O$ | f | 1.9 | 0.9 | 0.3 | 0.7 | 1.3 |

**Table 3.** *Average temperature calculations, data defining band in P-T space. Mineral end-members used are the same as in Table 2. Sd(T) is standard deviation on T estimate at the given P, f is the chi squared test.*

| Sample | | 8 | 10 | 12 | 14 | 15 | 16 | 18 | 20 | 22 kb |
|---|---|---|---|---|---|---|---|---|---|---|
| 67644 | $T_{ave}$ | 561 | 599 | 636 | 672 | 689 | 706 | 738 | 769 | 798 |
| core # 1 | Sd(T) | 82 | 63 | 45 | 31 | 30 | 28 | 41 | 61 | 84 |
| | f | 3.3 | 2.5 | 1.7 | 1.2 | 1.1 | 1.0 | 1.5 | 2.1 | 2.9 |
| 67644 | $T_{ave}$ | 576 | 612 | 647 | 681 | 697 | 712 | 742 | 770 | 796 |
| rim # 1 | Sd(T) | 78 | 58 | 39 | 26 | 26.5 | 27 | 44 | 66 | 90 |
| | f | 3.1 | 2.3 | 1.5 | 0.9 | 0.95 | 1.0 | 1.6 | 2.3 | 3.1 |
| 67644 | $T_{ave}$ | 562 | 600 | 637 | 673 | 690 | 707 | 740 | 770 | 799 |
| core # 2 | Sd(T) | 81 | 62 | 44 | 29 | 28 | 27 | 39 | 59 | 82 |
| | f | 3.2 | 2.4 | 1.7 | 1.1 | 1.0 | 0.9 | 1.4 | 2.1 | 2.8 |
| 67644 | $T_{ave}$ | 582 | 618 | 653 | 686 | 701 | 717 | 747 | 775 | 800 |
| rim # 2 | Sd(T) | 79 | 59 | 39 | 26 | 26.5 | 27 | 41 | 63 | 88 |
| | f | 3.2 | 2.3 | 1.5 | 0.9 | 0.9 | 0.9 | 1.5 | 2.3 | 3.1 |
| 67644 | $T_{ave}$ | 570 | 608 | 644 | 680 | 696 | 713 | 745 | 776 | 804 |
| core # 3 | Sd(T) | 83 | 64 | 46 | 30 | 28.5 | 27 | 36 | 56 | 79 |
| | f | 3.3 | 2.5 | 1.8 | 1.1 | 1.0 | 0.9 | 1.3 | 2 | 2.8 |
| 67644 | $T_{ave}$ | 601 | 636 | 670 | 702 | 717 | 733 | 762 | 789 | 814 |
| rim # 3 | Sd(T) | 83 | 63 | 43 | 26 | 26 | 26 | 34 | 56 | 80 |
| | f | 3.4 | 2.6 | 1.7 | 1.0 | 0.85 | 0.7 | 1.3 | 2.1 | 2.9 |

**Table 4.** *Average P-T loci calculations. Mineral end-members used are the same as in Table 2. Sd is standard deviation, f is the chi squared test and corr is the correlation coefficient.*

| Sample | $P_{ave}$ | Sd(P) | $T_{ave}$ | Sd(T) | corr | f |
|---|---|---|---|---|---|---|
| 67644 core # 1 | 15.5 | 1.4 | 701 | 37 | 0.661 | 1.02 |
| 67644 rim # 1 | 14.9 | 1.4 | 697 | 35 | 0.625 | 1.04 |
| 67644 core # 2 | 15.5 | 1.6 | 701 | 40 | 0.661 | 1.11 |
| 67644 rim # 2 | 15.1 | 1.3 | 704 | 34 | 0.621 | 0.94 |
| 67644 core # 3 | 15.7 | 1.5 | 711 | 39 | 0.656 | 1.08 |
| 67644 rim # 3 | 15.6 | 1.4 | 728 | 34 | 0.607 | 0.86 |
| 67662 rim # 3 | 16.5 | 2.5 | 706 | 96 | 0.847 | 0.49 |

**Table 5.** *The sets of independent reactions used in the average P and T calculations.*

Independent reactions used in average P-T loci and average P calculations in 44c1, 44c2, 44c3, 44r1 and 44r2.

1. 2san + 2hb = 2cel + py + 3di + cats + 2q
2. 3cel + di + cats + q = 3san + hb + 2$H_2O$
3. 2san + 2hb + 3hed = 2 cel + alm + 6di + cats + 2q
4. 2san + 2hb + ed = 2cel + py + parg + 4di + 2q

Independent reactions used in average P-T loci and average P calculations in 44r3.

1. 2san + 2hb = 2cel + py + 3di + cats + 2q
2. 7cel + 2cats + q = py + 7san + hb + 6$H_2O$
3. 2san + 2hb + 3hed = 2 cel + alm + 6di + cats + 2q
4. 2san + 2hb + ed = 2cel + py + parg + 4di + 2q

Independent reactions used in average T calculations in 44c1, 44c2, 44c3, 44r1, 44r2 and 44r3.

1. 4cel + cats = py + 4san + di + 4$H_2O$
2. cel + hb = py + san + 2di + q + 2$H_2O$
3. 12cel + alm + 3cats = 4py + 12san + 3hed + 12$H_2O$
4. 4cel + parg = py + 4san + ed + 4$H_2O$

Independent reactions used in average P-T loci and average P calculations in 62r3.

1. 3an = gr + q + 2ky
2. phl + 3an = mu + gr + py
3. 3east + 15an = mu + 2phl + 5gr + 12ky

# APPENDIX 1

## List of Abbreviations

| | |
|---|---|
| a | activity |
| $\gamma$ | activity coefficient |
| $\Delta G^{o}$ | Gibbs energy change for a reaction among end-member phases at the temperature and pressure of interest |
| K | Equilibrium constant for a balanced reaction |
| X | Mole fraction |

**MINERAL END-MEMBERS**

| | |
|---|---|
| gr | Grossular |
| alm | Almandine |
| py | Pyrope |
| san | Sanidine |
| ab | Albite |
| an | Anorthite |
| di | Diopside |
| hed | Hedenbergite |
| cats | Ca-Tschermak's |
| phl | Phlogopite |
| ann | Annite |
| east | Eastonite |
| mu | Muscovite |
| cel | Celadonite |
| hb | Hornblende |
| parg | Pargasite |
| ed | Edenite |
| q | Quartz |
| ky | Kyanite |

# APPENDIX 2

## Activity Calculations

For equilibrium thermodynamic calculations the following equilibrium relationship must be satisfied for each reaction of mineral end-members:

$$0 = \Delta G^\circ + RT\ln K$$

$\Delta G^\circ$ is supplied by the internally consistent thermodynamic data set, whereas the compositional term ($RT\ln K$) is variable. $RT\ln K$ can be written as:

$$RT\ln K = \Sigma RT\ln a_{products} - \Sigma RT\ln a_{reactants}$$

The activities of end-members in the equilibrium assemblage are calculated (see below) and then used as input for THERMOCALC.

Activity is defined as:

$$a_e^p = \gamma_e^p \,.\, X_e^p$$

where $X_e^p$ = mole fraction of end-member (e) in phase (p), calculated from mineral analyses using RECALC.

$\gamma_e^p$ = activity coefficient of end-member (e) in phase (p).

For assuming ideal mixing on sites $\gamma=1$. For non-ideal mixing $\gamma>1$ if pure end-members are more stable than a solid solution and $\gamma<1$ if a solid solution between two or more end-members together is the most stable arrangement.

The activity calculations used in this report are listed as follows.

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### A. IDEAL SOLID SOLUTION

Quartz

$a_q = 1$

Kyanite

$a_{ky} = 1$

Feldspar (T. Holland pers. comm. 1987)

$a_{san} = X_{san}$

$a_{ab} = X_{ab}$

Muscovite

$a_{mu} = 4X_K^A(X_V^{M2})(X_{Al}^{M1})^2(X_{Al}^{T1})(X_{Si}^{T1})$

$a_{cel} = X_K^A(X_V^{M2})(X_{Al}^{M1})(X_{Mg}^{M1})(X_{Si}^{T1})^2(X_{Si}^{T2})^2$

Clinopyroxene

$a_{di} = (X_{Ca}^{M2})(X_{Mg}^{M1})$

$a_{hed} = (X_{Ca}^{M2})(X_{Fe}^{M1})$

$a_{cats} = (X_{Ca}^{M2})(X_{Al}^{M1})$

Biotite

$a_{phl} = 4X_K^A(X_{Mg}^{M2})(X_{Mg}^{M1})^2(X_{Si}^{T1})(X_{Al}^{T1})$

$a_{ann} = 4X_K^A(X_{Fe}^{M2})(X_{Fe}^{M1})^2(X_{Si}^{T1})(X_{Al}^{T1})$

$a_{east} = X_K^A(X_{Al}^{M2})(X_{Mg}^{M1})^2(X_{Al}^{T1})^2$

Amphibole

$a_{hb} = 37.9X_v(X_{Ca}^{M2})^2(X_{Mg}^{M3})^3(X_{Mg}^{M1})(X_{Al}^{M1})(X_{Si}^{T1})^3(X_{Al}^{T1})$

$a_{parg} = 64X_{Na}(X_{Ca}^{M2})^2(X_{Mg}^{M3})^3(X_{Mg}^{M1})(X_{Al}^{M1})(X_{Si}^{T1})^2(X_{Al}^{T1})^2$

$a_{ed} = 9.48X_{Na}(X_{Ca}^{M2})^2(X_{Mg}^{M3})^3(X_{Mg}^{M1})^2(X_{Si}^{T1})^3(X_{Al}^{T1})$

### B. NON-IDEAL SOLID SOLUTION

Garnet

$a_{py} = (\gamma_{py}.X_{Mg}^{M2})^3(X_{Al}^{M1})^2(X_{Si}^{T1})^3$

$a_{alm} = (\gamma_{alm}.X_{Fe}^{M2})^3(X_{Al}^{M1})^2(X_{Si}^{T1})^3$

$a_{gr} = (\gamma_{gr}.X_{Ca}^{M2})^3(X_{Al}^{M1})^2(X_{Si}^{T1})^3$

activity coefficients after Newton and Haselton (1981).

$RT\ln(\gamma_{py}) = (3300-1.5T)X_{Ca}(1-X_{Mg})$

$RT\ln(\gamma_{alm}) = (3300-1.5T)X_{Mg}X_{Ca}$

$RT\ln(\gamma_{gr}) = (3300-1.5T)X_{Mg}(1-X_{Ca})$

Plagioclase

$a_{an} = \gamma_{an}X_{an}$, where $\gamma_{an} = 1.3$ for compositions of $X_{an} = 0.2-0.8$ (T. Holland pers. comm.1987)