Canadian Mineralogist
Vol. 29, pp. 615-632 (1991)

MODAL SPACE: APPLICATIONS TO ULTRAMAFIC AND MAFIC ROCKS

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ABSTRACT

Quantitative and semiquantitative modal analyses have long been cornerstones of petrographic study. Paragenetic investigations based on textural relationships, and on the spatial distributions of mineral assemblages, have led many investigators to reconstruct the modal evolution of a given rock or mineral deposit through time. The results are typically presented as a parallel array of two-dimensional sketches resembling a school of fish swimming along the time axis. The pinches and swells of the various "fish" are not independent, however, in systems that are constrained in chemical content. These modal interdependencies may be clarified by introducing the concept of "modal space", in which changes in modal abundance through time may be represented by a sequence of points defining a path in that space. In a system with no chemical constraints (a completely open system), the dimensionality of such a space is equal to the number of phases involved. In constrained systems, however, the dimensionality is commonly a lesser number, especially in systems that are completely closed, or open to but one or two components. Algebraic methods are presented for dealing with modal abundances in polyphase, multicomponent systems, and for the geometric representation of these in their appropriate modal spaces. This approach proves to have great utility in obtaining the reaction history from the textural interpretation of a thin section. This, in turn, can be a useful aid in determining a pressure - temperature - time (P-T-t) path.

Keywords: modal, mafic, ultramafic, lherzolite, basalt, pyroxene granulite, eclogite, amphibolite.

SOMMAIRE

Les analyses modales quantitatives et semi-quantitatives ont longtemps servi de piliers aux études pétrographiques. Les études de paragenèse fondées sur les relations texturales, et sur la distribution dans l'espace des assemblages de minéraux, ont inspiré plusieurs chercheurs à reconstruire l'évolution modale d'une roche ou d'un gîte minéral à travers le temps. Les résultats sont typiquement présentés en formes étirées parallèles en deux dimensions, qui font penser à un groupe de poissons nageant le long de l'axe qui représente le temps. Les gonflements et retrécissements des divers "poissons" ne sont toutefois pas indépendants dans tout système défini dans son contenu chimique. Ces interdépendances modales peuvent être rendues plus clairement au moyen du concept de l'espace modal, dans lequel tout changement en abondance d'une phase minérale avec le temps peut être représenté par une séquence de points qui définissent une trajectoire dans cet espace. Pour un système sans contraintes chimiques, et donc complètement ouvert, la dimensionalité d'un tel espace est égal au nombre de phases qui y participent. Dans tout système où il y a contrainte, par contre, la dimensionalité est généralement plus restreinte, spécialement dans un système qui est complètement fermé, ou ouvert à tout composant sauf un ou deux. Des méthodes algébriques permettent de manipuler les abondances modales dans des systèmes polyphasés et à plusieurs composantes, et de représenter ceux-ci géométriquement dans leur espace modal approprié. Cette approche a une grande utilité pour définir la séquence de réactions à partir de l'interprétation texturale d'une lame mince. Cette information peut ensuite fournir une aide précieuse dans l'élaboration de la trajectoire en termes de pression, température, et temps.

(Traduit par la Rédaction)

Mots-clés: composition modale, roches mafiques, roches ultramafiques, lherzolite, basalte, granulite à pyroxène, éclogite, amphibolite.

INTRODUCTION

With the aid of such devices as camera lucida drawings, point counters and, in rare cases, even a net of chicken wire spread over an outcrop, those of us who study rocks and mineral deposits have long ago put modal abundance on a quantitative basis. Most of us have then gone further and used textural and geological relationships (and perhaps quite a bit of wishful thinking) in order to determine how such modal abundances have evolved and varied through time. The classically honored way of displaying one's conclusions on such matters has been by means of an array of simple graphs (Fig. 1), in each of which the modal abundance of a single phase is plotted (vertically) against time (horizontally), in such a way that the modal abundance is shown more or less symmetrically about an arbitrary time axis. An array of such graphs bears, in many instances, a striking

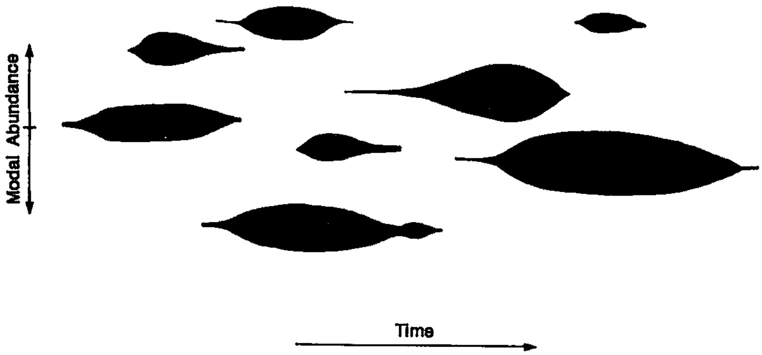

FIG. 1. The classical representation of modal changes with time. The pinches and swells of the figures record the waxings and wanings of the mineral phases with time.

resemblance to a school of fish that may be imagined as swimming, one way or the other, along their time axes (Fig. 2). We shall therefore refer to these herein as *fish diagrams*.

A problem with fish diagrams, however, is that they imply an independence among the various modal abundances that can be true only in systems open to any and all components. Let us consider the opposite extreme, a completely closed system that matter can neither enter nor leave. One phase (or fish) can here grow only at the expense of one or more of its fellows, creating a dreadful situation like that portrayed in Figure 3.

Modal space in a completely open system, where the abundance of each phase may vary independently of its neighbors, must have as many dimensions as there are phases in the assemblage. To obtain such a space for a completely closed system, on the other hand, we need to know the number of independent ways in which matter may be transferred from phase to phase within the system. Not all transfers, however, affect modal abundance, at least if measured in, say, the number of standard formula units of each phase present in the system. We must further distinguish, therefore, between *net-transfers*, which vary the quantities, as above measured, of two or more phases, and *exchanges*, which do not. These net-transfers and exchanges are, of course, the heterogeneous reactions that can take place within the closed system. Because only the net-transfer reactions can alter our measures of modal abundance, we will know the dimensionality of our modal space if we know the minimum number of net-transfer reac-

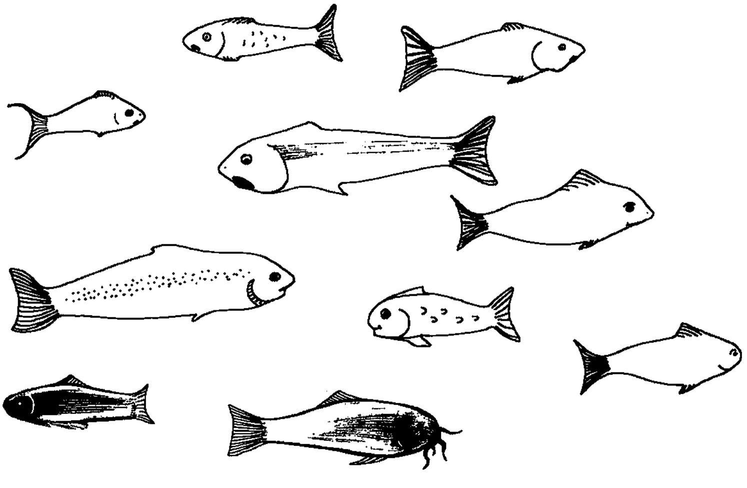

FIG. 2. Modification of Figure 1 as a fish diagram.

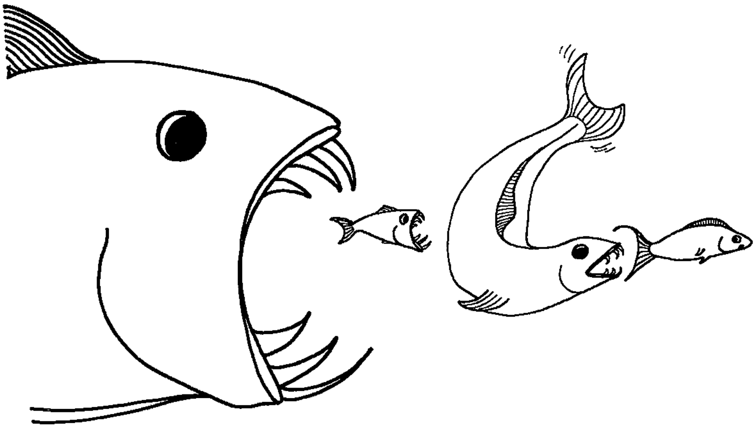

FIG. 3. Fish diagram for a closed system.

tions needed to define all possible changes in modal abundance within our closed system. Yes, you've guessed it, net-transfer reaction space and modal space are the same thing! We here give it a kinder, gentler name, a name that also emphasizes some of its more useful applications to petrological problems, especially in dealing with closed or but partially open systems.

Modal abundances expressed as numbers of formula units are of course not the same as volumetric abundances, as obtained by a point count or by a camera lucida drawing. If, however, we multiply each formula abundance by the number of oxygen (plus fluorine) atoms per formula unit, we will obtain new numbers that are roughly proportional to their volumetric abundances for most rock-forming minerals.

The theoretical basis has been presented at some length elsewhere (Thompson *et al.* 1982, Thompson 1982a,b), and need not be repeated here. We shall instead follow some of the procedures involved, as a refresher, and then explore some of the applications, emphasizing ones that earlier presentations have overlooked or dealt with too briefly.

SELECTION OF COMPONENTS

The results of chemical analyses of a mineral or rock (mineral assemblage) are typically presented in terms of a series of practical components (oxide components or, less commonly, elements) that may or may not be *independently variable* in the mineral or mineral assemblage in question. The actual variations of which a homogeneous phase is capable occupy a composition space whose dimensionality exceeds by one the number of independently variable (I.V.) components of that phase. A c-component space may thus be defined in terms of any c distinct components, each of which corresponds to a specific point in that space. By distinct, we mean that none lies in any subspace defined by the other ones. These points (see Thompson 1982a) may represent either compositions (additive components) that can be added to or removed from the phase in question, thus varying its modal abundance, or may represent operations (exchange components or operators) that vary the composition of that phase without varying its modal abundance.

To define such a space, we must select at least one additive component for each phase. The others may all be additive (the conventional choice), mixed, or all exchange (the unconventional choice we shall adopt here). If there is but a single additive component for each phase, it will then be the one that monitors the modal abundance of that phase, whereas the exchange components simply vary its composition.

It is generally convenient to select a simple, idealized, end-member composition as that of the additive component. Composition variables may then be defined as formula-unit ratios, exchange to additive, rather than as a conventional set of formula-unit fractions (or mass- or mole-fractions). Convention would thus describe feldspar in terms of mole fractions (X_{ii}) of the additive components $KAlSi_3O_8$–$NaAlSi_3O_8$–$CaAl_2Si_2O_8$ (or–ab–an), any two of which, say (X_{or}) and (X_{an}) may be taken as independent. We could equally well take $NaAlSi_3O_8$ as a single additive component, and the ratios (Y_{ii}) to it of the exchange components KNa_{-1} (ak), and $CaAlNa_{-1}Si_{-1}$ (pg). In this specific example, the results happen, in fact, to be numerically identical: $X_{or} = Y_{ak}$, and $X_{an} = Y_{pl}$. Olivine, on the other hand, may be described in terms of the additive components Mg_2SiO_4–Fe_2SiO_4 (fo–fa) and X_{fa}, or in terms of the single additive component Mg_2SiO_4 and the exchange component $FeMg_{-1}$ (fm). In this instance: $2X_{fa} = Y_{fm}$, and the two variables, though not identical, are very simply related.

A useful strategy, in the selection of the additive components for an assemblage of phases, is to select ones that lie in as simple a subsystem as possible. The task of identifying all possible net-transfer reactions, the only ones that vary the mode, is then one that can be carried out entirely within the confines of the simpler system. The simpler composition-space may also contain points corresponding to exchange components of one or more of the phases present. This is commonly so, and such exchange components should be included in the working set. It should be borne in mind, however, that these guidelines allow for a considerable freedom of choice. The most convenient additive component for a given phase may therefore depend on the nature of the assemblage in which it occurs and on the problem at hand. Table 1 lists some of the major mineral phases encountered in dealing with the metamorphism of mafic and ultramafic rocks, and the additive components selected for each. These phases, even to a first approximation, lie in a system involving at least eight practical oxide components. Their *additive* components, however, may be selected so that these all lie in the subsystem SiO_2–Al_2O_3–MgO–CaO, as indicated. Table 2 lists some of the principal exchange components in these minerals. Two of these exchange components, $CaMg_{-1}$ (pyroxene, amphibole, garnet) and $Al_2Mg_{-1}Si_{-1}$ (pyroxene, amphibole), also lie in this subsystem. Although the point $Mg_2Si_2O_6$ is not normally accessible to the composition of a natural clinopyroxene, it is nevertheless a point in the composition space in which clinopyroxenes vary and is indeed an I.V. component of such a pyroxene, as well as of an orthopyroxene. It may therefore be used as a monitor of total pyroxene, just as $Mg_7Si_8O_{22}(OH)_2$ may be used as a monitor of total amphibole.

TABLE 2. EXCHANGE COMPONENTS*

Formulas	Mineral Phases
$Al_2Mg_{-1}Si_{-1}$ or tk	Pyroxene, amphibole
$CaAlNa_{-1}Si_{-1}$ or pg	Plagioclase, pyroxene,amphibole
$NaAlSi_{-1}$ or ed	Amphibole
KNa_{-1} or ak	Amphibole, Feldspar
$CaMg_{-1}$ or cm	Pyroxene, amphibole, garnet
$FeMg_{-1}$ or fm	Most ferromagnesian minerals
$FeAl_{-1}$	Most ferromagnesian minerals
$TiFe_{-1}$	Most ferromagnesian minerals
$MnFe_{-1}$	Most ferromagnesian minerals
$CrFe_{-1}$	Most ferromagnesian minerals
H_4Si_{-1}	Calcic garnet

*See Thompson (1981, p. 161) for explanation of $TiFe_{-1}$ and $MnFe_{-1}$.

TABLE 1. ADDITIVE COMPONENTS OF MINERALS*

Minerals	Symbols	Components	Symbols
Quartz	Qtz	SiO_2	qtz
Plagioclase	Plg	$CaAl_2Si_2O_8$	plg
Pyroxene	Pyx	$Mg_2Si_2O_6$	pyx
Amphibole	Amp	$Mg_7Si_8O_{22}(OH)_2$	amp
Garnet	Grt	$Mg_3Al_2Si_3O_{12}$	grt
Olivine	Olv	Mg_2SiO_4	olv
Spinel	Spl	$MgAl_2O_4$	spl
Epidote	Epi	$Ca_2Al_3Si_3O_{12}(OH)$	epi
Chlorite	Chl	$Mg_5Al_2Si_3O_{10}(OH)_2$	chl

*Mineral symbols are slightly modified from those of Kretz (1983), because of need to distinguish mineral symbols and those of their corresponding additive components from those of all other components. Pyx and Amp refer to *total* pyroxene and amphibole.

Notation is a problem here and requires some minor revision of existing conventions in order to avoid conceptual difficulties. We will use three-letter symbols for the mineral phases, the initial letter capitalized (Table 1). These are either the symbols proposed by Kretz (1983), or include his symbols as their first two letters. Kretz gave no symbols for *total* amphibole or pyroxene (where more than one of either is present). For these we will use Amp and Pyx, respectively. We will use the same three letters, all lower case (Table 1), for the additive components of these minerals, in order to emphasize that these are the components that monitor the modal abundances. All other components will be assigned two-letter, lower-case symbols (Tables 2 and 5), in order to distinguish them from those that monitor modal abundances.

REDUCTION OF THE STOICHIOMETRIC EQUATIONS

Once a set of additive components has been selected for the assemblage in question, we may select a set of practical components (not necessarily independently variable) sufficient to define the compositions of the selected additive components, and of the exchange components that are also in their space. These may be selected as the chemical elements themselves, although judicious use of oxide components may yield a speedier solution. This may be illustrated by considering some of the major phases characteristic of silica-undersaturated mafic and ultramafic igneous rocks and their metamorphic derivatives. The likely assemblages include pyroxene, plagioclase, olivine, garnet, and spinel in various combinations. The additive components may be selected as indicated in Table 1. All of these lie in the subsystem defined by Si–Al–Mg–Ca–O, or, more compactly, by SiO_2–Al_2O_3–MgO–CaO. The space for this subsystem also contains the exchange components $CaMg_{-1}$ (cm), and $Al_2Mg_{-1}Si_{-1}$ (tk). The first is an I.V. component of both pyroxene and garnet, and the second, of pyroxene. Although more than one pyroxene may be present, we shall refer both to the same additive component, which will then monitor total pyroxene. We shall see later that the kind of pyroxene is usually obvious from other considerations, and that we can gain more than we lose by such simplification.

In Table 3, we see the compositions of the components in the subsystem in terms of the chemical elements as practical components. When we use the elements as practical components, this is simply a rewriting of the chemical formulas in equation form, displayed so as to emphasize the coefficient matrix. A Gauss–Jordan reduction of this set of equations yields the results shown in Table 4. The last three equations have no non-zero terms on the right-hand side. All the terms on the left represent I.V. components of the phases; hence these three equations are those of three distinct linear dependencies involving the additive components of these phases, and also those exchange components of these phases that lie in the same subsystem. The closed-system modal space in this example is therefore three-dimensional inasmuch as there are three distinct processes that can alter modal abundance without appeal to any external source or sink. The first four equations in Table 4 tell us that the subsystem can be described in terms of four practical components, rather than the five with which we started. Their right-hand sides, in fact, correspond to the formulas SiO_2, Al_2O_3, MgO, and CaO. Had we started with these, in fact, as practical components, we could have achieved equivalent results more compactly. In each of these first four equations, the terms on the left are components that are I.V. in one or more of the phases present. The *entire* right-hand side of each is therefore a linear combination of I.V. components and hence is itself a possible choice as an I.V. component of both the subsystem and of the larger system in which the assemblage lies. It is thus evident that SiO_2, Al_2O_3, MgO, and CaO are all I.V. in this system. Had we used a different ordering of the initial equations, a different ordering or selection of practical components, or had we, on our computer, used a different method of reduction, we would be likely to obtain our results in a different but equivalent form. We would still obtain the same number of independent net-transfer reactions (and hence the same dimensionality for our modal space), but the reactions might appear as linear recombinations of the ones in Table 4. By the same token, we will obtain the same number of I.V. components for the subsystem, but a set that again may involve recombination of the ones in Table 4. In any case, the number of I.V. components in the assemblage that are also in the selected subsystem is equal to the rank of the coefficient matrix in the initial equations, and the dimensionality of the modal space is equal to its row-nullity. There is, happily, still some room for individual choice here, inasmuch as the set of I.V. components, or the set of reactions that is first obtained, though these are sufficient, may often be improved upon by appropriate linear recombination. We will return to this matter below when considering modal spaces for mafic and ultramafic rocks.

LHERZOLITES

Lherzolites are peridotites consisting primarily of olivine, orthopyroxene and clinopyroxene, but

TABLE 3. STOICHIOMETRIC EQUATIONS

Component		Si	Al	Mg	Ca	Ox
pyx	=	2	0	2	0	6
tk	=	-1	2	-1	0	0
olv	=	1	0	2	0	4
cm	=	0	0	-1	1	0
grt	=	3	2	3	0	12
spl	=	0	2	1	0	4
plg	=	2	2	0	1	8

TABLE 4. REDUCED EQUATIONS

Components		Si	Al	Mg	Ca	Ox
pyx - olv	=	1	0	0	0	2
tk + 0.5 pyx	=	0	2	0	0	3
olv - 0.5 pyx	=	0	0	1	0	1
cm + olv - 0.5 pyx	=	0	0	0	1	1
grt - 2 pyx - tk	=	0	0	0	0	0
spl - olv - tk	=	0	0	0	0	0
plg + olv -2 pyx - tk - cm	=	0	0	0	0	0

TABLE 5. SOME ADDITIVE COMPONENTS*

Formulas	Symbols
$NaAlSi_3O_8$	ab
$KAlSi_3O_8$	or
$CaAlSi_2O_8$	an
$CaMgSi_2O_6$	di
$Mg_2Si_2O_6$	en
Mg_2SiO_4	fo
Fe_2SiO_4	fa
$Ca_2Mg_5Si_8O_{22}(OH)_2$	tr
$Mg_7Si_8O_{22}(OH)_2$	oa

*Most of the above, are standard components as used in the calculation of a "CIPW" norm as introduced by Cross *et al.* (1902); the last two are normative amphibole components in the spirit of the "mesonorm" of Barth (1959).

not uncommonly containing small amounts of garnet, spinel or plagioclase. An assemblage of all these phases allows four independent net-transfer reactions, which would correspond to a four-dimensional modal space. We can simplify the problem, however, by referring both pyroxenes to the same additive component, which means that one of these reactions can be taken as the trivial one based on:

$$\mathrm{pyx_{Cpx}} = \mathrm{pyx_{Opx}} \tag{1}$$

The reaction defined by (1) may be neglected if we initially concern ourselves only with total pyroxene. This is a sacrifice, but a sacrifice that will prove to be a minor one inasmuch as we shall find that the kinds of pyroxene that correspond to a point in the simpler space are usually fairly obvious. With pyx (no subscript) thus monitoring only *total* pyroxene, we may then obtain from Table 4 the following three equations for net-transfer reactions that, in turn, define a three-dimensional modal space:

$$\mathrm{grt} = 2\mathrm{pyx} + \mathrm{tk} \tag{2}$$

$$\mathrm{olv} + \mathrm{tk} = \mathrm{spl} \tag{3}$$

and

$$\mathrm{plg} + \mathrm{olv} = 2\mathrm{pyx} + \mathrm{cm} + \mathrm{tk} \tag{4}$$

The components in equations (2) and (3) above are Ca-free, and hence their effects may be visualized in the three-component system MgO–Al_2O_3–SiO_2, as shown in Figure 4 (see Burt 1988).

From equations (2) and (4) we may also obtain:

$$\mathrm{plg} + \mathrm{olv} = \mathrm{grt} + \mathrm{cm} \tag{5}$$

where both terms on the right-hand-side are I.V. components of garnet and could be combined as $CaMg_2Al_2Si_3O_{12}$. Further equations may be derived as linear recombinations of (1), (2) and (3). Some of interest are:

$$\mathrm{grt} + \mathrm{olv} = 2\mathrm{pyx} + \mathrm{spl} \tag{6}$$

$$\mathrm{plg} + 2\mathrm{olv} = 2\mathrm{pyx} + \mathrm{spl} + \mathrm{cm} \tag{7}$$

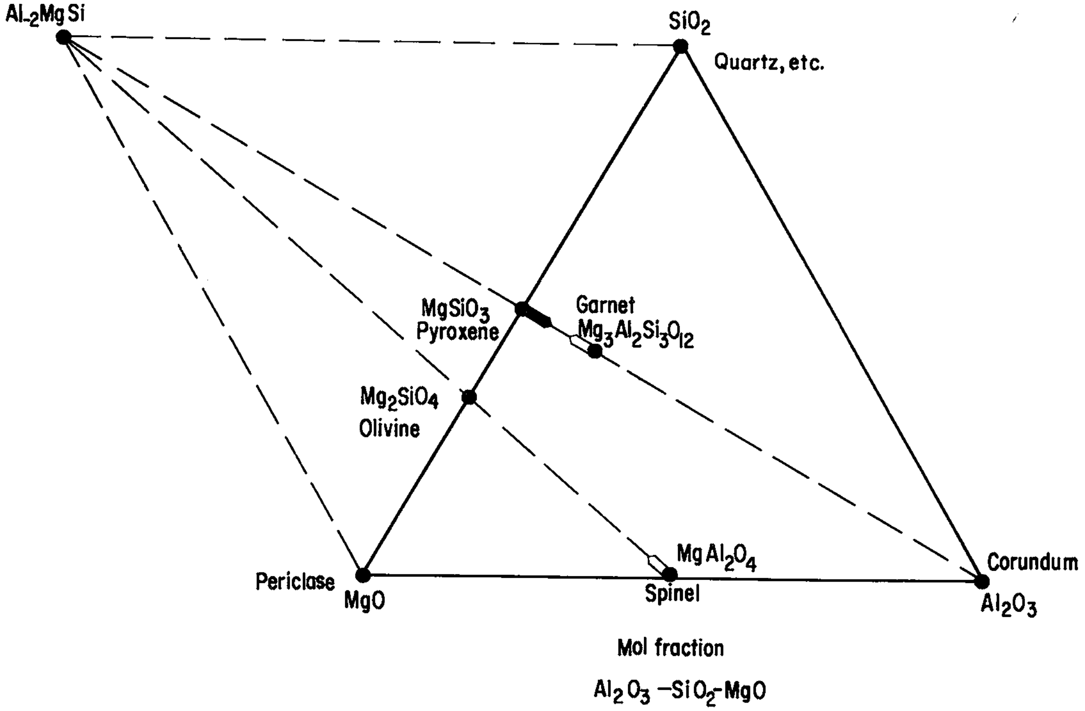

FIG. 4. The composition plane SiO_2–Al_2O_3–MgO. The point $Al_{-2}MgSi$ is negative tk; therefore, "adding" tk is a motion, in this plane, *away* from $Al_{-2}MgSi$ (see Burt 1988, p. 563). Equation (2) in the text deals with the solubility of garnet in orthopyroxene (see Wood & Banno 1973, O'Hara & Howells 1978), and equation (3) shows that the proportions of olivine and spinel may be varied in the presence of a phase such as pyroxene that has tk-exchange capacity.

and

$$2\mathrm{grt} + \mathrm{cm} = 2\mathrm{pyx} + \mathrm{spl} + \mathrm{plg} \tag{8}$$

We may note that reactions corresponding to (2) and (3) are independent of each other and do not alter modal plagioclase. The same arguments apply to (3) and (5) with respect to pyroxene, to (3) and (4) with respect to garnet, to (2) and (8) with respect to olivine, and to (2) and either (4) or (5) with

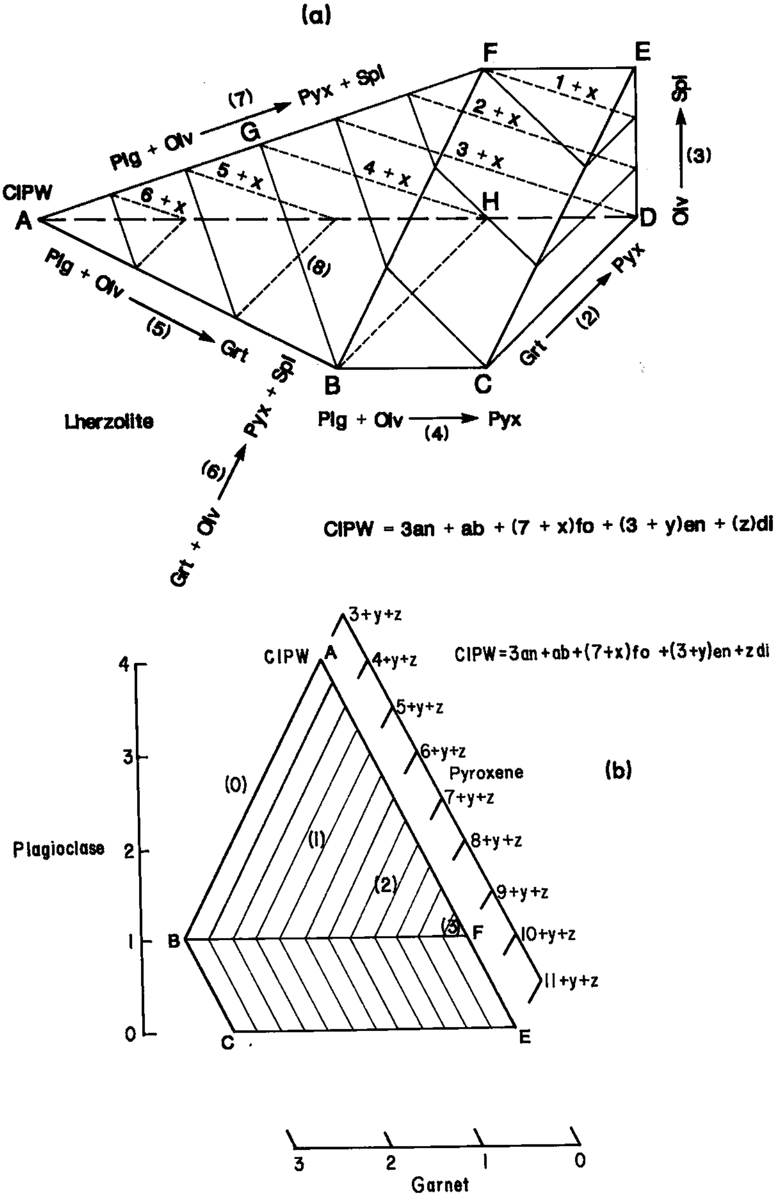

FIG. 5. Two views of a modal space for lherzolites as discussed in text. The internal inclined planes in 5a are olivine isopleths; spinel isopleths are parallel to the base and shown as contours in 5b. Plagioclase lherzolites lie near the A vertex, garnet lherzolites lie near the line BC, and spinel lherzolites lie near the line EF.

respect to spinel. Reactions corresponding to (6), (7), and (8), any two of which are independent, are all possible where any pyroxene is free of Al and thus at the low-aluminum limit [tk–] of its tk exchange capacity. Reactions corresponding to (4) and (6) are possible where any plagioclase or pyroxene is at the sodic limit [pg–] of its pg exchange capacity. In this last case, (4) is equivalent to:

$$NaAlSi_3O_8 + Mg_2SiO_4 = Mg_2Si_2O_6 + NaAlSi_2O_6 \quad (4a)$$

That this last is equivalent to (4) may be surprising, but makes sense when we realize that $NaAlSi_3O_8$ may be written as plg - pg, and that $NaAlSi_2O_6$ may be written as pyx + cm + tk - pg.

In Figure 5 we see two views of a (closed-system) modal space for the CIPW normative composition (see Table 5) indicated at A, and for which (2), (3), and (5) provide convenient basis-vectors. As drawn, (2) and (3) are orthogonal, and (5), though normal to (3), is inclined to (2). The accessible space is within the polyhedron. Three of the bounding faces of the polyhedron are zero isopleths. The plane CDE is the zero isopleth for plagioclase; the basal plane ABCD is the zero isopleth for spinel, and the plane ADEF is the zero isopleth for garnet. Spinel isopleths are horizontal and shown by contours in Figure 5b. The other two bounding surfaces arise where a limit to an exchange capacity is reached. In the plane ABF, a pyroxene is at the limit [tk–], and in the plane BCEF, plagioclase and pyroxene are at the limit [pl–]. Point A corresponds to an idealized "CIPW" lherzolite having the mineralogy and modal abundance implied by the classical normative calculation (Cross *et al.* 1902). A real igneous rock that has crystallized at or near the earth's surface, however, contains somewhat less plagioclase than the amount implied by its norm, and thus corresponds to a point slightly displaced from A along the line AD, the missing plagioclase being hidden or "occult" as a Ca–Al component in pyroxene. Garnet lherzolites lie on or near the line BC, and spinel lherzolites, on or near the line EF (see O'Hara 1968, and Wyllie 1970, and references therein, for relevant experimental results). Those near the plane DEF must have an omphacitic component in the clinopyroxene, and at the D vertex, all normative plagioclase would be "occult" in pyroxene. A plagioclase in the plane BCEF can only be pure ab, and, inasmuch as sodic plagioclase is known to coexist with Ca–Al pyroxene, any plagioclase in the entire triangular prism between CDE and BFH is probably very nearly pure ab.

In Figure 5a, the inclined internal planes are olivine isopleths. The one labeled BGH is at a modal abundance of $(4 + x)$. If x were zero, the zero isopleth for olivine would pass through the E vertex, if greater than zero, it would miss the polyhedron entirely, and if less than zero it would truncate the polyhedron. Similarly, if $(y + z)$ were zero, the zero isopleth for pyroxene would pass through the edge AB, parallel to the edge DE. If $(y + z)$ were greater than zero, it would miss the polyhedron entirely, and if $(y + z)$ were less than zero, it would truncate the polyhedron. The initial abundances of the major phases, pyroxenes and olivine, may thus vary widely with little or no effect on the appearance of the accessible modal space. Such variations, even though they may cause truncation of the polyhedron, simply alter the labeling of the isopleths, not their orientation. One's concern is commonly to deduce the reaction history of a rock from the textural evidence of modal change. In this instance, the shape of the accessible region is a matter of little interest, and the orientation of the isopleths with respect to each other and the reaction coordinates is the key to the problem.

We may also note that generalization of the compositions of the phases by the presence of exchange components such as KNa_{-1} (ak), $FeMg_{-1}$ (fm), $FeAl_{-1}$, $CrAl_{-1}$, $FeMn_{-1}$, $TiFe_{-1}$, $CaAlNa_{-1}Si_{-1}$ (pg), $NaAlSi_{-1}$ (ed), and others, does not alter the isopleth orientation in modal space, because these isopleths record only variations in the additive components of the phases (see Thompson 1982a, p. 22 for clarification of $FeMn_{-1}$ and $FeTi_{-1}$). There may, however, be other truncations if all phases having these components reach an extreme limit of exchange capacity. We have an example of this in the plane BCEF in Figure 5, where both plagioclase and pyroxene have reached the sodic end of the substitution $CaAlNa_{-1}Si_{-1}$ (pg). Varying normative ab while holding all else constant produces the effects shown in Figure 6. In Figure 6b, the modal space is as in Figure 5, whereas in Figure 6a, the ab is wholly removed. If x is at least two, then Figures 6c and 6d result from adding one and two formula units of ab, respectively. The substitution $FeMg_{-1}$ (fm) has no effect on the appearance of the modal space. All net-transfer reactions that are written in terms of Mg-bearing components could equally well be written in terms of equivalent Fe-bearing components.

It should by now be evident that the modal spaces for a wide variety of ultramafic rocks have a great deal in common, and that their precise form may be anticipated from the normative composition. Everything we have said applies with equal force, for example, to harzburgites, by simply setting z at zero, or to the "pyrolite" compositions of Green & Ringwood (1967b). The assemblages indicated in Figure 5 include everything likely to

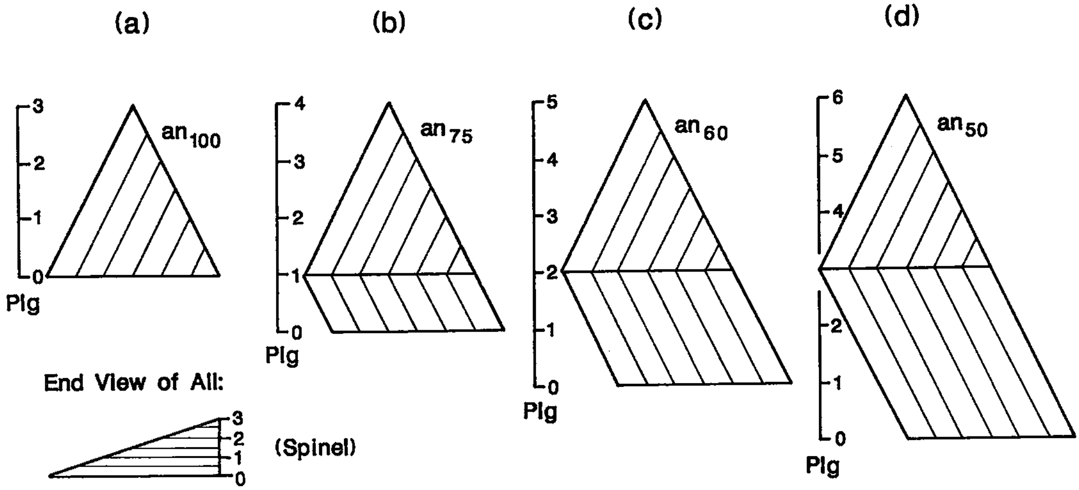

FIG. 6. Lherzolite spaces obtained by removing ab from (6a), or adding it to (6c,d), the normative composition (6b) of the lherzolite in Figure 5. The inset labeled "end view" may also be regarded as a two-dimensional modal space based on equations (2) and (3) and the composition space of Figure 4.

form in the crust or uppermost mantle. Deeper in the earth, plagioclase is out of the picture entirely. The compositional constraints on spinel and garnet are less severe at extremely high pressures, where both may show variations in tk sufficient to allow spinel to encompass olivine compositions, and garnet (majorite) to encompass pyroxene compositions. Other R_2O_3 phases, having either the corundum-ilmenite or perovskite structures, also may appear, and our modal spaces may be adapted to allow for them, if we so wish.

BASALTS, PYROXENE GRANULITES, ECLOGITES

The mineral phases and the reactions that have just been discussed also occur in olivine basalts. The space of Figure 6d could, in fact, with x equal to 2, and y equal to 0, indeed be that for the metamorphism of an olivine-rich basalt at the boundary of the nepheline-normative region. In Figure 7, we have the modal space to deal with the closed-system metamorphism of a similar basalt that is also at the boundary of the nepheline-normative region. It differs, however, from the basalt consistent with Figure 6d in having less normative olivine, and hence is truncated by the zero isopleth for olivine.

For quartz-bearing basalts, devoid of olivine and spinel, we find, by the same methods, that a reaction corresponding to (2) is possible, but that reactions (3) and (4) are replaced by a single reaction that can be taken either as:

$$2\text{plg} = \text{grt} + 2\text{cm} + \text{tk} + 2\text{qtz} \tag{9}$$

or as

$$\text{plg} = \text{pyx} + \text{cm} + \text{tk} + \text{qtz} \tag{10}$$

We may also obtain:

$$\text{plg} + \text{pyx} = \text{grt} + \text{cm} + \text{qtz} \tag{11}$$

If reactions corresponding to (2) and (9) are selected as orthogonal basis-vectors, we obtain the two-dimensional modal space shown in Figure 8, with isopleths as indicated, for a basalt that is at the boundary of the quartz-normative region. The edges CD and DA are zero isopleths for plagioclase and garnet, respectively. The edge AB is at the limit [tk–], and the edge BC is at [pg–]. Note that these bounds correspond closely to those in Figure 4 or Figure 7. The zero isopleth for quartz is a horizontal line passing through A.

The bulk compositions for Figures 7 and 8 differ only in silica content, the normative olivine (fo) in Figure 7 being replaced by normative orthopyroxene (en) in Figure 8. In Figure 9, we have four intermediate steps, spaced at regular intervals in silica content. In 9a, the zero isopleths for olivine, spinel, and plagioclase all meet at the edge CD. At the C vertex, the assemblage is garnet–omphacite, a perfect eclogite, and at the D vertex, it is orthopyroxene–omphacite, an assemblage in which *all* normative plagioclase is occult in pyroxene.

For a basalt composition appropriate to Figure 9c, the mineral content at the A vertex would be:

Plagioclase: 6 an + 6 ab

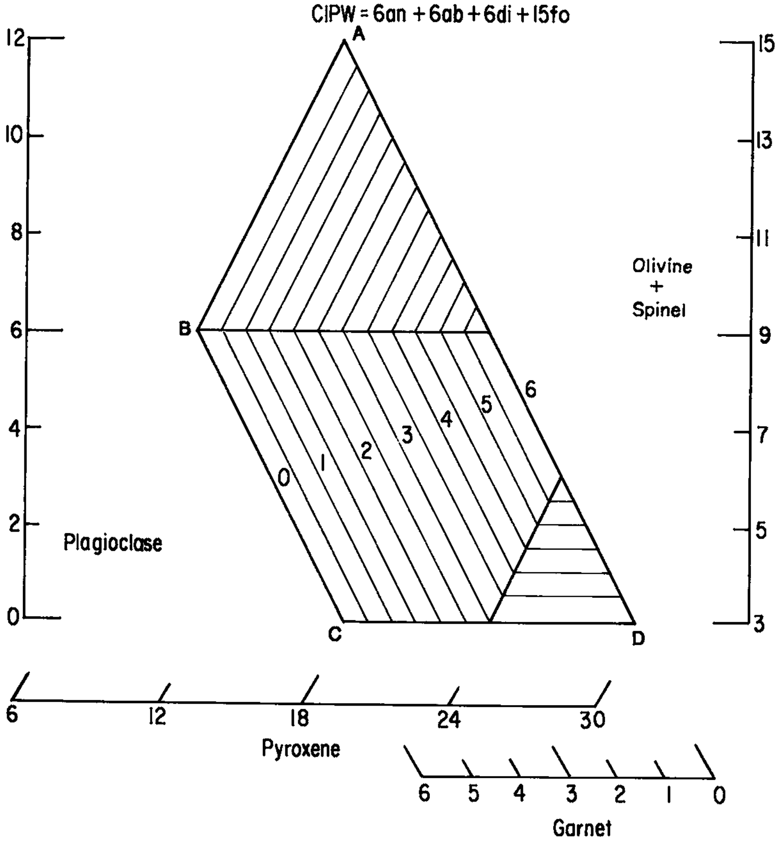

FIG. 7. A modal space for an olivine basalt. The reactions serving as basis-vectors are as in the lherzolite spaces. Note the similarity to Figure 6d.

Pyroxene: 6 di + 9 en
Olivine: 6 fo

in other words, that which is implied by the CIPW norm itself. At point E, midway on the line at which the two modal spaces meet, the mineral content would be, approximately:

Plagioclase: 6 ab
Pyroxene: 9 di + 9 en + 3 $CaAl_2SiO_6$
Olivine: none
Garnet: 3 $Mg_3Al_2Si_3O_{12}$

In this the plagioclase could be slightly calcic owing to pg-exchange with pyroxene, as the garnet could also be by cm-exchange with pyroxene. Points to the left of E would have more garnet, those to the right, less. The phase compositions may, of course, be generalized by the operation of exchange components such as $FeMg_{-1}$ and others, without altering the modal space. The pyroxene would probably be a two-phase mixture of augite and minor orthopyroxene. The assemblage is thus that of a fairly typical two-pyroxene garnet granulite.

At the C vertex, the mineral content would probably be:

Quartz: 6 SiO_2
Plagioclase: none
Pyroxene: 12 di + 3 en + 6 $NaAlSi_2O_6$
Garnet: 6 $Mg_3Al_2Si_3O_{12}$

in which the pyroxene would probably be a two-phase mixture of omphacitic clinopyroxene and minor orthopyroxene. If the 6 di were eliminated from the original composition, the clinopyroxene at C would be an omphacite. In each of the Figures, 7 through 9, the transformation from A to C is from a CIPW-type assemblage through a pyroxene granulite assemblage to an eclogitic assemblage (see Green & Ringwood 1967a, for some relevant experimental results).

AMPHIBOLITES

By adding 6 SiO_2 and 6 H_2O to the bulk composition for Figure 8, and introducing two new

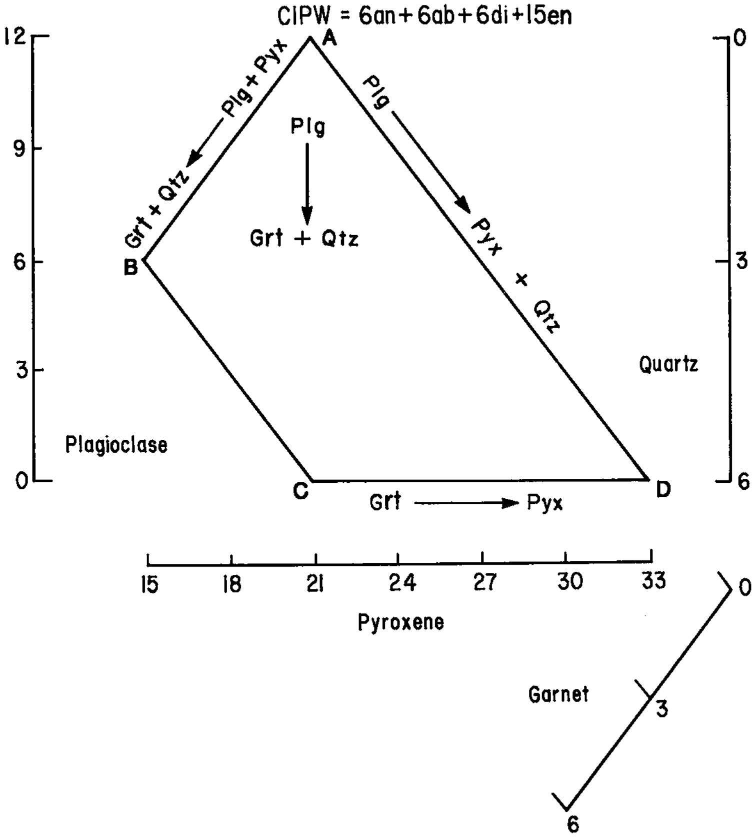

FIG. 8. A modal space for a silica-saturated basalt. The composition is obtained from that of Figure 8 by adding 15 SiO_2.

"normative" amphibole components: $Ca_2Mg_5Si_8O_{22}(OH)_2$ or *tr*, and $Mg_7Si_8O_{22}(OH)_2$ or *oa*, we may replace all the pyroxene of Figure 8 by amphibole. Because amphibole, like pyroxene, has both tk- and pg-exchange capacity we may, on the basis of equations (2) and (9), construct a two-dimensional, closed-system modal space as shown in Figure 10. This space is analogous to that for Figure 8, but enables us to deal with assemblages containing amphibole as well as quartz, plagioclase, garnet, and pyroxene. Because we are using total amphibole and there are no other hydrous phases, the total modal amphibole necessarily must remain constant in a closed system. Its composition, however, can vary widely, as we shall see. This is also why a triangular area on the left side of the space in Figure 8 is missing in Figure 10. The line ABC is here the zero isopleth for pyroxene, and is a bound to the modal space because amphibole cannot be transformed isochemically into garnet.

Amphiboles, however, allow an exchange component, $NaAlSi_{-1}$, or ed, that is not present in pyroxenes. Because it is a second sodic exchange component, in addition to pg, we should, to be safe, add Na_2O as a further practical component in our procedure for determining the net-transfer reactions. We then find that our amphibole assemblages have a third closed-system net-transfer reaction that may be written:

$$4\text{qtz} + \text{pg} + \text{ed} = \text{plg} \qquad (12)$$

Because pg-exchange capacity may be provided by both plagioclase itself and amphibole, equation (12) tells us that plagioclase may be converted into quartz in a closed system containing amphibole. With a reaction corresponding to (12) as a third basis-vector, we obtain the three-dimensional modal space of Figure 11. Figure 10 may now be regarded as simply its base, at the limit [ed−] of ed-exchange capacity. Figure 12 is then the left-hand face of the polyhedron of Figure 11,

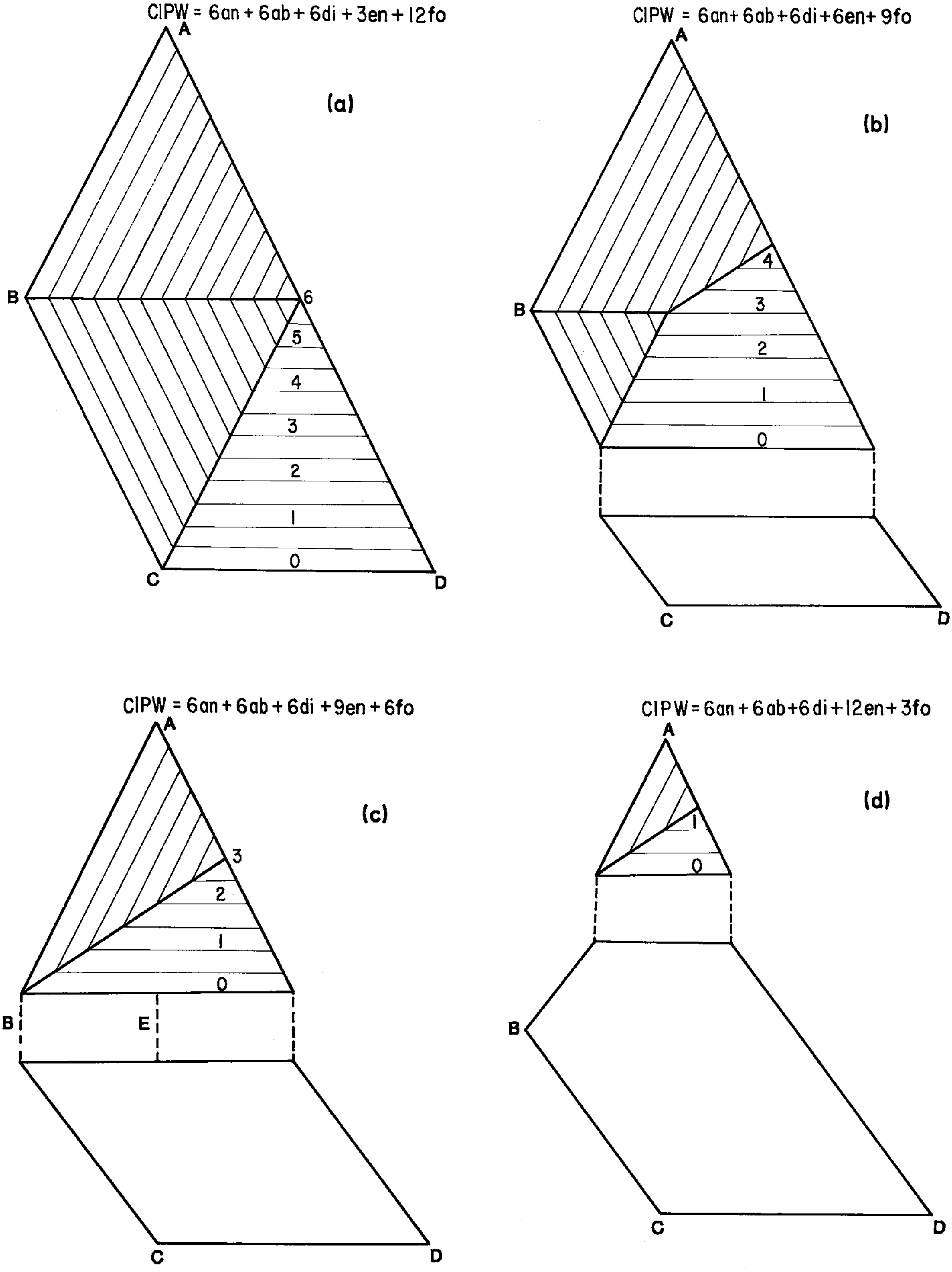

FIG. 9. Modal spaces for olivine basalts intermediate to those of Figures 7 and 8, at intervals of 3 SiO_2.

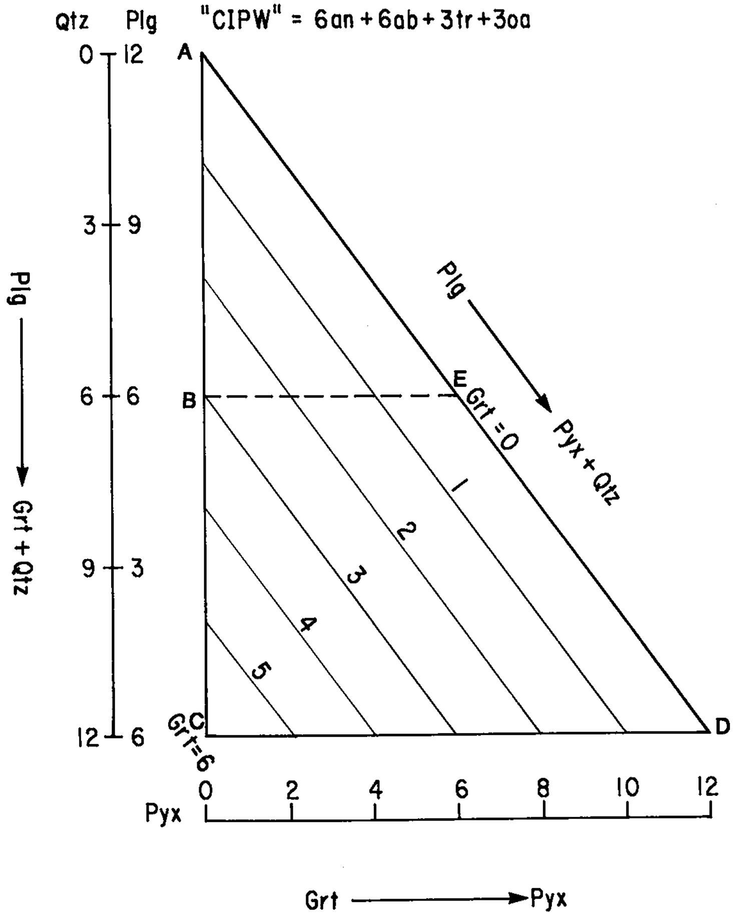

FIG. 10. A partial modal space for a high-silica basalt in which normative pyroxene is replaced by amphibole (see text).

which is also the zero isopleth for pyroxene. The zero isopleth for garnet is the back face, and the top is the exchange limit [ed+], where the A sites of the amphibole are fully occupied by sodium atoms. Plagioclase isopleths are parallel to the plane CDFG, and quartz isopleths, parallel to the line CD, dip more gently, as shown in Figures 11 and 12.

Along the line AH, as plagioclase is converted into quartz, we regain, as quartz, all of the silica, and more, that we have added since we began with the olivine basalt composition of Figure 7, the one that was at the boundary of the nepheline-normative region. Had we simply added 6 H_2O to that basalt, converting all its initial pyroxene to amphibole, its closed-system modal space would then be the volume in Figure 11 that lies above the quartz isopleth labeled (1). This isopleth then becomes the zero isopleth for quartz. Similarly, had we added 6 H_2O to the basalt of Figure 8, the modal space would have as its zero isopleth for quartz the one that is labeled (6) in Figure 11. Adding 6 H_2O to the basalts of Figure 9 provides the intermediate cases corresponding to the isopleths labeled (2) through (5) in Figure 11. It is thus evident that the modal space of Figure 11 can cope with basalt compositions ranging from quartz-normative to nepheline-normative, thanks to the exchange capacity of amphibole!

Our results are, in fact, more realistic than they may seem. Let us consider the basalt of Figure 9c, with 6 H_2O added so as to form an amphibolite. The zero isopleth for quartz is then the one at (4) in Figure 11 that passes through the edge CD. The mineral content would then be:

Plagioclase: 6 an + 3 ab
Amphibole: 3 $Ca_2Mg_5Si_8O_{22}(OH)_2$ +
3 $Mg_7Si_8O_{22}(OH)_2$ + 3 $NaAlSi_{-1}$

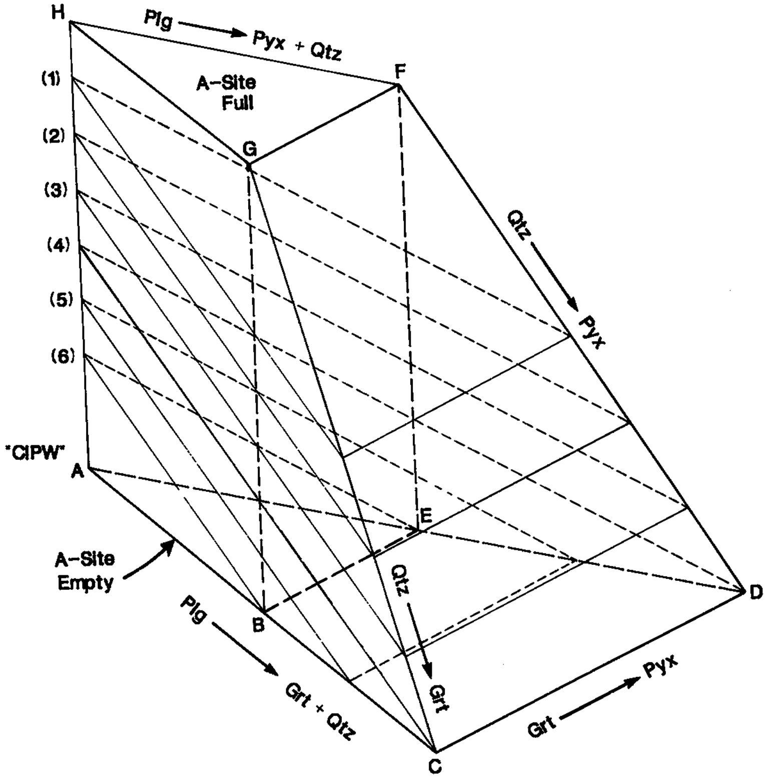

FIG. 11. The full modal space for the basaltic composition of Figure 10 (see text).

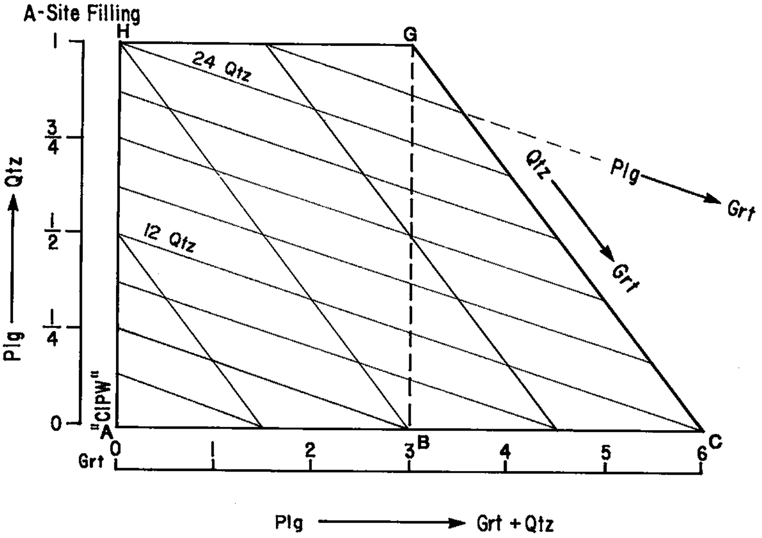

FIG. 12. The left-hand face of the polyhedron in Figure 11.

in other words a sodic andesine and two or more amphiboles, one of which would be a hornblende with a partially filled *A* site. The other amphiboles could be anthophyllite, gedrite, cummingtonite, or some combination thereof, as in the assemblages considered by Robinson & Jaffe (1969), by Stout (1971, 1972), and by others (see Robinson *et al.* 1982, for further references). At a point midway between (4) and the vertex C, the mineral content would be:

Plagioclase: 4.5 ab
Garnet: 3 $Mg_3Al_2Si_3O_{12}$
Amphibole: 6 $Ca_2Mg_{4.5}AlSi_{7.5}O_{22}(OH)_2$ +
1.5 $NaAlSi_{-1}$

in which the amphibole would be a single-phase hornblende. Finally, at the C vertex, we obtain:

Plagioclase: none
Garnet: 6 $CaMg_2Al_2Si_3O_{12}$
Amphibole: 3 $Na_2Mg_3Al_2Si_8O_{22}(OH)_2$ +
3 $Ca_2Mg_5Si_8O_{22}(OH)_2$

All of the above may be generalized and made yet more realistic by the operation of exchange components such as $FeMg_{-1}$, $FeAl_{-1}$, $TiFe_{-1}$, and others that do not alter the modal space. At C, the amphibole would be either a single-phase winchite or a mixture of glaucophane and actinolite. If we were to modify the composition at the A vertex in Figure 11 by removing the 3 tr, the amphibole at (4), then at the limit [ed+], would be: 3 $NaMg_7AlSi_7O_{22}(OH)_2$, that at the midpoint would be: 3 $Na_{0.5}Ca_2Mg_4Al_{2.5}Si_{6.5}O_{22}(OH)_2$, and that at the C vertex would be glaucophane. Note that total amphibole remains constant and that the net effect is the transformation of plagioclase into garnet, a feat that is possible thanks to the remarkable exchange-capacity of amphibole. Although the total remains constant, the *kind* of amphibole varies greatly as plagioclase is destroyed and garnet is created. A similar role is played by pyroxene in the anhydrous assemblages. Some relevant experimental work has recently been presented by D.M. Jenkins (1990). The reactions that make this possible are based on equations (5) and (9) above, and have much in common with the garnet–plagioclase reactions used by Ghent (1976) in pelite geobarometry.

Epidote is an additional phase that is characteristic of many garnet amphibolites and garnet glaucophanites. Its presence adds, inconveniently, one more dimension to the modal space of the amphibolite. The extra reaction equation, however, may be written simply as:

$$\text{amp} + \text{qtz} + 4\ \text{cm} + 3\ \text{tk} = 2\ \text{epi} \qquad (13)$$

and we may partially visualize this larger modal space by eliminating one of the reactions considered in Figure 11. In Figure 13, a three-dimensional section of the larger space has been constructed with basis-vectors on equations (2), (9), and (13), but omitting (12).

OPEN-SYSTEM MODAL SPACES

It is recommended that closed-system modal spaces be investigated before considering open or

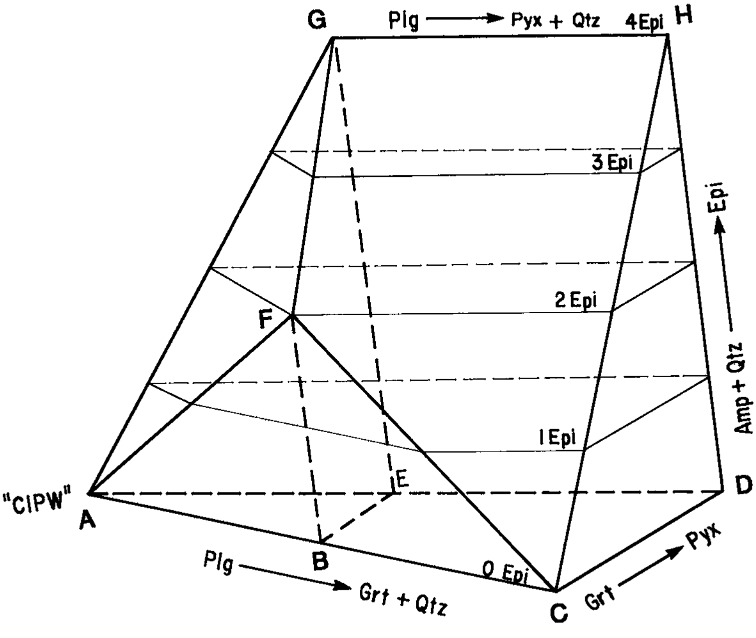

FIG. 13. A partial modal space for epidote-bearing amphibolites (see text).

partially open systems. The closed-system space may well contain the answers we seek, in which case there is no need to go further. However, if we wish to consider the transformation of anhydrous granulites into amphibolites, or *vice versa,* it is necessary to allow, at least, for open-system reactions that permit the gain or loss of H_2O. To do this, we may add H_2O as an *environmental* component to the list of phase components in the initial stoichiometric equations. If H_2O is I.V. in the assemblage (not always so), an open-system reaction involving H_2O will be obtained. One is always sufficient. If two are obtained, then H_2O can be eliminated between them, yielding one open-system and one closed-system reaction. The hydrous and anhydrous assemblages discussed above can be related, if quartz is present, by the equation:

$$2\ \mathrm{amp} = 7\ \mathrm{pyx} + 2\ \mathrm{qtz} + 2\ H_2O \qquad (14)$$

or, in any case, by:

$$4\ \mathrm{amp} + \mathrm{ed} + \mathrm{pg} = 14\ \mathrm{pyx} + \mathrm{plg} + 4\ H_2O \qquad (15)$$

Lower-grade amphibolites, such as those considered in an earlier paper (Thompson *et al.* 1982), commonly contain chlorite. Chlorite may be related to garnet by either:

$$2\ \mathrm{chl} + 4\ \mathrm{qtz} + \mathrm{tk} = 3\ \mathrm{grt} + 8\ H_2O \qquad (16)$$

or by:

$$2\ \mathrm{chl} + \mathrm{plg} + \mathrm{tk} = 3\ \mathrm{grt} + \mathrm{ed} + \mathrm{pg} + 8\ H_2O \qquad (17)$$

as may be appropriate to the assemblage.

In both (16) and (17), thirty-six oxyequivalents of chlorite replace thirty-six oxyequivalents of garnet or *vice versa,* a very nearly constant-volume replacement. The accompanying effect, left-to-right, is the consumption of quartz or plagioclase, or both, with the release of the same number of oxyequivalents of water, an apparent conversion, therefore, of quartz or plagioclase to water! These processes are thus somewhat reminiscent of a long ago event (Exodus, xvii, 1-7), and may therefore be referred to as Sinai reactions. The exchange operator or component, H_4Si_{-1}, is found in calcic garnet, and possibly in other silicates having isolated SiO_4 tetrahedra. It leads to the simplest of Sinai reactions, namely:

$$\mathrm{qtz} + H_4Si_{-1} = 2\ H_2O \qquad (18)$$

and

$$\mathrm{plg} + 4\ H_4Si_{-1} = 8\ H_2O + \mathrm{ed} + \mathrm{pg} \qquad (19)$$

We also may write, from (16) and (18):

$$3\ \mathrm{grt} + 4\ H_4Si_{-1} = 2\ \mathrm{chl} + \mathrm{tk} \qquad (20)$$

in which the two components on the right-hand side sum to a chlorite midway between an idealized clinochlore and an idealized corundophyllite. It is thus clear that it is saturation with respect to chlorite that prevents Fe–Mg garnet from showing significant variation from its anhydrous compositions by means of the operator H_4Si_{-1}. Chlorite simply forms instead. Variation by H_4Si_{-1} does occur, however, in calcic garnet because there are no calcic chlorites. Interestingly, some further pairs of phases are, like garnet and chlorite, related by H_4Si_{-1}, and hence related by equations analogous to (16) and (17). These include cordierite (anhydrous) and sudoite:

$$Mg_2Al_4Si_5O_{18} + 2\ H_4Si_{-1} = Mg_2Al_4Si_3O_{10}(OH)_8 \qquad (21)$$

suggesting that some pinite alterations of cordierite may contain sudoite rather than an ordinary chlorite. Orthopyroxene and lizardite (or antigorite) are similarly related:

$$3\ MgSiO_3 + H_4Si_{-1} = Mg_3Si_2O_5(OH)_4 \qquad (22)$$

as are olivine and brucite (*via* the hydroxy-humite series):

$$Mg_2SiO_4 + H_4Si_{-1} = 2\ Mg(OH)_2 \qquad (23)$$

This last relationship is perhaps the reason why variation by H_4Si_{-1} is absent or minor in olivine.

FURTHER APPLICATIONS

The foregoing discussion has been based primarily on considerations of material balance and of the constraints imposed by crystal chemistry on the chemical variability of minerals. Very little has been said or even implied about thermodynamic equilibrium, kinetics, or other matters of petrological concern. A path through modal space that represents a succession of equilibrium states, either in experimental results or in natural occurrence, is a special case of considerable interest, either as a way of displaying modal aspects of the experimental results, or as an aid in deciphering the P–T–t history of a metamorphic rock (Thompson *et al.* 1982, Ferry 1983, 1984, Chamberlain 1986, Schneiderman 1990). It has also been shown recently that the distribution of oxygen isotopes is profoundly influenced by variations in modal abundance (Chamberlain *et al.* 1990).

ACKNOWLEDGEMENTS

I thank D.M. Burt, R.F. Martin, and two anonymous reviewers for helpful comments on the manuscript. I also thank those students of recent years who, as captive audiences, have responded so helpfully to my obsession with the above approach, and especially Jo Laird and Alan Thompson, who were in on it from the start! My thanks too to Hugh Greenwood, always ready to listen to the unconventional (or even outrageous) in the hope that something useful might come of it. And thank you again, Hugh, for those early forays of yours into linear algebra (1967, 1968) that inspired me to begin the trend of thought here presented!

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Received January 28, 1991, revised manuscript accepted August 8, 1991.