Amphibole compositional space

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Summary. The basic formula of an amphibole is completely defined by stating the number of sodium atoms in X positions and the numbers of aluminium atoms in Y and Z. These three numbers are coordinates in a compositional space that can easily be represented. The alkali amphiboles are re-defined as having at least one atom of sodium in X in the basic formula unit. A systematic nomenclature for the calciferous and alkali amphiboles is suggested using existing end-member names.

IT has been shown (Phillips and Layton, 1964) that the major compositional affinities of calciferous and alkali amphiboles are more easily appreciated by deriving from the chemical analysis what was termed the *basic atomic formula*. Regarding these amphiboles as the result of various substitutions in the tremolite structure, the basic atomic formula is obtained by converting all substitutions in the Z position to equivalent aluminium, all substitutions in Y to equivalent aluminium or magnesium, and substitutions in A and X to equivalent sodium. It was suggested that the basic atomic formula could be related to pure end-member compositions on a simple two-axis diagram plotting total sodium atoms against total aluminium atoms in the formula.

A disadvantage of this method is that in certain cases two different basic formulae plot at the same point on the diagram. This occurs when the same numbers of sodium and aluminium atoms occupy different lattice positions in the two formulae, as, for example, in the case of edenite-κ, $NaCa_2Mg_5Si_7Al$, and $Tr_{50}G_{50}$, $CaNaMg_4AlSi_8$ (cations only are given and the abbreviations are those suggested in the above paper). To discriminate between such compositions a method of representation is required that will distinguish between Na^A and Na^X and between Al^Y and Al^Z. Now in the basic formula the relationship $Na^A+Al^Y = Na^X+Al^Z$ must hold. Knowing any three of these values, the fourth is completely determined because of the need for balanced substitution.

The variations of basic formula composition may therefore be regarded as occurring in a three-dimensional amphibole-compositional space. Fig. 1 shows how this space may conveniently be represented relative to orthogonal axes X, Y, and Z in a conventional orientation,

representing the numbers of atoms Na^X, Al^Y, and Al^Z in the basic formula. The figure may easily be duplicated to scale by tracing over an isometric graph paper.

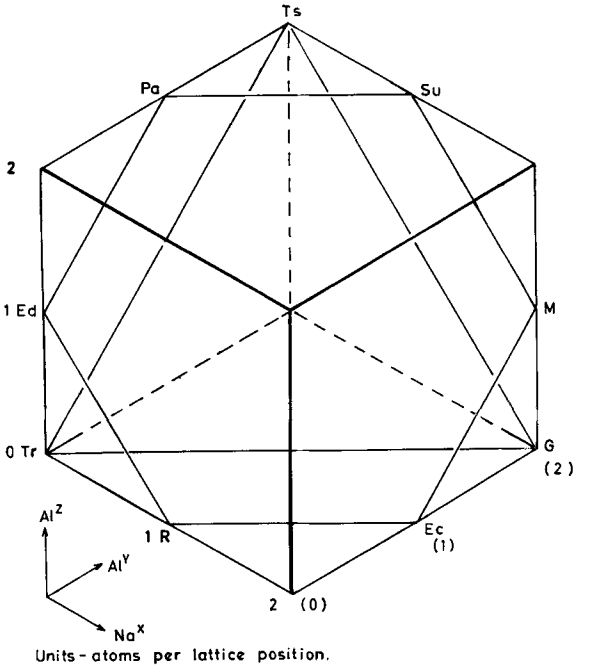

FIG. 1. Amphibole compositional space within the bounding cube.

The compositional space is an oblique slice through a cube, bounded by faces equivalent to crystallographic {100} and {111} planes. The limits are set by the number of X positions in the lattice and by assumptions (Phillips, 1963) about the limits of substitution in Y and Z positions.

It is immediately obvious from fig. 1 that a given basic formula (and consequently the atomic formula of any amphibole) can be matched by more than one combination of the end-member compositions suggested by Phillips and Layton, 1964. However, this is a disadvantage that exists in any ternary or high-order system with solid solution where *compounds* of the primary components are regarded as end-members for descriptive purposes. In most normal cases the number of end-members is small and the most convenient choice of a combination of end-members is fairly obvious. The choice is usually also influenced by a knowledge of the range of solid solution and the frequency of occurrence of certain

compositions or ranges of composition. These points are demonstrated in fig. 2 with reference to the system FeO–Fe_2O_3–TiO_2; the difficulty is accentuated in the amphibole group because of the large number of end-members involved and because we have as yet only a limited knowledge of the true range of solid solutions and their association with particular

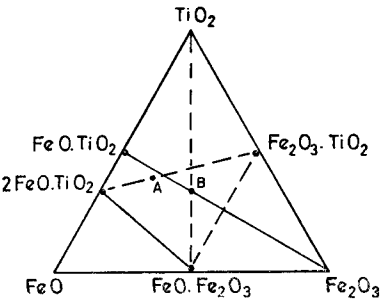

FIG. 2. The system FeO–Fe_2O_3–TiO_2 illustrates how a given composition, e.g. *A* or *B*, can be expressed in terms of more than one combination of end-members when these are not the primary components of the system. Because of the known range of composition of Fe–Ti oxide minerals in rocks, composition *A* would normally be expressed in terms of the three end-members magnetite, hematite, ilmenite, even though it could be expressed more simply as an ulvospinel–pseudobrookite solid solution.

geological environments. It may be that as our knowledge increases, and especially for a particular study, certain simple combinations of end-members will be found to be more useful than others, but this has yet to be established.

For some purposes it may be more convenient to fix the relative positions of basic formulae by specifying for each the three coordinates *X*, *Y*, and *Z* rather than by having to determine the proportions of a larger number of end-members required to match each formula.

It is useful at this point to consider the question of the boundary between the calciferous and the alkali amphiboles. Phillips and Layton, 1964, suggested that no compositional break exists between these groups as previously defined, but it is nevertheless convenient for certain purposes to make the distinction. In this earlier paper an arbitrary division was set at a total of $1\frac{1}{2}$ sodium atoms in the basic formula. It now seems that a much more satisfactory division can be made on the basis of the sodium in *X* alone. Calciferous amphiboles are therefore redefined as having less than 1·00 atoms of sodium in *X* in the basic formula, whilst

alkali amphiboles have 1·00 or more. Fig. 3 shows the position of the dividing plane. The compositions $Tr_{50}G_{50}$, $Ts_{50}G_{50}$, and $Su_{50}R_{50}$, which could not be distinguished from Ed, Pa, and G respectively on the two-axis diagram, are now seen to lie on this plane.

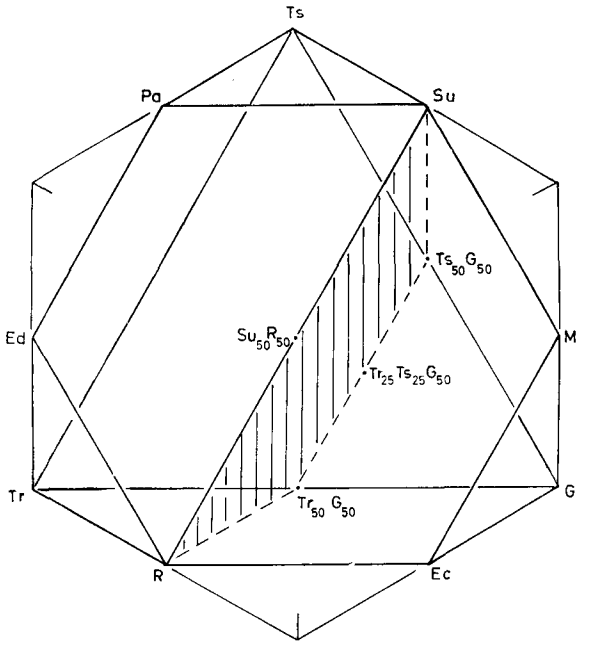

FIG. 3. The plane $Na^X = 1$ as the boundary between the calciferous and alkali amphibole sub-spaces.

The term *sensu extenso* was suggested by Phillips and Layton to denote a composition containing at least 50 % of a named end-member. Thus Tr s.e. denotes a composition containing 50 % or more of the end-member tremolite-κ. We may now consider the application of a *sensu extenso* nomenclature to subdivisions of the compositional space just defined.

The first major division has already been defined as the plane $X = 1$, separating the calciferous and alkali amphibole subspaces. The second logical division is by means of a plane midway between and parallel to the Tr, Ts, G triangle and the hexagon. Further boundaries required are provided by three diagonal planes of the cube parallel respectively to the X, Y, and Z axes. Fig. 4 shows the traces of the dividing planes on the

Tr, Ts, G triangle and the hexagon. It is difficult to represent clearly on a diagram the extension of these boundaries into the body of the cube, but in fig. 5 sections have been drawn at half atom intervals to indicate relationships in the solid.

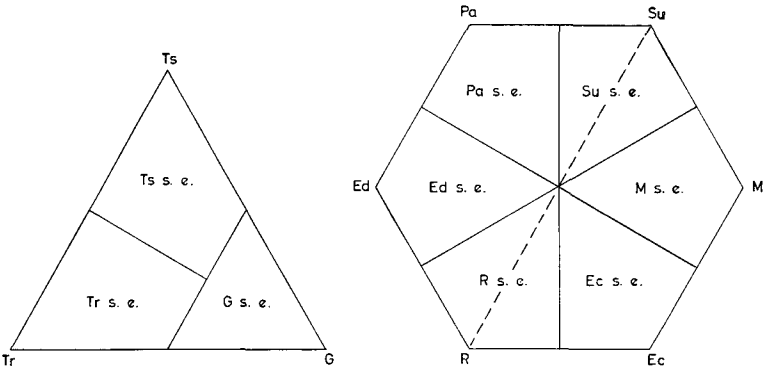

FIG. 4. The traces of the dividing planes on the Tr–Ts–G triangle and the hexagon.

For practical application of the nomenclature it is only necessary to refer to table I, which sets out the various limits together with simple conditions governing the position of a point relative to the oblique limiting planes. In the case of the two end-members richterite and sundiusite lying on the calc : alkali dividing plane, the name ranges across the division. If it should for any reason be necessary to make a distinction between compositions in different parts of these two fields, the names may be prefixed calciferous or alkali as appropriate, e.g. alk. R s.e., calc. Su s.e., etc.

As an example consider the basic formula shown by Phillips and Layton (1964, p. 1108) to be equivalent to $G_{36}Su_{33}Pa_{27}Ts_4$. It is no longer necessary to write out the basic formula at length—we can say that the basic formula is 1·05, 1·73, 1·28 if we adopt the convention of quoting X, Y, and Z in that order. Since $X > 1$, the formula is that of an alkali amphibole. Reference to table I shows that G, M, and Su are possible names. Conditions A and B are not satisfied, therefore the name (alkali) Sundiusite s.e. is appropriate.

If we now wish to express the composition in terms of end-members, by writing out the basic formula in full and comparing with the end-member formulae it is easily seen that the sodium in A restricts the amount of Su in the composition to 60 %. After deducting this and

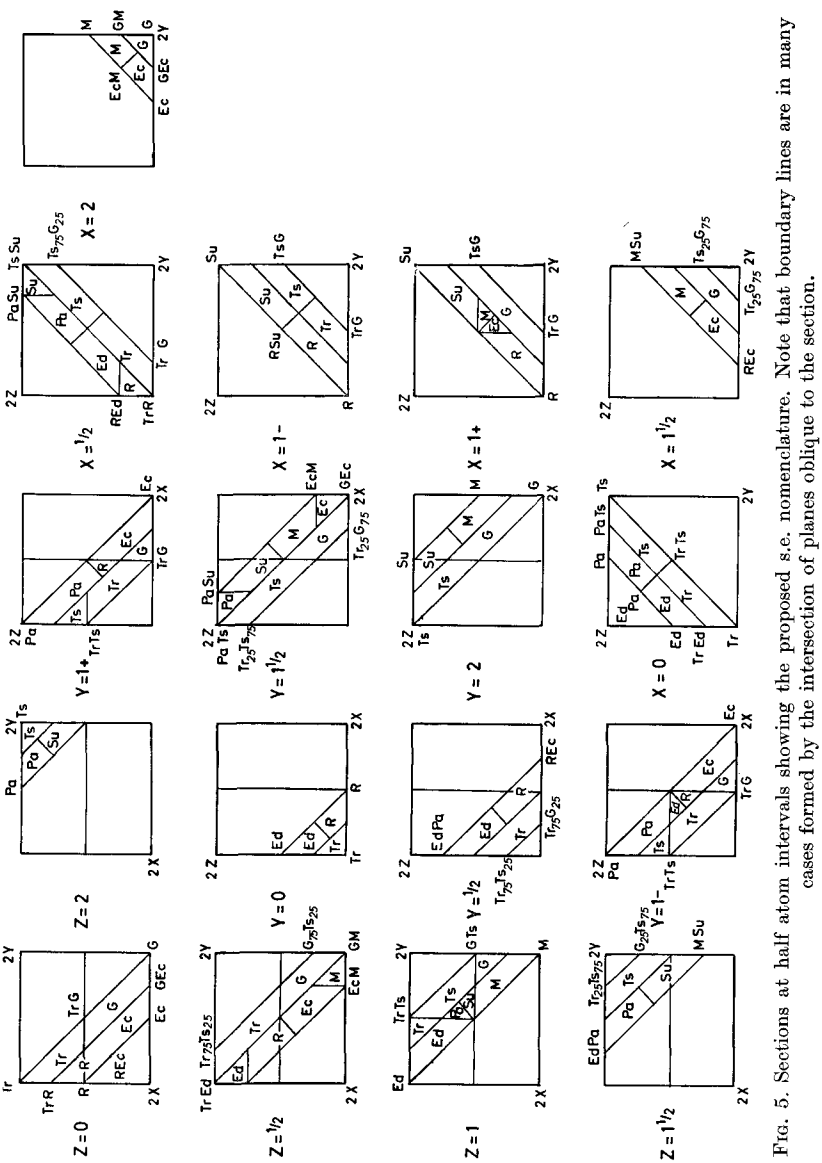

FIG. 5. Sections at half atom intervals showing the proposed s.e. nomenclature. Note that boundary lines are in many cases formed by the intersection of planes oblique to the section.

bearing in mind the position at which the analysis plots, a trial and error match can very quickly be made and leads to the combination $Su_{60}G_{22\cdot5}Tr_{13\cdot5}Ts_4$. For many practical purposes the analysis can be regarded as lying in the triangle Su–G–Tr.

TABLE I. Compositional limits for s.e. amphibole nomenclature
$X < 1{\cdot}00$. *Calciferous amphiboles*

		Conditions satisfied						
Y	*Z*	Unique	A+C	A	B	C	D	Otherwise
$X = 0$–$0{\cdot}50$								
0–0·50	0–0·50	.	.	Tr	R	.	.	Ed
	> 0·50–1·00	.	.	Tr	.	.	.	Ed
	> 1·00–1·50	Ed	.	.	.	.	.	.
> 0·50–1·00	0–1·50	Tr	.	.	.	.	.	.
	> 0·50–1·00	.	.	Tr	.	.	.	Ed
	> 1·00–1·50	.	Tr	Ts	.	Ed	.	Pa
	> 1·50–2·00	Pa	.	.	.	.	.	.
> 1·00–1·50	0·50–1·00	.	Tr	.	.	.	.	Ts
	> 1·00–1·50	.	.	Ts	.	.	.	Pa
	> 1·50–2·00	.	.	Ts	.	.	.	Pa
> 1·50–2·00	1·00–1·50	Ts	.	.	.	.	.	.
	> 1·50–2·00	.	.	Ts	.	.	Pa	Su
$X = > 0{\cdot}50 < 1{\cdot}00$								
0–0·50	0–0·50	.	.	Tr	.	.	.	R
	> 0·50–1·00	.	.	.	R	.	.	Ed
> 0·50–1·00	0–0·50	.	.	Tr	.	.	.	R
	> 0·50–1·00	.	.	Tr	R	.	.	Ed
	> 1·00–1·50	.	.	.	.	Ed	.	Pa
> 1·00–1·50	0–0·50	Tr	.	.	.	.	.	.
	> 0·50–1·00	.	Tr	Ts	R	.	Pa	Su
	> 1·00–1·50	.	.	Ts	.	.	Pa	Su
	> 1·50–2·00	.	.	.	.	.	Pa	Su
> 1·50–2·00	0·50–1·00	Ts	.	.	.	.	.	.
	> 1·00–2·00	.	.	Ts	.	.	.	Su

The more general condition $0 \leqslant x-y+z \leqslant 1$ must be satisfied in all cases if the basic formula is to lie within the compositional space as defined.

In using the tables, always work from left to right in checking the conditions satisfied.

Although rather different from the end-member combination suggested by Phillips and Layton, both are equally valid, but the present method leads to a combination more appropriate to the s.e. name. It still does not give a unique choice in all cases, for reasons given earlier, but work on this problem is continuing and further comment must be left for the future.

Many amphibole analyses do not satisfy the criteria for a reliable analysis suggested by Phillips, 1963. Derivation of the basic formula in such cases may be difficult to make in accordance with the rules so far given, but this problem is to be discussed in a later communication. Since any errors will tend to be pushed down into the A position, it is still possible for the X, Y, and Z values to plot within the compositional space, so that a name can be given. Also, if the plot is outside the space,

TABLE I (*cont.*)

$X \geqslant 1{\cdot}00$. *Alkali amphiboles*

		Conditions satisfied					
Y	Z	Unique	A	B	C	D	Otherwise
$X = 1{\cdot}00$–$1{\cdot}50$							
0–0·50	0–0·50	R	.	.	.	.	.
> 0·50–1·00	0–0·50	.	G	.	.	R	Ec
	> 0·50–1·00	.	.	.	.	R	Ec
> 1·00–1·50	0–0·50	.	G	.	.	.	Ec
	> 0·50–1·00	.	G	.	Ec	.	M
	> 1·00–1·50	.	.	M	.	.	Su
> 1·50–2·00	0–0·50	G	.	.	.	.	.
	> 0·50–1·00	.	G	.	.	.	M
	> 1·00–1·50	.	G	M	.	.	Su
	> 1·50–2·00	Su	.	.	.	.	.
$X = > 1{\cdot}50$–$2{\cdot}00$							
0·50–1·00	0–0·50	Ec	.	.	.	.	.
> 1·00–1·50	0–0·50	.	G	.	.	.	Ec
	> 0·50–1·00	.	.	.	Ec	.	M
> 1·50–2·00	0–0·50	.	G	.	Ec	.	M
	> 0·50–1·00	.	G	.	.	.	M
	> 1·00–1·50	M	.	.	.	.	.

Conditions—A $z \leqslant y-x+\frac{1}{2}$ C $z \leqslant 2-y$
B $z \leqslant x$ D $y \leqslant 2-x$

it will normally be possible to choose a suitable s.e. name from the adjacent named space. The problem of extending the compositional space into more dimensions to take account of other major substitutions also remains for future discussion. At least for the moment a relatively simple basic formula nomenclature is provided that can be used with uniformity by all workers and has fewer disadvantages than the scheme previously suggested.

References

PHILLIPS (R.), 1963. Min. Mag., vol. 33, p. 701.
—— and LAYTON (W.), 1964. *Ibid.*, p. 1097.

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