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CHARACTERIZATION OF PARTLY-OPEN-SYSTEM CHEMICAL VARIATIONS IN CLINOPYROXENE AMPHIBOLITE BOUDINS, THREE VALLEY GAP, BRITISH COLUMBIA, USING THOMPSON SPACE CALCULATIONS

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ABSTRACT

Garnet – clinopyroxene amphibolite boudins crop out near Three Valley Gap, British Columbia. They are as large as 13 m in maximum dimension and occur within metasedimentary gneisses. The metasedimentary rocks contain K-feldspar + sillimanite, and muscovite is not stable. The boudins have assemblages dominated by amphibole (tschermakitic hornblende, tschermakite, magnesio-hornblende, some with a rim of secondary actinolitic hornblende), unzoned to weakly zoned plagioclase (ΔAn < 5) in the andesine–bytownite range, and smaller amounts of diopside, quartz and Fe–Ti oxides. Accessory phases include biotite, epidote, enstatite, apatite and garnet. The presence of enstatite in the mineral assemblage indicates peak metamorphic conditions at the boundary between amphibolite and granulite facies. Geobarometric–thermometric estimates, based on mineral equilibria, indicate metamorphic conditions near 0.8 GPa and 700°C. A single boudin is chemically heterogeneous on the thin section, hand sample and outcrop scales. The variations in element ratios cannot be explained by original, internal, igneous processes. Plots of the compositions derived from chemical analysis of hand-specimen-size samples and of compositions derived from modal analysis in Thompson space reveal differences in composition similar to those between intermediate igneous rocks (approximately andesite), tholeiitic basalts and undersaturated basalts, all from a single boudin. These variations are the result of metamorphic or metasomatic processes.

Keywords: amphibolite – granulite facies transition, amphibole, plagioclase, clinopyroxene, orthopyroxene, quartz, modes, partly open system, Thompson space, British Columbia.

SOMMAIRE

Des boudins d'amphibolite à grenat + clinopyroxène affleurent près de Three Valley Gap, en Colombie Britannique. Ils atteignent 13 m en dimension maximale et sont inclus dans des gneiss métasédimentaires. Les roches métasédimentaires contiennent feldspath potassique + sillimanite et sont sans muscovite stable. Dans les boudins, une amphibole (hornblende tschermakitique, tschermakite, magnésio-hornblende, avec dans certains cas une bordure de hornblende actinolitique) et un plagioclase (andésine – bytownite) homogène ou faiblement zoné (ΔAn < 5) prédominent, et sont accompagnés de quantités moins importantes de diopside, quartz et oxydes de Fe–Ti. Parmi les minéraux accessoires, nous trouvons biotite, épidote, apatite et grenat. La présence d'enstatite dans l'assemblage signalerait des conditions métamorphiques à la transition amphibolite – granulite. Les évaluations géobarométriques et thermométriques, fondées sur les équilibres parmi les phases minérales, indiquent des conditions voisines de 0.8 GPa et 700°C. Chaque boudin est chimiquement hétérogène, à l'échelle d'une lame mince, d'un échantillon ou d'un affleurement. Les variations dans les rapports d'éléments ne peuvent s'expliquer par des processus ignés internes. Une approche faisant appel aux diagrammes dans l'espace de Thompson, qui montrent la composition chimique des échantillons et leur composition modale, révèle des différences en composition semblables à celles qui distinguent les roches intermédiaires (andésitiques), les basaltes tholéitiques et les basaltes sous-saturés, toutes à l'intérieur d'un seul boudin. Ces variations résulteraient de processus métamorphiques ou métasomatiques.

(Traduit par la Rédaction)

Mots-clés: transition amphibolite – granulite, amphibole, plagioclase, clinopyroxène, orthopyroxène, quartz, analyses modales, système partiellement ouvert, espace de Thompson, Colombie Britannique.

INTRODUCTION

Chemical, mineralogical and textural variations are evident in boudins that crop out near Three Valley Gap, British Columbia, approximately 20 km west of Revelstoke; for a locality map, see Ghent *et al.* (1977, Fig. 1). Processes contributing to these observed variations may include original closed-system igneous processes, later open-system metamorphic or metasomatic processes, or a combination of all three. In this paper, we apply Thompson space calculations to an integrated body of chemical, mineralogical, and modal data from a set of rocks with a relatively simple geological setting. These calculations provide an assessment of the consistency of the different types of data and can thereby illustrate the extent of variation and support or negate the several postulated causes of the variations present in the boudins. The boudins are up to 13 m in maximum dimension and occur within metasedimentary gneisses. The metasedimentary rocks contain K-feldspar + sillimanite, and muscovite is not stable. Ghent *et al.* (1977) reported rock compositions, modes, mineral compositions and estimates of the physical conditions attending metamorphism. They concluded that the amphibolite boudins were originally dolerites.

Because automated modal analyses with the electron microprobe (Nicholls & Stout 1986) provide improved estimates of mineralogical variability, new modes have been obtained. Modal analyses with the automated electron microprobe resulted in the identification of sporadically occurring orthopyroxene, not previously found with the optical microscope. Consequently, we report the first discovery, to our knowledge, of granulite-facies rocks in the Shuswap terrane. In addition, we present updated pressure–temperature estimates using newer methods, fluid-inclusion measurements, and further interpretation of the nature of the protolith.

MODES AND THEIR VARIATIONS

The boudins have assemblages dominated by amphibole (tschermakitic hornblende, tschermakite, magnesio-hornblende, some with a rim of secondary actinolitic hornblende), unzoned to weakly zoned plagioclase (ΔAn < 5) in the andesine–bytownite range, and smaller amounts of diopside, quartz and Fe–Ti oxides. Accessory phases include biotite, epidote, enstatite, apatite and garnet. Not all the accessory phases are present in every sample. Pyroxene names comply with the IMA rules of nomenclature (Morimoto 1989), but petrologists are cautioned that the enstatite in these rocks is quite Fe-rich, near Fs_{45}.

Modes were determined for all four samples by automatic counting on the electron microprobe. One-second counts on Ca, K, Na, Ti, Si, Al, Fe and Mg were ranked and compared to the ranking expected for the minerals in the rocks, *i.e.*, standard lines (Nicholls & Stout 1986). Counting was done on a 200-μm grid spacing, and greater than 93% of the spots were identified in each sample. The results are listed in Table 1 and illustrated in Figure 1.

The areas selected for modal analysis were chosen to avoid quartz veins that cut through these rocks. To analyze the homogeneity of mineral distribution within a sample, modes for the four quadrants of an area can be displayed separately (Fig. 2). With the exception of the high amount of clinopyroxene and the very low amount of quartz present in sample BR-4 (Fig. 1), the variability

TABLE 1. MODES OF THREE VALLEY GAP AMPHIBOLITES IN VOLUME PERCENTAGES

Sample	Pl	Amph	Cpx	Opx	Qtz	Bt	Ep	Grt	Ap	Opaque	Chl
BR-2	28.230	51.730	9.490	0.050	8.660		0.030		0.550	0.100	1.170
Q1	24.219	57.616	4.541		12.488				0.095	0.189	0.851
Q2	23.744	54.680	10.148		8.670		0.099		0.690	0.197	1.733
Q3	34.800	45.241	11.259	0.102	6.960				0.716		0.921
Q4	30.682	48.760	12.397	0.103	6.198				0.723		1.136
BR-3	35.810	43.920	8.010	0.830	10.970	0.020	0.090	0.030	0.080	0.080	0.160
Q1	37.139	41.092	9.536		11.857		0.251		0.063		0.063
Q2	37.643	41.508	8.935	0.444	11.090		0.063	0.063	0.063		0.190
Q3	33.250	48.692	7.597	0.498	9.340		0.062		0.125	0.249	0.187
Q4	35.260	44.282	5.972	2.414	11.626	0.064		0.064	0.064	0.064	0.191
BR-4	36.260	46.520	15.940	0.082	0.492		0.040		0.310	0.040	0.310
Q1	41.318	42.042	14.389		0.965				0.643	0.080	0.563
Q2	37.490	43.431	17.657		0.921		0.084		0.251	0.084	0.084
Q3	36.438	44.853	17.810	0.327					0.245		0.327
Q4	29.633	55.927	13.940		0.083		0.083		0.083		0.250
BR-5	26.960	54.760	8.120	0.029	9.550		0.180		0.120	0.060	0.230
Q1	26.067	52.018	10.035	0.115	11.534		0.115				0.115
Q2	25.935	56.893	8.645		7.944		0.117			0.234	0.234
Q3	24.253	56.782	8.966		9.080		0.345		0.460		0.115
Q4	31.710	53.325	4.751		9.620		0.119				0.475

Q1 - Q4 are quadrants of the thin section. Abbreviations of mineral names are from Kretz (1983) except for Amph = amphibole and Opaque = opaque minerals.

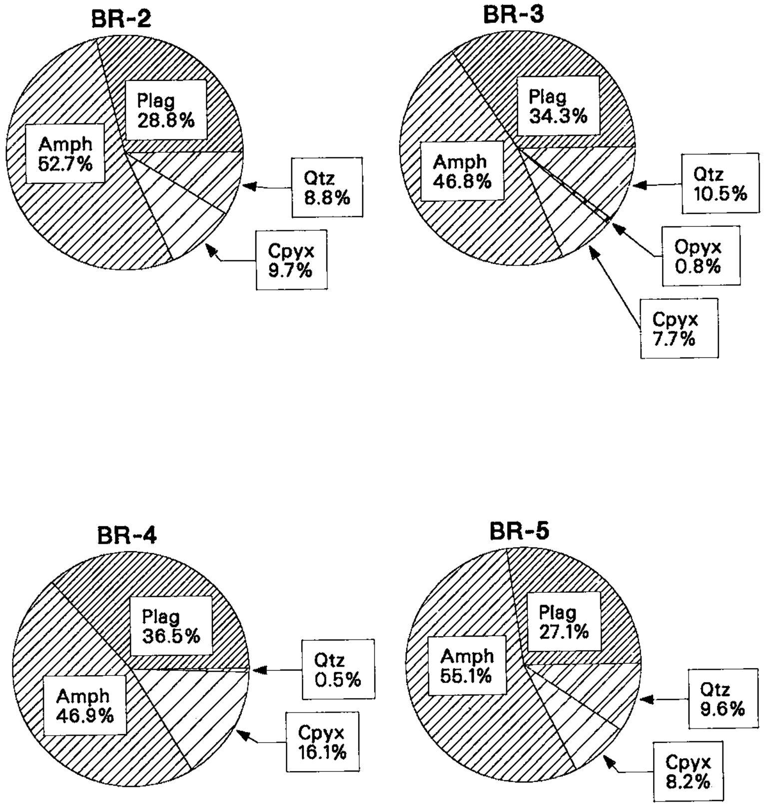

FIG. 1. Results of electron-microprobe-generated automated modal analyses of amphibolite boudins from Three Valley Gap. Each circular diagram represents one sample. Analyses done using one-second counts on a 200-μm grid spacing.

within a thin section, as shown by modes from quadrants of the thin section of BR-2 (Fig. 2), is as great as the variability between samples.

Plots of the distribution of the major minerals show pyroxene and quartz distributed throughout an amphibole – plagioclase framework. The distributions are not homogeneous, however. For example, in BR-2 there is a greater density of identified clinopyroxene and plagioclase spots near a diagonal of the thin section, whereas amphibole and quartz are more concentrated off the diagonal (Fig. 3).

MINERAL CHEMISTRY

Coexisting amphibole, clinopyroxene, orthopyroxene and plagioclase were analyzed using an ARL SEMQ 8-channel electron microprobe. Analytical techniques and calculation of detection limits and precision are described in Nicholls & Stout (1988). Tables of the complete mineral compositions of the four samples used in this study are available from the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2. Additional mineral compositions of these and four other samples, which were all analyzed previously, are published in Ghent *et al.* (1977), along with details of the petrography, mineralogy and mineral chemistry.

Pyroxene standard lines entered in a computerized modal analysis program (Nicholls & Stout 1986) allowed us to identify orthopyroxene despite its rare and sporadic occurrence in these rocks. By using the position coordinates of the microprobe stage that were recorded in the modal analysis program, we could locate and analyze the orthopyroxene grains. Because there are no previous microprobe data on the orthopyroxene from these boudins, the compositions are presented in Table 2.

Similar to the other silicate minerals in these boudins, the orthopyroxene is quite homogeneous. With the exception of higher concentrations of Al

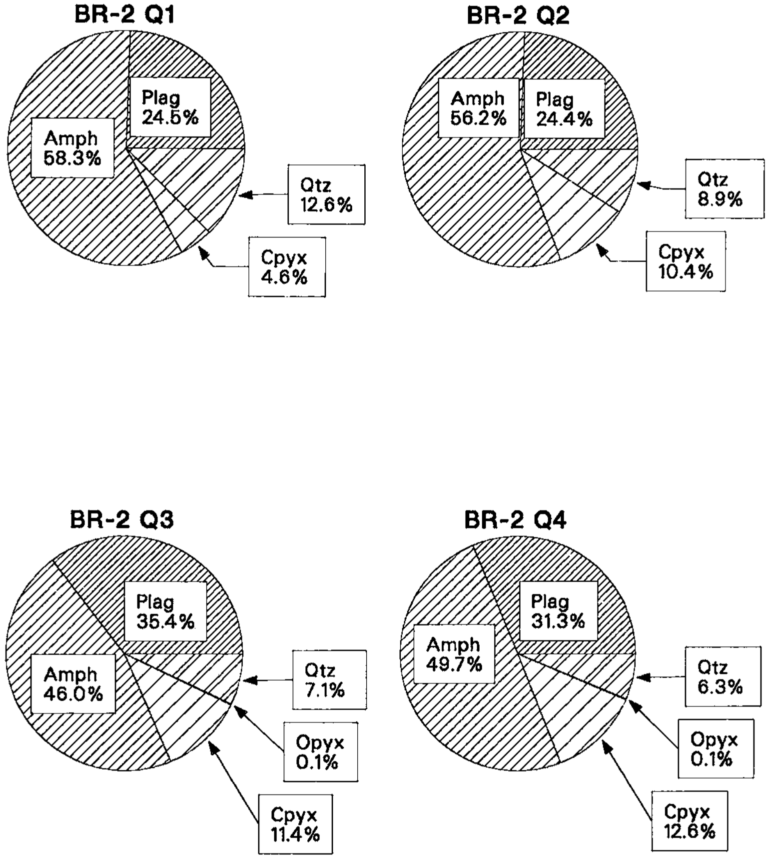

FIG. 2. Illustration of the variability in mineral distribution within one sample (BR-2). Each circular diagram represents one quadrant of the complete sample (Q1 through Q4).

occasionally found in the interior of some crystals, there is little intercrystalline and intracrystalline variation.

PRESSURE–TEMPERATURE CONDITIONS

P–T conditions attending the metamorphism of the amphibolite boudins and associated metasedimentary rocks were estimated by Ghent *et al.* (1977). Since that time, there has been an extensive and critical revision of geothermobarometers. Using more recent calibrations, peak P–T conditions have been estimated for both the boudins and the adjacent pelitic gneisses that contain the assemblage quartz + K-feldspar + plagioclase + biotite + garnet + sillimanite. The program GEØ-CALC (version PTXss) with the data-base of Berman *et al.* (1987) was used to calculate P–T relations in these rocks.

P–T results are given in Table 3. The mineral assemblages in these rocks suggest peak metamorphic conditions at the transition between amphibolite and granulite facies, near 0.8 GPa and 700°C.

FLUID INCLUSIONS

Microthermometric measurements were made on fluid inclusions present in quartz from the matrix of two samples (BR-2, BR-3) and in a vein in BR-2. The quartz grains are very fractured, and there is no discernible pattern to the fractures or to the trails of fluid inclusions. Both fractures and trails of fluid inclusions cross grain boundaries. Evidence of decrepitation, leaking and necking down of inclusions is observed in all samples. However, apparently intact inclusions do occur.

These latter inclusions are very similar in size, shape and composition in the matrix and vein quartz. The inclusions range in size from 5 to 10

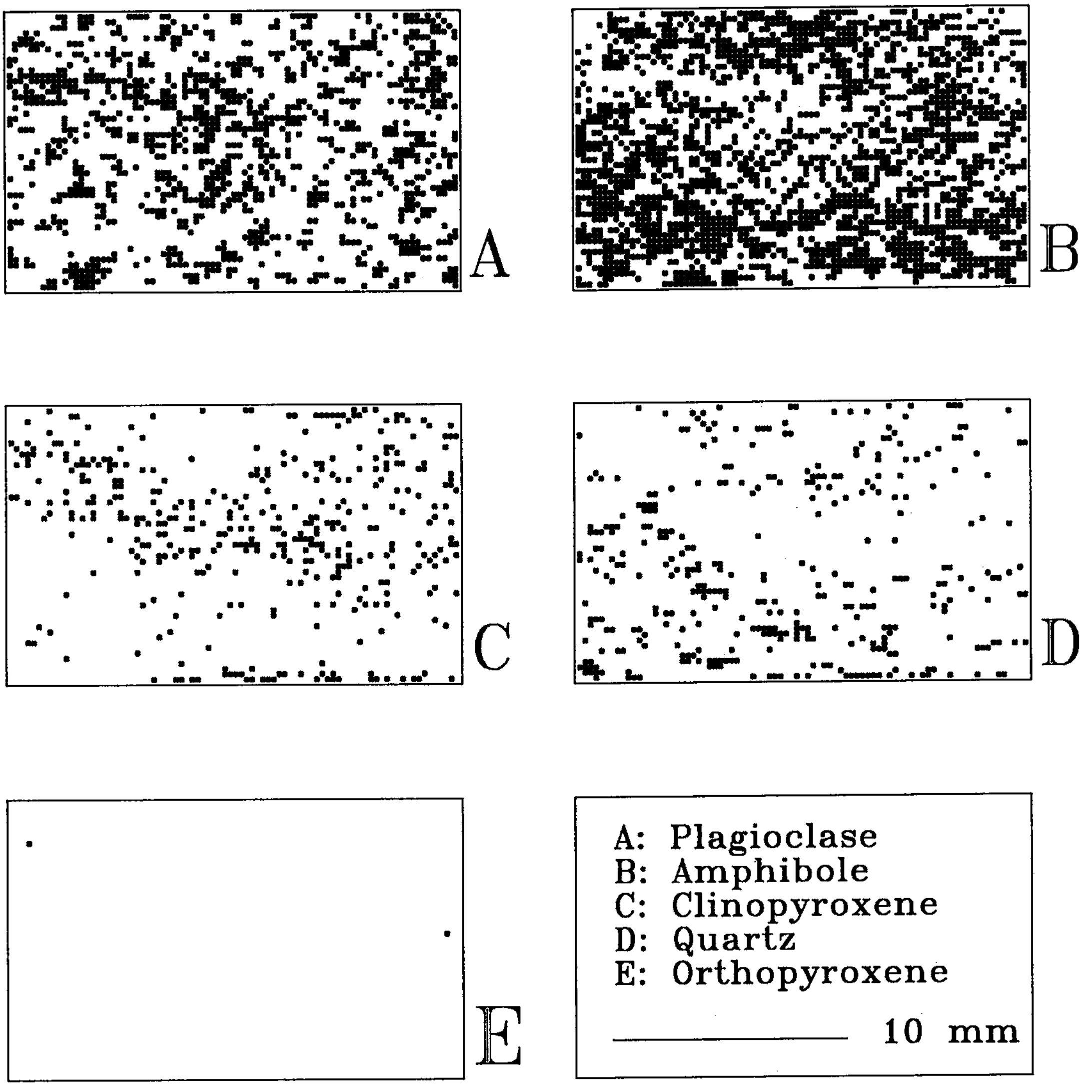

FIG. 3. Maps of the locations where the major phases were identified on a thin section from BR-2. Adjacent locations on the maps are 200 μm apart. Note that the phases are not homogeneously distributed across the thin section.

μm and in shape from round to irregular. Sample preparation and procedures follow the methods described by Hollister *et al.* (1981) and Stout *et al.* (1986). Density, $X(H_2O)$, wt.% NaCl equivalents and isochores were calculated with the computer programs of Nicholls & Crawford (1985).

Melting and homogenization temperatures indicate the presence of both slightly saline H_2O-rich and essentially pure CO_2-rich fluids in the inclusions in both matrix and vein quartz. No clathrate was observed in the H_2O-rich inclusions, and no melting-temperature depression was observed in the CO_2-rich inclusions nor in some of the H_2O-rich inclusions. The wt.% NaCl equivalents range from zero to approximately 2, but most H_2O-rich inclusions have melting temperatures of near -0.03 ± 0.2°C, indicating a wt.% NaCl equivalent of less than 0.4.

The range in densities of these inclusions also is similar in both matrix and vein quartz, but the H_2O-rich inclusions are more dense (0.90 to 0.95 g cm^{-3}) than the CO_2-rich inclusions (0.66 to 0.74 g cm^{-3}). Isochores show that neither compositional set of inclusions could have formed near the pressures and temperatures of metamorphism estimated from the mineral assemblages in these

TABLE 2. ELECTRON MICROPROBE COMPOSITIONS OF ORTHOPYROXENES, THREE VALLEY GAP BOUDINS

	BR-3 c	BR-3 m1	BR-3 m2	BR-3 ma	BR-3 r
SiO_2	50.84	50.98	50.28	50.44	51.08
TiO_2	0.02	0.04	0.03	0.04	0.03
Al_2O_3	1.56	1.18	3.23	2.26	1.43
FeO	27.71	27.95	26.64	27.43	28.02
MnO	0.89	0.88	0.70	0.80	0.91
MgO	18.66	18.41	17.60	17.96	18.49
CaO	0.58	0.58	0.58	0.58	0.55
Na_2O	<0.02	<0.02	<0.02	<0.02	<0.02
Total	100.26	100.02	99.06	99.51	100.51
Number of ions on the basis of 12 positive charges					
Si	1.945	1.957	1.933	1.941	1.951
Al^{iv}	0.055	0.043	0.067	0.059	0.049
Sum	2.000	2.000	2.000	2.000	2.000
Ti	0.001	0.001	0.001	0.001	0.001
Al	0.015	0.011	0.080	0.043	0.015
Fe^{2+}	0.887	0.897	0.857	0.883	0.895
Mn	0.029	0.029	0.023	0.026	0.029
Mg	1.064	1.053	1.009	1.030	1.053
Ca	0.024	0.024	0.024	0.024	0.023
Na	—	—	—	—	—
Sum	2.020	2.015	2.994	2.007	2.016
Thompson Components					
Di	1.0000	1.0000	1.0000	1.0000	1.0000
mc	0.9767	0.9765	0.9759	0.9763	0.9778
tk	0.0351	0.0274	0.0746	0.0520	0.0325
fm	0.8698	0.8840	0.8629	0.8765	0.8809
mt	0.0006	0.0011	0.0009	0.0011	0.0008
mm	0.0283	0.0282	0.0230	0.0259	0.0290

c = core; m = middle; r = rim; a = average

rocks. The isochores of the low-density CO_2-rich inclusions intersect the isochores of the higher-density H_2O-rich inclusions at approximately 750 bars and 150 to 200°C.

The most obvious interpretation of these data is that the inclusions formed during a late event associated with a low-pressure - low-temperature influx of fluid, or with the disruption and consequent breakdown of original high-pressure - high-temperature fluid inclusions, or both. This interpretation is consistent with the highly fractured texture of the quartz in both the matrix and veins and with the disrupted nature of many of the fluid inclusions.

CHEMICAL VARIATIONS AND THEIR CAUSES

Bulk-rock compositions and element ratios are listed in Table 4. The ratios Ti/Al and P/Al are relatively constant in comparison with uncertainty expected from the analytical procedures. The standard deviation for the Ti/Al values from samples BR-2 to BR-5 is 0.001, whereas the uncertainty arising from the analytical procedures also is 0.001. The analogous values for P/Al are 0.002 and 0.001. The confidence level for rejecting the hypothesis: *the variance in the ratios is less than expected from analytical uncertainty* is 65% for Ti/Al and 79% for P/Al (see Meyer 1975, Russell & Nicholls 1988). If we use a 95% confidence level as a criterion for rejection, then there is no evidence that the ratios are different from rock to rock. Therefore, Al, Ti and P are conserved elements, that is, the boudin acted as a system closed to these elements.

Chemical variations produced by igneous processes acting on basaltic systems are controlled by the stoichiometry of olivine, pyroxene and plagioclase (see Pearce 1968, Russell & Nicholls 1988), which produce distinctive trends on Pearce element-ratio diagrams. None of the element-ratio diagrams designed to show the effects of the sorting of igneous minerals display the trends expected for igneous rocks (*e.g.*, Fig. 4). We conclude that the chemical variations in the boudin are not due to internal igneous processes because:

1. Plagioclase fractionation or accumulation (sorting) would require a variation in Al. This conclusion is true whether or not other phases fractionated or accumulated. As shown above, Al is conserved. Therefore, plagioclase cannot have accumulated or fractionated.
2. The ratio (Fe + Mg)/Al (Fig. 4A) does not define a coherent trend. Consequently, fractionation or accumulation of ferromagnesian igneous assemblages cannot have produced the variation. This conclusion depends on the truth of point 1, because scatter could be generated by plagioclase accumulation.
3. Augite sorting, with or without olivine, cannot account for the variation because the [0.5 (Fe + Mg) + Ca]/Al *versus* Si/Al diagram shows no trend. If augite and olivine fractionation or accumulation caused the chemical variations, the data should define a slope of one on Figure 4B.
4. Because Ti is conserved, oxide fractionation or accumulation cannot be the cause of the variation.
5. Assimilation of pelitic country-rocks is not a viable hypothesis because Al is conserved.

The chemical variations among the boudin samples cannot be ascribed to igneous processes. Consequently, we turn to metamorphic processes as the cause.

THOMPSON SPACE

Thompson (1982a, b) showed that compositions of rocks and minerals can be mathematically transformed into a set of additive and exchange components. The additive components, one per mineral phase, correspond to standard end-member mineral formulae; for example, $CaMgSi_2O_6$ is an additive component for pyroxenes. In addition to representing a chemical composition, the additive components also represent the amount of the

TABLE 3. PRESSURE-TEMPERATURE ESTIMATES OF METAMORPHISM OF THREE VALLEY GAP AMPHIBOLITES

Sample/ Rock Type	P GPa	T°C	Mineral Assemb	Solution Model	Reference
Pelitic Gneiss		745	Grt-Bt		Ferry & Spear (1978)
Pelitic Gneiss		685	Grt-Bt		Thompson (1976)
Pelitic Gneiss	0.61	(700)	Grt-Pl-Sil-Qtz		Ghent *et al.* (1979)
Amphibolite		710	Grt-Cpx	$K_D = 6.9 \pm 0.45$	Ellis & Green (1979)
Amphibolite		820	Opx-Cpx		Wood & Banno (1973)
Amphibolite		850	Opx-Cpx		Wells (1977)
Amphibolite		710			Lee & Ganguly (1988)
Amphibolite		770			Lee & Ganguly (1988)
Amphibolite	0.8	700	Grt-Pl-Sil-Qtz	1) Grt 2) Pl	Ghent *et al.* (1979)
			Grt-Bt		Ferry & Spear (1978)
Amphibolite BR-3	0.77	(700)	Cpx-Pl-Grt-Qtz	1) Grt 2) Pl 3) Cpx	Berman *et al.* (1987)
Amphibolite BR-3	0.83	(700)	Opx-Pl-Grt-Qtz	1) Grt 2) Pl 3) Opx	Berman *et al.* (1987)
Pelitic Gneiss	0.8	(700)	Cpx-Pl-Grt-Qtz	1) Grt 2) Pl 3) Cpx	Berman *et al.* (1987)
Pelitic Gneiss BR-1Y, BR- 2Y	0.82-0.825	(700)	Opx-Pl-Grt-Qtz	2) Pl 3) Opx 4) Grt	Berman *et al.* (1987)

1) Crystalline solution model, Berman (unpublished)
2) Crystalline solution model, Fuhrman & Lindsley (1988)
3) Ideal solution model, Wood (1976)
4) Solution model, Ganguly & Saxena (1984)
Abbreviations of mineral names are from Kretz (1983).

mineral phase. Assigning a value to $CaMgSi_2O_6$, for example, fixes the amount of pyroxene in the system. The exchange components correspond to the elemental substitutions in minerals; for example, $NaSiCa_{-1}Al_{-1}$ represents the coupled substitution in feldspar. The advantage of transforming rock, mineral and modal compositions to Thompson space lies in the common chemical frame of reference the space provides. Modes, rock compositions and mineral compositions can be compared directly for consistency. In this section, examples of the transformation from rock composition or mineral formula to Thompson space are described. Names of the additive components begin with a capital letter and are written in standard type (*e.g.*, Di for $CaMgSi_2O_6$), whereas exchange components are distinguished by lowercase letters and italic type. The names of the exchange components are two letters from the name of a phase or end member that is characterized by that substitution, for example, *pl* and *tk* for plagioclase and tschermak represent the exchanges $NaSiCa_{-1}Al_{-1}$ and $Al_2Mg_{-1}Si_{-1}$, or are the first letters of the elements in the exchange, for example, *fa* and *ca* represent the exchanges $FeAl_{-1}$ and $CrAl_{-1}$ (see Table 5).

We will illustrate the use of Thompson space by calculating the spaces that represent the Three Valley Gap boudin. First, the rock compositions are converted to Thompson spaces, and then Thompson spaces for the constituent minerals are calculated, with specific examples for feldspars and amphiboles. From the set of Thompson components that corresponds to the mineral assemblages in the rocks, we relate the modes to the limiting boundaries of the space and show that there have been significant changes in composition within the boudin.

TABLE 4. COMPOSITIONS OF THREE VALLEY GAP AMPHIBOLITES, IN WEIGHT PERCENT, AND THEIR ELEMENT RATIOS AND THOMPSON COMPONENTS

	BR-2	BR-3	BR-4	BR-5
SiO_2	53.60	52.80	55.14	51.36
TiO_2	0.61	0.63	0.68	0.67
Al_2O_3	14.06	14.47	14.49	14.57
Fe_2O_3	1.04	1.22	1.30	1.29
FeO	7.33	7.75	7.71	8.35
MnO	0.17	0.12	0.12	0.18
MgO	7.92	7.33	5.98	8.16
CaO	10.83	10.65	8.93	10.42
Na_2O	1.83	2.57	2.84	2.34
K_2O	0.60	0.65	1.03	0.97
P_2O_5	0.16	0.08	0.10	0.10
Total	98.15	98.27	98.32	98.41
	Element Ratios			
Si/Al	3.235	3.096	3.229	2.991
Ti/Al	0.028	0.028	0.030	0.029
Fe/Al	0.417	0.434	0.435	0.463
Mn/Al	0.009	0.006	0.006	0.009
Mg/Al	0.712	0.641	0.522	0.708
Ca/Al	0.700	0.669	0.560	0.650
Na/Al	0.214	0.292	0.322	0.264
K /Al	0.046	0.049	0.077	0.072
P /Al	0.008	0.004	0.005	0.005
	Thompson Components, normalized to 100 moles of oxygens atoms			
Di	3.803	6.291	2.965	8.530
An	9.603	7.760	10.249	6.075
mc	3.974	3.713	3.488	4.394
tk	−2.815	−0.289	−2.497	1.500
pl	2.593	3.512	4.083	3.510
fm	3.685	3.916	3.860	4.245
kn	0.460	0.501	0.787	0.752
mt	0.276	0.286	0.306	0.306
fa	0.471	0.555	0.586	0.590
mm	0.087	0.061	0.061	0.093
Ap	0.027	0.014	0.017	0.017

TABLE 5. THOMPSON COMPONENTS IN BASALT AND AMPHIBOLITE ASSEMBLAGES

Initial Assemblage:			**Metamorphic Assemblages:**		
Additive Components			Additive Components		
Diopside	$CaMgSi_2O_6$	(Di)	Diopside	$CaMgSi_2O_6$	(Di)
Anorthite	$CaAl_2Si_2O_8$	(An)	Anorthite	$CaAl_2Si_2O_8$	(An)
Apatite	$Ca_5P_3O_{12}(OH)$	(Ap)	Apatite	$Ca_5P_3O_{12}(OH)$	(Ap)
			Tremolite	$Ca_2Mg_5Si_8O_{22}(OH)_2$	(Tr)
			Quartz	SiO_2	(Q)
			Grossular	$Ca_3Al_2Si_3O_{12}$	(Gr)
Exchange Components			Exchange Components		
$MgCa_{-1}$	(*mc*)		$MgCa_{-1}$	(*mc*)	
$Al_2Mg_{-1}Si_{-1}$	(*tk*)		$Al_2Mg_{-1}Si_{-1}$	(*tk*)	
$NaSiCa_{-1}Al_{-1}$	(*pl*)		$NaSiCa_{-1}Al_{-1}$	(*pl*)	
$FeMg_{-1}$	(*fm*)		$FeMg_{-1}$	(*fm*)	
KNa_{-1}	(*kn*)		KNa_{-1}	(*kn*)	
$MgTiAl_{-2}$	(*mt*)		$MgTiAl_{-2}$	(*mt*)	
$FeAl_{-1}$	(*fa*)		$FeAl_{-1}$	(*fa*)	
$MnMg_{-1}$	(*mm*)		$MnMg_{-1}$	(*mm*)	
$BaCa_{-1}$	(*bc*)		$NaAlSi_{-1}$	(*ed*)	
			$BaCa_{-1}$	(*bc*)	

The initial, pre-metamorphic, assemblage is a hypothetical assemblage expected for a basaltic composition.

THOMPSON COMPONENTS FOR A ROCK COMPOSITION

The easiest procedure to implement on a computer is to pick an initial set of Thompson components and convert all rock compositions to this set. The initial set may or may not be the most appropriate set for the rock in question. However, any other set of Thompson components can be obtained from linear combinations of components in the initial set. An example of this operation will be provided later. For the moment, our concern is

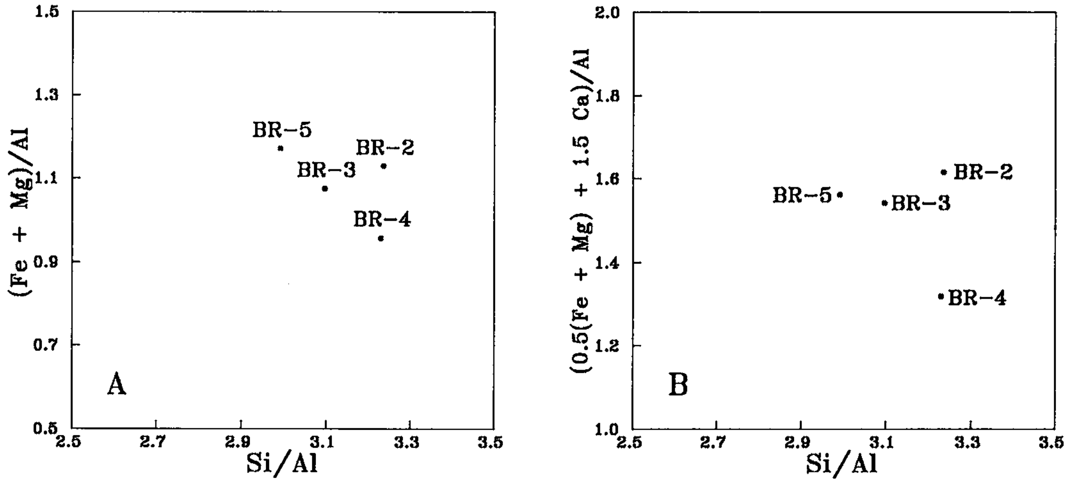

FIG. 4. A. Plot of (Fe + Mg)/Al *versus* Si/Al. B. Plot of [0.5(Fe + Mg) + 1.5 Ca]/Al *versus* Si/Al. If the sorting of pyroxene and olivine caused the chemical variations in the boudins, the data should define trends with a positive slope in 4A and a slope of one in 4B.

the selection of the initial set into which we will transform our rock composition.

The restrictions on the set of Thompson components that we calculate from a rock composition are few. There must be at least one additive component (Thompson 1982a, p. 20); the other components needed to represent the rock composition can be exchange components. In spite of the relative simplicity of one additive component per composition, it is more in keeping with traditional views of geochemical constituents that we assign one additive component to represent the mafic phases and a second to represent the felsic phases. An obvious example of this dichotomy is Bowen's reaction series. We will use $CaMgSi_2O_6$ and $CaAl_2Si_2O_8$ as the two additive components in the initial set of Thompson components for each rock composition because the chemistry of the boudins suggests a basaltic protolith (Ghent *et al.* 1977) and because basalts, which are essentially plagioclase–pyroxene assemblages, are among the most abundant rocks on earth.

P_2O_5 is present in detectable amounts in basalts only in apatite. Consequently, there is no convenient exchange component involving phosphorus that occurs in any abundance in the major phases. To account for the P_2O_5 in a rock, we will use a third additive component, $Ca_5P_3O_{12}(OH)$, but ignore the OH when making the conversion from oxide weight percentages to Thompson components.

Given a rock composition in weight percent oxides, the first step is to convert from weight percentages to moles of oxides by dividing by the appropriate molecular weights. The second step, transformation from moles to Thompson components, is a simple change of basis that can be accomplished by a matrix multiplication. In general, the number of Thompson components must equal the number of oxides reported. If the oxides are: SiO_2, TiO_2, Al_2O_3, Fe_2O_3, FeO, MnO, MgO, CaO, Na_2O, K_2O, and P_2O_5, then eleven Thompson components are required to represent the rock composition. The set of initial components and the formulae are listed in Table 5. As we will see later, this equality in number of oxides and Thompson components is not always required because mineral stoichiometry forces us to use fewer Thompson components than the number of oxide concentrations that result from a typical analysis.

To transform the oxides into the designated set of Thompson components, we require an (11 × 11) transformation matrix. The easiest way to proceed is to write down the matrix that would transform a set of Thompson components back into oxides and then find the inverse. The matrix that would transform a vector of Thompson components:

$$[\mathrm{Di}, \mathrm{An}, mc, tk, pl, fm, kn, mt, fa, mm, \mathrm{Ap}]^T \tag{1}$$

into a vector of oxide mole numbers:

$$[\mathrm{SiO_2}, \mathrm{TiO_2}, \mathrm{Al_2O_3}, \mathrm{Fe_2O_3}, \mathrm{FeO}, \mathrm{MnO}, \mathrm{MgO}, \mathrm{CaO}, \mathrm{Na_2O}, \mathrm{K_2O}, \mathrm{P_2O_5}]^T \tag{2}$$

can be written down immediately and is:

$$\mathbf{A} = \begin{vmatrix} 2 & 2 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & -1/2 & 0 & 0 & -1 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & -1 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\ 1 & 1 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 5 \\ 0 & 0 & 0 & 0 & 1/2 & 0 & -1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3/2 \end{vmatrix} \tag{3}$$

In other words, if one is supplied with a column of numbers representing a set of Thompson components for a rock, then the oxides can be recovered by multiplying the column by matrix **A**.

The inverse of matrix **A** converts a vector of mole numbers of oxides into the vector of Thompson components:

$$\mathbf{A}^{-1} = \begin{vmatrix} -1 & -1 & 1/2 & 1/2 & 3/2 & 3/2 & 3/2 & 3/2 & 11/2 & 11/2 & -5 \\ 1 & 1 & 0 & 0 & -1 & -1 & -1 & -1 & -4 & -4 & 10/3 \\ 0 & 0 & 1/2 & 1/2 & 1/2 & 1/2 & 1/2 & -1/2 & -1/2 & -1/2 & 5/3 \\ -1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 5 & 5 & -10/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2/3 \end{vmatrix} \tag{4}$$

If we name the column vector of oxides **O** and the vector of Thompson components **T**, then the two are related by the multiplication operations:

$$\mathbf{O} = \mathbf{A}\,\mathbf{T} \tag{5}$$

$$\mathbf{T} = \mathbf{A}^{-1}\,\mathbf{O} \tag{6}$$

The initial set of Thompson components for the compositions of the Three Valley Gap boudins are listed in Table 4. The initial set of components has been normalized to 100 moles of oxygen atoms. Notice that three compositions have negative amounts of *tk* in the initial set (BR-2, BR-3, and BR-4). Experience demonstrates that basaltic compositions with normative Q (see CIPW norms in Ghent *et al.* 1977) produce negative values for *tk* in the initial set of Thompson components. The deficiency in *tk* can be removed in a fashion analogous to the desilication steps in the CIPW norm by converting a component in the initial set into at least one new component in Thompson space. In this instance, the presence of quartz in the rocks and Q in the norms suggests a conversion based on the reaction:

$$\mathrm{An} = \mathrm{Di} + \mathrm{Q} + tk \tag{7}$$

An equivalent set of Thompson components for BR-2 is:

	New (Q-bearing)	Old (*tk*-bearing)
Di	6.618	3.803
An	6.788	9.603
Q	2.815	0.0
tk	0.0	-2.815

The remaining components in the new set are identical to those in the initial set. Notice that the new set could represent a plagioclase - pyroxene - quartz assemblage and that the procedure very much mimics a desilication step in the CIPW norm; the amount of plagioclase (An) is decreased, and the amounts of pyroxene (Di) and quartz (Q) increased until the negative amount of *tk* is increased to zero.

If the rock for which we have a composition consists of the assemblage garnet - plagioclase - quartz (no pyroxene), then a transformation such as:

$$\mathrm{Di} + \mathrm{An} = \mathrm{Gr} + \mathrm{Q} + \mathrm{mc} \tag{8}$$

will change the initial set of Thompson components into a new set that matches the mineral assemblage of the rock. For example, the composition of BR-2 can be cast as the components:

	Gr + An-bearing	Qtz-bearing	Pl + Augite-bearing
Di	0.0	6.618	3.803
An	0.170	6.788	9.603
Q	9.433	2.815	0.0
Gr	6.618	0.0	0.0
tk	0.0	0.0	-2.815
mc	10.592	3.974	3.974

The main point of this discussion is: Thompson space can represent the composition of a single rock in a variety of ways. The representation can be chosen to best reflect the mineral assemblage found in the rock.

Some transformations that can be used to convert the initial set of Thompson components to sets that can represent other assemblages are:

Fo $2\,\mathrm{Di} + mc + tk = \mathrm{An} + \mathrm{Fo}$ Olivine (9)

Ne $2\,\mathrm{Di} + 2\,tk + pl = \mathrm{An} + \mathrm{Ne}$ Nepheline (10)

Sp $2\,\mathrm{Di} + 2\,tk + mc = \mathrm{An} + \mathrm{Sp}$ Spinel (11)

Co $\mathrm{Di} + 2\,tk + mc = 2\,\mathrm{Co}$ Rhombohedral oxide (12)

THOMPSON COMPONENTS IN MINERALS

The Thompson components of minerals could be constructed with the same matrix operations and matrices used to define the components of a rock composition. This procedure would not take advantage of the stoichiometry of minerals, however. A Di component in plagioclase would not make much sense. Stoichiometry in minerals creates dependencies in the amounts of the elements in a given amount of phase. For example, the ratio of divalent cations (Fe, Mg, Ca, Ni, *etc.*) to Si in olivine is two. Consequently, transformation of a mineral composition into a set of Thompson components for that mineral generally requires fewer equations than the number of cations reported.

Standard chemical formulae for minerals, based on the number of moles of oxygen atoms, explicitly show the stoichiometry. Transformations of mineral compositions into Thompson components can take advantage of the stoichiometry if the starting positions are the mineral formulae rather than a composition in weight percentages of the oxides. It is implicit in the following discussion that a mineral composition has been converted to a standard formula (see Table 2).

THOMPSON COMPONENTS IN FELDSPARS

The expected substitutions in feldspars are the coupled substitution, Na + Si = Ca + Al (*pl*), and the cation substitutions, Ba = Ca (*bc*) and K = Na (*kn*). To represent a feldspar composition as a set of Thompson components, we need a method of calculating four numbers: An (the required additive component), *pl*, *kn* and *bc* (three exchange components). Equations relating element abundances and abundances of the Thompson components in a feldspar are:

$$2\,\mathrm{An} + pl = \mathrm{Si} \tag{13}$$

$$2\,\mathrm{An} - pl = \mathrm{Al} \tag{14}$$

$$\mathrm{An} - pl - bc = \mathrm{Ca} \tag{15}$$

$$pl - kn = \mathrm{Na} \tag{16}$$

$$kn = \mathrm{K} \tag{17}$$

$$bc = \mathrm{Ba} \tag{18}$$

where Si, Al, Ca, *etc.*, are the number of cations in a feldspar formula, based on eight moles of oxygen atoms.

There are more equations than unknowns; the system is overdetermined. The easy way to proceed is to realize that the amount of feldspar can be determined from the amounts of Si plus Al or from the amounts of the cations, Ca, Na, K and Ba. With this consideration, it is easy enough to show that we can calculate An from either of the two relations:

$$\mathrm{An} = (\mathrm{Si} + \mathrm{Al})/4 \tag{19}$$

$$\mathrm{An} = \mathrm{Ca} + \mathrm{Na} + \mathrm{K} + \mathrm{Ba} \tag{20}$$

The question is, which of the two is the better to use? Propagation of typical analytical errors from a microprobe analysis of plagioclase in basalt gives approximate uncertainties in the calculated value of An (as a Thompson Component) of 0.021 from the Si + Al calculation and 0.016 from the equation based on principal cations (see, for example, Nicholls & Stout 1988). Consequently, the second of the two is preferable.

Having calculated An with either Equation (19) or Equation (20), Equations (16)–(18) can be used to find the remaining Thompson components for a feldspar formula. The final step is to normalize the result so that the set of Thompson components for the feldspar has eight moles of oxygen atoms. This means that we normalize the results so that An is one. Thompson components for the Three Valley Gap minerals are listed in Table 6.

THOMPSON COMPONENTS IN AMPHIBOLES

We assume that the structural formula of an amphibole can be adequately represented by the cations: Si, Ti, Al, Fe^{3+}, Fe^{2+}, Mn, Mg, Ca, Na, K, OH, F, and Cl. The Thompson components representing amphibole compositions are: Tr, *mc*, *tk*, *pl*, *fm*, *kn*, *mt*, *fa*, *mm*, *ed*, *fh*, and *ch*, where $fh = \mathrm{F(OH)}_{-1}$, $ch = \mathrm{Cl(OH)}_{-1}$ and the remaining abbreviations are defined in Table 5.

The transformation matrix that converts an amphibole formula based on 46 negative charges into the listed set of Thompson components is:

$$\begin{array}{cccccccccc|c}
\mathrm{Si} & \mathrm{Ti} & \mathrm{Al} & \mathrm{Fe}^{3+} & \mathrm{Fe}^{2+} & \mathrm{Mn} & \mathrm{Mg} & \mathrm{Ca} & \mathrm{Na} & \mathrm{K} & \\
2/23 & 2/23 & 3/46 & 3/46 & 1/23 & 1/23 & 1/23 & 1/23 & 1/46 & 1/46 & \mathrm{Tr} \\
-3/23 & -3/23 & 7/46 & 7/46 & 10/23 & 10/23 & 10/23 & -13/23 & -13/46 & -13/46 & mc \\
7/23 & 30/23 & 11/23 & 11/23 & -8/23 & -8/23 & -8/23 & -8/23 & -4/23 & -4/23 & tk \\
7/23 & 7/23 & -1/46 & -1/46 & -8/23 & -8/23 & -8/23 & -8/23 & 15/46 & 15/46 & pl \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & fm \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & kn \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & mt \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & fa \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & mm \\
-7/23 & -7/23 & 1/46 & 1/46 & 8/23 & 8/23 & 8/23 & 8/23 & 31/46 & 31/46 & ed
\end{array} \tag{21}$$

TABLE 6. THOMPSON COMPONENTS OF MINERALS

		BR-2 Cores			BR-3 Cores	
	Pl	Amph	Cpx	Pl	Amph	Cpx
pl	0.3811		0.0173	0.5121		0.0295
kn	0.0081	0.1779		0.0201	0.2162	
mc		0.1171	0.0661		0.1544	0.1086
tk		0.8980	0.0433		0.9264	0.0662
fm		1.5316	0.2537		1.7432	0.3200
mt		0.1027	0.0022		0.1118	0.0025
mm		0.0323	0.0113		0.0352	0.0119
fa		0.1591			0.1448	
ed		0.5480			0.6455	
$pl^{\mathrm{Di}}/pl^{\mathrm{An}}$		0.0454			0.0576	
$kn^{\mathrm{An}}/kn^{\mathrm{Tr}}$		0.0455			0.0930	
$mc^{\mathrm{Di}}/mc^{\mathrm{Tr}}$		0.5645			0.7034	
$tk^{\mathrm{Di}}/tk^{\mathrm{Tr}}$		0.0482			0.0715	
$fm^{\mathrm{Di}}/fm^{\mathrm{Tr}}$		0.1656			0.1836	
		BR-4 Cores			BR-5 Cores	
	Pl	Amph	Cpx	Pl	Amph	Cpx
pl	0.5858	0.0000	0.0160	0.5206	0.0000	0.0167
kn	0.0103	0.2388		0.0177	0.2029	
mc		0.1410	0.0687		0.0894	0.0656
tk		0.9023	0.0284		0.9748	0.0276
fm		1.7206	0.3151		1.5728	0.3081
mt		0.1329	0.0014		0.0952	0.0011
mm		0.0377	0.0130		0.0312	0.0124
fa		0.1268			0.2055	
ed		0.6593			0.5341	
$pl^{\mathrm{Di}}/pl^{\mathrm{An}}$		0.0273			0.0321	
$kn^{\mathrm{An}}/kn^{\mathrm{Tr}}$		0.0431			0.0872	
$mc^{\mathrm{Di}}/mc^{\mathrm{Tr}}$		0.4872			0.7338	
$tk^{\mathrm{Di}}/tk^{\mathrm{Tr}}$		0.0315			0.0283	
$fm^{\mathrm{Di}}/fm^{\mathrm{Tr}}$		0.1831			0.1959	

The additive components (An, Tr and Di) for all the phases are equal to one. Abbreviations of mineral names are from Kretz (1983) except for Amph = amphibole

The rows and columns of the matrix used to convert Cl and F to $\mathrm{Cl(OH)}_{-1}$ and $\mathrm{F(OH)}_{-1}$ are left out to save space. The augmented matrix can be obtained by putting a 1 in the appropriate position, and 0 elsewhere.

There is obviously a correlation between Thompson components and the procedure used to calculate the amphibole formula. For example, if all the iron is left as FeO, as measured with a microprobe, then the amphiboles in the Three Valley Gap boudins have negative values for *pl*. If the Fe is apportioned to have Fe^{2+} and Fe^{3+} consistent with maximum degree of oxidation, then *pl* is equal to zero. Without measured values of Fe^{2+} and Fe^{3+}, amounts of the calculated Thompson components in an amphibole composition remain as uncertain as the values of Fe^{2+} and Fe^{3+} in a structural formula.

Methods used to convert the structural formulae of pyroxene and garnet are given in the Appendix.

THOMPSON COMPONENTS IN THREE VALLEY GAP MINERALS

Thompson components for the major minerals in the Three Valley Gap boudin are listed in Tables 2 and 6. Like other components, Thompson components can be treated as thermodynamic variables (Thompson 1982b). Consequently, the distribution of a particular component, *pl* for example, between two phases at equilibrium should depend on P, T and the nature of the phases. If the Thompson components behave approximately ideally and if the parts of the boudin all formed under the same conditions, then the ratios of the Thompson components between two phases should be approximately constant. The ratios of several Thompson components between two phases are listed in Table 6. The distributions are qualitatively consistent, the *pl* exchange component in plagioclase (pl^{An}) is always greater than the amount of *pl* in pyroxene (pl^{Di}) for example, but with the exception of the *fm* component, the ratios vary by factors in the range 1.5–2.5. The *fm* component, on the other hand, varies by a factor of approximately 1.2. It has been generally accepted that the Fe–Mg substitution in silicate minerals is commonly roughly ideal, whereas most other substitutions are nonideal. Presumably at least part of the variations in the ratios can be attributed to the nonideal nature of the solid solutions. Consequently, conversion of mineral compositions to Thompson components need not produce a more nearly ideal representation of a solid solution.

THOMPSON SPACE AND REACTION VARIABLES

Our ability to choose a set of Thompson components that can represent any mineral assemblage provides a way to describe a reaction space defined by the limits that a given rock composition can reach in terms of mineral abundances. A rock composition can be expressed in any number of different sets of Thompson components, each set corresponding to a different reaction-space. We pick a set that corresponds with the actual mineral assemblage in the rock. A fixed rock composition can be represented by different modal amounts of a mineral assemblage, depending on the conditions of formation (*e.g.*, pressure and temperature). The amounts assigned to the Thompson components can be changed to mimic the actual modal composition of the rock. In fact, a one-to-one relationship between the amounts of the Thompson components and the modal amounts can be devised. Consequently, Thompson components can represent mineral assemblages and modes as well (*e.g.*, Thompson *et al.* 1982).

The links between modal amounts and concentrations of Thompson components are chemical transformations involving additive ± exchange components. Within the initial set of Thompson components, there are no reactions we can write. Consequently, only one set of values can be assigned to the initial concentrations of the Thompson components. These are listed in Table 5 for the Three Valley Gap amphibolites. In order to write a reaction, we have to add another component to the set. If the component is an additive one, corresponding to another phase, then a net-transfer reaction results. Because quartz is a phase common to all the amphibolites in the study, it is realistic to add Q to the set of Thompson components. The resulting reaction is:

$$\mathrm{Di} + tk + \mathrm{Q} - \mathrm{An} = 0 \qquad (22)$$

This net-transfer reaction is equivalent to $CaAl_2SiO_6 + SiO_2 = CaAl_2Si_2O_8$. This reaction can also form one basis-vector, V_1, in the amphibolite reaction-space because a basis-vector is defined as a net-transfer reaction (Thompson 1982b). When amphibole becomes a stable phase, a second basis-vector is generated. The second basis-vector introduces another component, H_2O, to the system. If there is no possibility of making an exchange of the new component between phases, then the component is called an open-system component (Thompson 1982a). Two vectors in reaction space are:

$$V_1\!: \ \mathrm{Di} + tk + \mathrm{Q} - \mathrm{An} = 0 \qquad (23)$$

$$V_2\!: \ \mathrm{Tr} + 3\mathrm{Q} + ed - (7/2)\mathrm{Di} - \mathrm{An} - (3/2)\,mc - pl - \mathrm{H_2O} = 0 \qquad (24)$$

The second vector, V_2, can be written as a combination of:

$$4\,\mathrm{Q} + ed - \mathrm{An} - pl = 0$$

and:

$$\mathrm{Tr} - \mathrm{Q} - (7/2)\mathrm{Di} - (3/2)mc - \mathrm{H_2O} = 0$$

indicating that three independent basis-vectors are required to span the Thompson space of amphibolites. By combining these last two basis-vectors, we can quantitatively represent the modes on a two-dimensional diagram at the cost of combining modal amounts of two phases, Q and An (see below, p. 648).

EQUATIONS FOR LIMITING BOUNDARIES OF REACTION SPACE

The limiting boundaries of reaction space are constrained by the amounts of the Thompson components in the initial set. The extents to which the values of V_1 and V_2 [Equations (23) and (24)] can be changed from zero depend on the initial amounts of the components preceded by a negative sign [An in Equation (23) and An, Di, *mc*, and *pl* in Equation (24)]. The following equations define the zero isopleths or the limiting constraints [Equation (29)] required by mineral stoichiometry in the assemblages under consideration (see below):

$$\text{An} = 0{:}\quad V_2 = -V_1 + \text{An}_o \tag{25}$$

$$\text{Q} = 0{:}\quad V_2 = -(1/3)V_1 \tag{26}$$

$$\text{Top:}\quad V_2 = \min(mc_o, pl_o) \tag{27}$$

$$\text{Left:}\quad V_1 = -tk_o\ (tk = 0) \tag{28}$$

$$[pl]{:}\quad V_2 = V_1 - (\text{An}_o - pl_o) \tag{29}$$

$$\text{Di} = 0{:}\quad V_2 = (2/7)\,V_1 + \text{Di}_o \tag{30}$$

where $\min(mc_o, pl_o)$ is the smaller value for *mc* or *pl* in the initial set of Thompson components. The subscript o on the component symbol indicates an amount in the initial assemblage. The limiting boundaries for the reaction space for BR-2 are shown on Figure 5.

As an example, consider the isopleth for An = 0. Each unit change of V_1 in the positive direction causes the loss of one unit of An in the

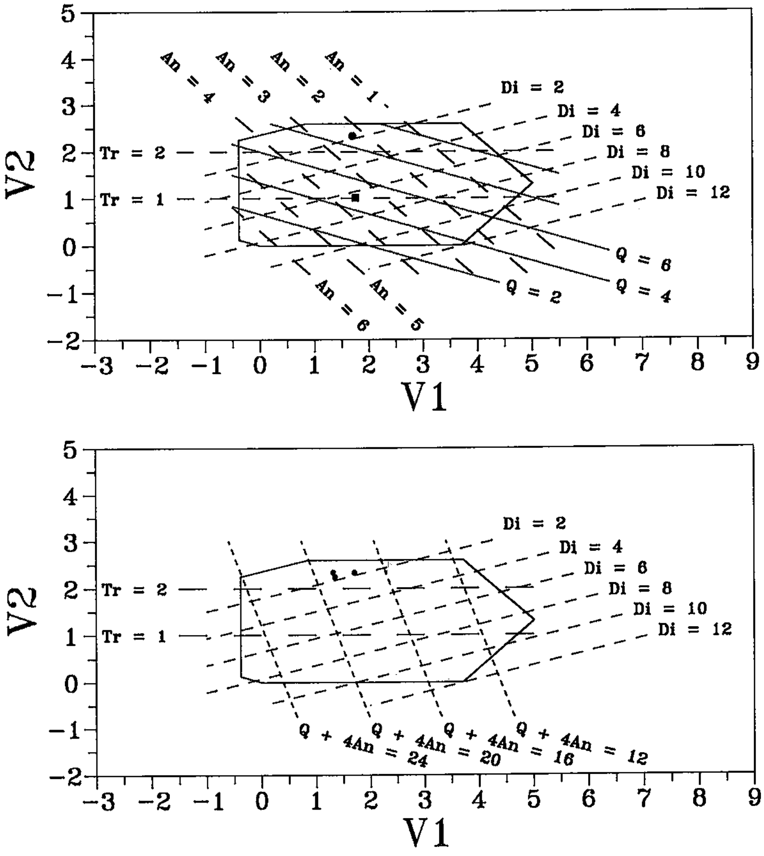

FIG. 5. Reaction space and isopleths for a basaltic composition derived from the modal composition of BR-2. Upper diagram shows the isopleths with An and Q contents as independent quantities. Dot marks the intersection of the Di and Tr isopleths for the modal amounts measured in thin section. The square marks the intersection of the An and Q isopleths for the modal amounts measured in thin section. The lower diagram is drawn with the amounts of Q and An constrained by Equation (45). Dots mark the intersections of the Tr and Di, the (Q + 4 An) and Tr, and the (Q + 4 An) and Di isopleths for the modal amounts of the minerals in the rock (Table 8). The zero isopleths are coincident with the solid lines marking the boundaries to the reactions spaces.

initial set of Thompson components. V_1 can change, at $V_2 = 0$, until it has a value equal to An_0, the initial amount of An calculated from the rock composition. V_2 also requires one unit of An for every unit increase in value. Consequently, concurrent changes in V_1 and V_2 are constrained by the sum:

$$V_1 + V_2 = An_0 \qquad (31)$$

A trivial rearrangement produces Equation (25). The other boundaries, limited by zero isopleths, are defined in an analogous manner (see Fig. 6).

Of particular interest is the limitation placed on the size of the reaction space by the *pl* component ($NaSiCa_{-1}Al_{-1}$). When $V_2 = 0$, the only phases in the boudins that can contain Na are plagioclase and pyroxene. In SiO_2-saturated basaltic and in amphibolitic rocks, the pyroxenes generally contain negligible amounts of Na. Consequently, at $V_2 = 0$, there must always be sufficient An to hold the initial amount of *pl* in the initial set of Thompson components. If we restrict the reaction space to assemblages reached by basaltic compositions in the amphibolite facies, then the maximum extent of V_1 is given by $An_0 - pl_0$. In amphiboles from the amphibolite facies, *pl* can be accommodated by a substitutional scheme such as (Thompson 1982a):

$$Tr + pl + ed = Na_2CaMg_5Si_8O_{22}(OH)_2 \qquad (32)$$

For a unit advance in V_2, there is created a unit of Tr that can accommodate one unit of *pl*. At

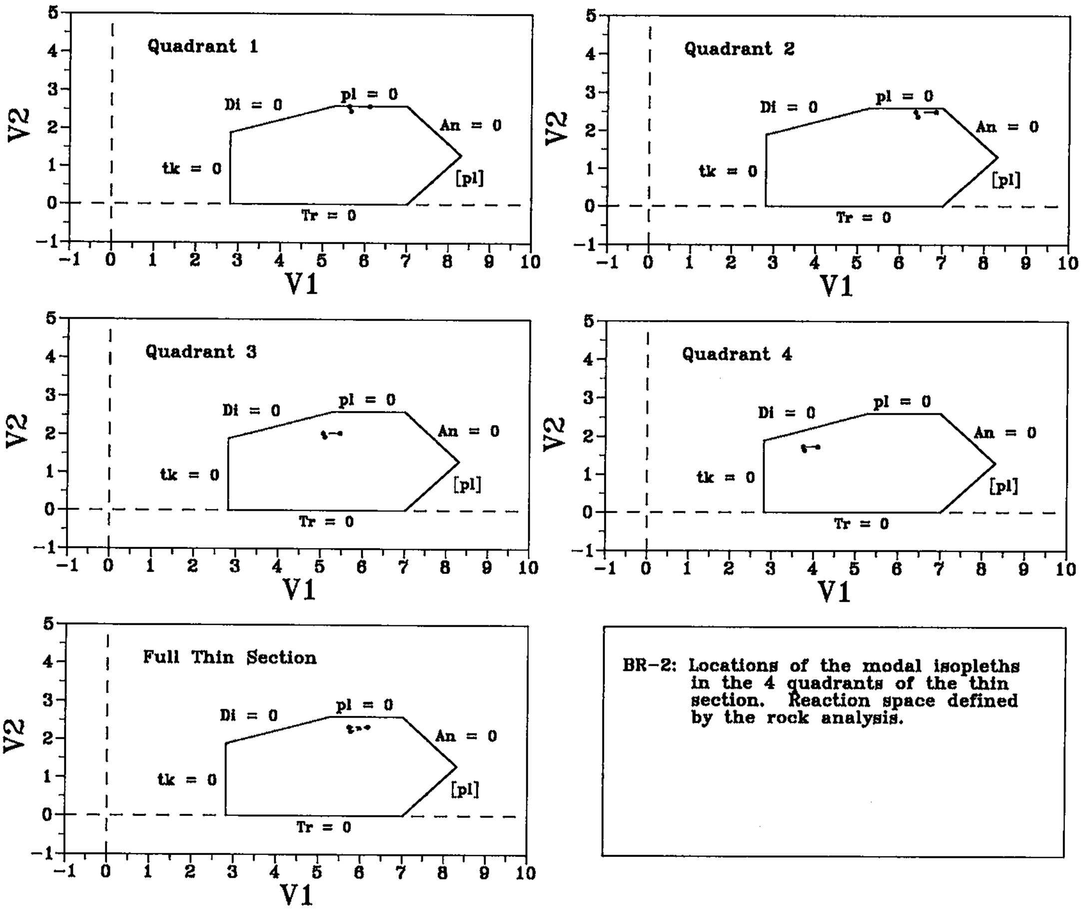

FIG. 6. Reaction space defined by the chemical compositions of BR-2 (see Table 4). Dots mark the intersections of the Tr and Di, the Tr and (Q + 4 An), and the Di and (Q + 4 An) isopleths defined by the modal amounts of these phases in the four quadrants of the thin section (see Table 1).

$V_2 = 1$, then, V_1 can increase by one more unit than it can at $V_2 = 0$. The limit placed on the reaction space where Na is essentially absent in pyroxene is a line given by Equation (29). If the reaction space is to represent assemblages where Na can enter the pyroxenes (*e.g.*, eclogites), then the [*pl*] limit will not apply, and the reaction space will extend along the V_1 axis until $V_1 = An_o$.

The top of the reaction space can be limited by several zero isopleths, depending on the initial composition of a rock. Because Di is produced by changes along V_1 and consumed by changes on V_2, the Di = 0 isopleth will intersect the An = 0 isopleth. If mc_o or pl_o is smaller than V_2 at the point of intersection, the top of the reaction space will be flat where V_2 is equal to the minimum of mc_o or pl_o. Otherwise, the top of the reaction space will be defined by the An = 0 and Di = 0 isopleths (*cf.* Figs. 6, 7).

EQUATIONS FOR MODE ISOPLETHS

Because a fixed composition (except for open-system components, *e.g.*, H_2O) can sustain only a limited amount of change along the basis-vectors of a reaction space, the boundaries usually mark a curve or surface along which a particular Thompson component is zero. Inside the space, the particular Thompson component is nonzero and, if it is an additive component for a phase, its amount lies on an isopleth for that phase. We can compare the modal amount of a phase as measured in thin section with the amount given by the isopleth in reaction space if both are converted to the same scale. The initial set of Thompson components are normalized to 100 moles of oxygen atoms. Consequently, modal amounts in volume percent need to be converted and normalized to the same value.

Molar properties of the amphibole, pyroxene, feldspar and garnet solid-solutions are easily obtained from representations in Thompson space. The molar volume, for example, is given by:

$$v = v_A + \Sigma x_i v_i \tag{33}$$

where v is the molar volume of the solid solution, v_A is the molar volume of the additive component, v_i is the molar volume of the exchange component i, and x_i is the number of moles of i in the solid solution relative to one mole of additive component (see Thompson 1982b). The volumes of the exchange components can be obtained from the volumes of the standard additive end-members of a solid solution. For example, the volume of the *pl* exchange component in feldspars is given by:

$$v_{pl} = v_{Ab} - v_{An} \tag{34}$$

where v_{Ab} and v_{An} are the molar volumes of albite and anorthite, respectively. The volumes used to calculate the compositions from the modes are listed in Table 7 (data from Robie *et al.* 1967, 1978, Berman 1988). Modes were recalculated to moles/100 moles of oxygen atoms by assigning 8 moles of oxygen atoms to feldspar, 6 to pyroxene, 22 to amphibole and 2 to quartz.

The equations for the isopleths can be derived from expressions relating the amount of a phase to the basis-vectors. For example, the pyroxene isopleth is given by:

$$Di = V_1 - (7/2)\, V_2 + Di_o \tag{35}$$

Rearranging:

$$V_2 = (2/7)\, V_1 + (2/7)(Di_o - Di) \tag{36}$$

where Di is the modal amount of Di in the rock.

Given the mode of the rock, in moles per 100 moles of oxygen atoms, where:

Tr = modal amphibole
Di = modal pyroxene
Q = modal quartz
An = modal plagioclase

The equations for the isopleths are:

$$V_2 = Tr \quad \text{Amphibole isopleth} \tag{37}$$

$$V_2 = -(1/3)\, V_1 + Q/3 \quad \text{Quartz isopleth} \tag{38}$$

$$V_2 = (2/7)\, V_1 + (2/7)(Di_o - Di) \quad \text{Pyroxene isopleth} \tag{39}$$

$$V_2 = -V_1 + (An_o - An) \quad \text{Feldspar isopleth} \tag{40}$$

Modes, in moles per 100 moles of oxygen atoms, chemical compositions derived from the modes, and the corresponding initial Thompson com-

TABLE 7. MOLAR VOLUMES OF THOMPSON COMPONENTS (cm^3)

	Q	An	CDi	ODi	Tr	Gr	Ap
	22.6900	100.7900	66.1900	66.1900	272.7000	125.3500	159.2000
mc		−3.5500	−3.5500	−4.0100	−4.0567		
tk			−2.6300	−2.6300	0.2400		
pl		−0.3600	−3.1600	−3.1600	−1.3800		
fm			2.1100	1.6400	1.9660	0.6433	
kn		8.2900			8.2900		
mt			3.9600	4.4300	4.1040	5.4267	
fa					0.4100	1.8850	
mm			1.9200	3.8380	1.9200	1.6567	
ed					2.0700		
ca			1.7575	1.7575			
nm							
bc		9.6600					
fh					−1.1200		
ch					4.6600		

CDi = Clinodiopside, ODi = Orthodiopside.

ponents are listed in Table 8. An example of a reaction space for an amphibolite with isopleths for quartz (Q), amphibole (Tr), pyroxene (Di) and plagioclase (An), is shown on Figure 5.

Ideally, the isopleths for each of the phases should intersect at a single point. Because the composition derived from a modal analysis need not coincide with the composition of a hand sample, the isopleths representing the measured modal amounts usually do not intersect at a point. The points of intersection can be obtained by solving the isopleth equations in pairs. Each intersection of a pair of isopleths represents an estimate of the consistency between the mode and the rock composition.

The intersections of the Di, An and Tr isopleths are given by:

$$\text{An, Tr:}\quad \begin{aligned} V_1 &= \mathrm{Tr} + (\mathrm{An_o} - \mathrm{An}) \\ V_2 &= \mathrm{Tr} \end{aligned} \qquad (41)$$

$$\text{Di, Tr:}\quad \begin{aligned} V_1 &= (7/2)\mathrm{Tr} - \mathrm{Di_o} + \mathrm{Di} \\ V_2 &= \mathrm{Tr} \end{aligned} \qquad (42)$$

$$\text{Di, An:}\quad \begin{aligned} V_1 &= (7/9)(\mathrm{An_o} - \mathrm{An}) - (2/9)(\mathrm{Di_o} - \mathrm{Di}) \\ V_2 &= -V_1 + \mathrm{An_o} - \mathrm{An} \end{aligned} \qquad (43)$$

where $\mathrm{An_o}$ and $\mathrm{Di_o}$ are the calculated amounts of the additive components in the initial set of Thompson components.

TABLE 8. MODES, RECALCULATED INTO UNITS OF MOLES/100 MOLES OF OXYGEN ATOMS, ROCK COMPOSITIONS, AND THOMPSON COMPONENTS CALCULATED FROM THE MEASURED MODES, IN VOLUME PERCENT, AND FROM THE MEASURED MINERAL COMPOSITIONS

	BR-2	BR-3	BR-4	BR-5
	Modes in moles/100 moles of oxygen atoms			
Pl	3.526	4.403	4.491	3.331
Cpx	1.799	1.498	2.988	1.520
Amph	2.336	1.947	2.073	2.443
Qtz	4.802	5.991	0.269	5.239
	Rock Compositions calculated from modes and mineral compositions (Weight %)			
SiO_2	51.89	54.01	50.04	52.66
TiO_2	0.52	0.49	0.60	0.50
Al_2O_3	14.49	14.88	14.60	13.82
FeO	8.53	8.47	9.14	9.30
MnO	0.18	0.18	0.22	0.18
MgO	8.48	6.88	8.12	8.08
CaO	12.44	10.84	12.66	11.56
Na_2O	1.85	2.59	2.90	2.10
K_2O	0.56	0.66	0.68	0.70
H_2O+	1.05	1.01	1.04	1.09
	Initial Thompson Components			
Di	8.268	5.867	13.408	7.994
An	6.299	5.100	2.444	6.505
mc	3.923	3.505	3.588	4.011
tk	0.394	–0.880	5.078	0.149
pl	2.596	3.509	3.973	2.999
fm	4.307	4.240	4.676	4.703
kn	0.434	0.502	0.530	0.542
mt	0.238	0.218	0.274	0.299
mm	0.094	0.090	0.115	0.093

Abbreviations of mineral names are from Kretz (1983) except for Amph = amphibole.

The isopleths for amphibole and pyroxene in the Three Valley Gap boudin define points in reaction space distinct from the points defined by the intersection of the isopleths for the felsic minerals, quartz (Q) and plagioclase (An) (see Fig. 5, which shows the reaction space for the composition derived from the mode of BR-2). The intersection of the Tr with the Di isopleth and the intersection of the An with the Q isopleth are marked with a dot and square, respectively, and are separate in the reaction space.

A large part of the discrepancy in location of the two intersections comes from the equivalence of Q and An as additive components:

$$\underset{\mathrm{Q}}{4\,\mathrm{SiO_2}} + \underset{ed}{\mathrm{NaAlSi_{-1}}} = \underset{\mathrm{An}}{\mathrm{CaAl_2Si_2O_8}} + \underset{pl}{\mathrm{NaSiCa_{-1}Al_{-1}}} \qquad (44)$$

In other words, by transferring exchange components between feldspar and amphibole, the mode can be adjusted to change the amounts of Q and An. Consequently, for a given mode, the amounts of Q and An are not independent (see above, p. 644). If Equation (44) is written as:

$$V_3\text{: } 4\,\mathrm{Q} + ed - \mathrm{An} - pl = 0 \qquad (45)$$

then the modal amount of Q in Thompson space is given by:

$$\mathrm{Q} = V_1 + 3\,V_2 + 4\,V_3 \qquad (46)$$

and the amount of An by:

$$\mathrm{An} = \mathrm{An_o} - V_1 - V_2 - V_3 \qquad (47)$$

The isopleths for constant amounts of (Q + 4 An) will be represented by contours in reaction space defined by:

$$V_2 = -3\,V_1 + 4\,(\mathrm{An_o} - \mathrm{An}) - \mathrm{Q} \qquad (48)$$

From the modes and mineral compositions, a chemical composition can be derived and compared to the composition from the rock analysis. The differences show up as different shapes for the reaction space if the two estimates of the rock composition are not consistent. Figure 6 shows the reaction space defined by the chemical composition of BR-2. Also shown on the diagrams are the locations of the intersections of the Tr-Di, Tr-(Q + 4 An) and Di-(Q + 4 An) isopleths defined by the modal amounts of the major minerals in the four quadrants of the thin section (see Table 1). If the reaction space were appropriate for all four quadrants (*i.e.*, if the results of the rock analysis represent the composition of the rock and the compositions derived from the modes of the four quadrants), then the different locations of the intersections would be the result of different conditions of crystallization (*e.g.*, P and T) in the various parts of the thin section. Because this seems unlikely, the different modes represent different compositions for the parts of the thin section; there are thus chemical gradients on the scale of the thin sections of the rocks.

Figure 7 shows a comparison of reaction spaces defined by the chemical compositions of the rocks

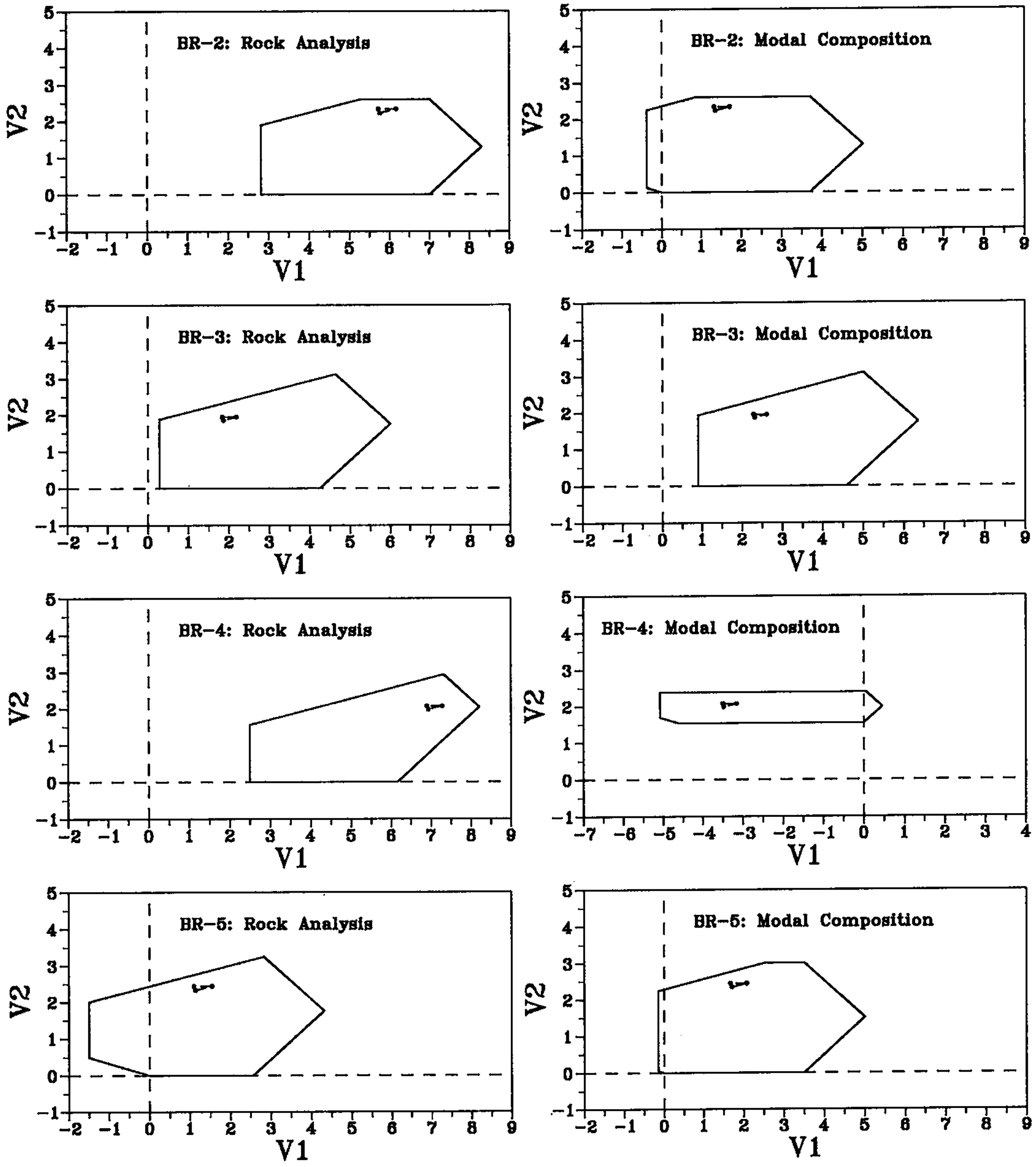

FIG. 7. Comparison of reaction spaces defined by the chemical compositions of the rocks and by the compositions derived from the modal amounts of the major minerals in the rocks (see Table 8).

with those defined by the compositions derived from the modal amounts of the major minerals in the rocks (see Table 8). In general, more Q-rich assemblages lie to the right and above the origin of the coordinate system (see Fig. 5). In BR-2 and BR-4, more quartz occurred in the rock sampled for analysis than was found in thin section (Fig. 7). In BR-3 and BR-5, the opposite occurred; more quartz was found in thin section than in the analyzed sample.

Although the differences between the reaction spaces based on the mode and those based on the rock compositions depend to some extent on all the oxides, BR-4 is especially different. The difference between the reaction spaces for this sample stems largely from the small amount of quartz found in thin section and the large amount of pyroxene in the assemblage (see Fig. 1). The reaction space based on the mode has its odd shape and position because *pl* exceeds An in the initial set of Thompson components (Table 8). The composition represented by the mode of this rock cannot be represented by a dry pyroxene–plagioclase assemblage because the base of the reaction space is above the Tr = 0 isopleth. In addition, the composition cannot become pyroxene-free because the Di = 0 isopleth lies above the reaction space. Consequently, if the boudin was once a silica-saturated basaltic flow, metasomatic changes on the scale of the thin section have operated to a sufficient degree to move the composition from the silica-saturated condition. That is, the composition derived from the mode of this sample of the boudin could be represented by a dry, undersaturated assemblage that includes Ne or Fo (see p. 642).

CONCLUSIONS

Thompson space polygons illustrate the extent of reaction space available to a specific bulk-composition. Comparison of the shapes of the reaction spaces derived from the Three Valley Gap rock compositions with the shapes derived from compositions of basalts suggests that BR-5 is most like a tholeiitic basalt. The other samples have shapes that are similar to more intermediate, more silica-saturated igneous rocks, such as andesites (see Fig. 8, with illustrations of Thompson spaces for rocks ranging from tholeiitic picrite to basaltic andesite). If the boudin was once a chemically homogeneous igneous rock, then the heterogeneities now present are such that we cannot reconstruct that original composition from the samples available.

Variations in element ratio preclude igneous processes as the cause of the chemical variations within the boudin. The boudin acted as a system closed to Al, Ti and P, within analytical uncertainty, which thus excludes fractionation and accumulation of feldspar and Fe-Ti oxides and the assimilation of country rocks as causes of the variations. Further, fractionation and accumulation of olivine ± augite are excluded because of the lack of a coherent trend with a slope of one, defined by the element ratios representing these processes, on Pearce element-ratio diagrams. Con-

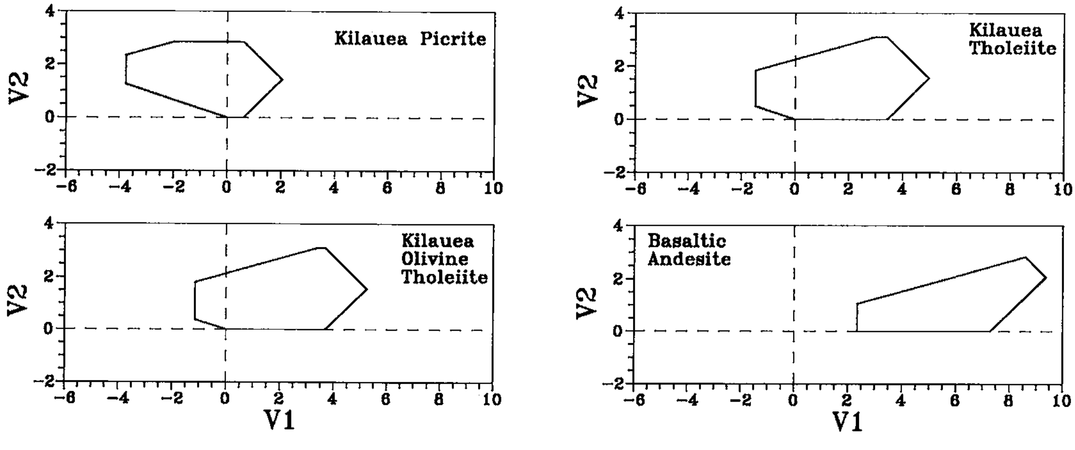

FIG. 8. Reaction-space polygons for a tholeiitic picrite, olivine tholeiite, tholeiite basalt and a basaltic andesite. Compositions of the Kilauean rocks from Wright (1971, Table 4: HM68-4, olivine tholeiite; HM68-12, tholeiite) and Wright *et al.* (1975, Table 3: Hi68-12, picrite). The basaltic andesite composition is from Lowder & Carmichael (1970, Table 2: 339).

sequently, the chemical variations that do occur must have resulted from metamorphic processes.

Because Thompson space illustrates the reaction space available to a specific bulk-composition, we can compare measured modal amounts of analyzed minerals with whole-rock compositions. The difference between compositions derived from mineral compositions and modal amounts and that from a chemical analysis of a hand sample can produce significantly different reaction-space polygons. Figure 7 shows the reaction spaces for compositions derived from the modal analysis using compositions of the minerals and the spaces derived from the results of a rock analysis. One obvious difference illustrated by these reaction spaces is the variation in amounts of quartz. Both BR-2 and BR-4 have less quartz in thin section than in the analyzed samples, whereas BR-3 and BR-5 have more. A comparison of the distribution of modal minerals within the quadrants of a thin section (BR-2) to the whole-rock composition is made by plotting isopleth intersections within the whole-rock reaction space. Again, differences are illustrated by the variations in the positions of the intersections. The suggested protolith, a silica-saturated basaltic flow, is approximately consistent with BR-2, -3 and -5. In contrast, the reaction-space polygon representing BR-4 differs markedly from the other samples in both shape and location, reflecting its silica-undersaturated nature that results from the high concentration of amphibole.

The sporadic presence of orthopyroxene with abundant clinopyroxene indicates that the Three Valley Gap boudins are on the P–T boundary between amphibolite and granulite facies, *i.e.*, the P–T of dehydration. The P–T conditions derived from the mineral compositions (700°C and 0.8 GPa) are almost directly on the high-T side of the amphibolite-facies envelope drawn by Turner (see Verhoogen *et al.* 1970), surely a remarkable bit of insight on his part.

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APPENDIX:

PROCEDURES FOR CONVERTING MINERAL FORMULAE TO THOMPSON COMPONENTS

Thompson components in garnets

We consider a garnet formula to consist of the cations Si, Ti, Al, Fe, Mn, Mg, and Ca. The Thompson components are then:

Gr = $Ca_3Al_2Si_3O_{12}$
mc = $MgCa_{-1}$
tk = $Al_2Mg_{-1}Si_{-1}$
fm = $FeMg_{-1}$
mt = $MgTiAl_{-2}$
mm = $MnMg_{-1}$

The matrix giving the element abundances of a garnet in terms of the Thompson components is:

$$\mathbf{A} = \left|\begin{array}{cccccc} 3 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 2 & 0 & 2 & 0 & -2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & -1 & 1 & -1 \\ 3 & -1 & 0 & 0 & 0 & 0 \end{array}\right|$$

As usual, there are more equations than unknowns: the number of Thompson components is 6, whereas the number of elements is 7. Consequently, we delete the Si equation, because Si has the poorest precision and accuracy in the results of a microprobe analysis. The matrix we need to invert in order to calculate Thompson components from element abundances is:

$$\mathbf{B} = \left|\begin{array}{cccccc} 0 & 0 & 0 & 0 & 1 & 0 \\ 2 & 0 & 2 & 0 & -2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & -1 & 1 & -1 \\ 3 & -1 & 0 & 0 & 0 & 0 \end{array}\right|$$

The inverted matrix with which we calculate Thompson components for a garnet composition is:

$$\mathbf{B}^{-1} = \left|\begin{array}{cccccc} 0 & 1/8 & 1/4 & 1/4 & 1/4 & 1/4 \\ 0 & 3/8 & 3/4 & 3/4 & 3/4 & -1/4 \\ 1 & 3/8 & -1/4 & -1/4 & -1/4 & -1/4 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{array}\right|$$

If we let T be the column vector of Thompson components, and **E** the column vector of elements:

E = [Ti, Al, Fe, Mn, Mg, Ca]$_{-1}$
Then:
T = $\mathbf{B}_{-1}\,\mathbf{E}$

Thompson components in pyroxenes

We assume that the structural formula of a pyroxene can be adequately represented by the cations: Si, Ti, Al, Fe, Mn, Mg, Ca, Na and Cr. The Thompson components representing pyroxene compositions are:

Di = $CaMgSi_2O_6$
mc = $MgCa_{-1}$
tk = $Al_2Mg_{-1}Si_{-1}$
pl = $NaSiCa_{-1}Al_{-1}$
fm = $FeMg_{-1}$
mt = $MgTiAl_{-2}$
mm = $MnMg_{-1}$
ca = $CrAl_{-1}$

There are nine cations in the standard formula and only eight Thompson components. In order to calculate Thompson components from a structural formula, we need to eliminate one cation from the list. As is now apparent, we eliminate the cation that, in general, is the least precisely known, Si. The matrix for converting cation numbers to Thompson components is:

$$\mathbf{A} = \left|\begin{array}{cccccccc} 0 & 1/4 & 1/2 & 1/2 & 1/2 & 1/2 & 3/4 & 1/4 \\ 0 & 1/4 & 1/2 & 1/2 & 1/2 & -1/2 & -1/4 & 1/4 \\ 1 & 1/2 & 0 & 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right|$$