Thermodynamically Valid Projections of Extensive Phase Relationships

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Abstract

A direct calculation is presented for the production of projections of phase relations. The projections obey the phase rule and take into account all phases not explicitly shown provided their chemical potentials are constant. The approach is a generalization of the method used by Thompson (1957) in deriving the immensely useful AFM projection.

The calculation is a simple matrix multiplication followed by normalization and permits construction of projections suitable for specific problems, avoiding the need to rely upon projections devised by others for different problems with different constraints.

Introduction

Since the introduction of the AFM projection (Thompson, 1957), petrologists have had a powerful tool for the graphical analysis of the mineralogic phase relations in pelitic schists. This analysis is applicable to mineral assemblages that can be described in terms of the system $SiO_2-Al_2O_3-MgO-FeO-K_2O-H_2O$, provided that quartz and muscovite are present and provided that H_2O is either present (or was present) as a pure phase or that H_2O has the same chemical potential (or equilibrium pressure) in all assemblages compared.

The great utility of this projection is attested by the fact that virtually every paper on the petrology of pelitic schists since 1957 has used the AFM projection, or a closely related version, projecting from K-feldspar instead of muscovite in K-feldspar bearing rocks without muscovite. It is not rare, however, to have need for a projection not constrained by the requirements of the AFM projection, or to need to look at the phase relations from a different point of view.

This paper presents a method, illustrated by the 6-component pelite system but applicable to all systems, for generating projections suitable to any specific need. It is then unnecessary to adopt existing representations of phase relations simply because the diagrams have been previously prepared, thus avoiding the likelihood of misrepresenting the relations by choice of an unsuitable projection.

Requirements of a "Legal" Projection

The requirement that any valid representation of phase relationships must obey the first two laws of thermodynamics suggests the use of the word "legal" in connection with projections. "Illegal" projections break one or more thermodynamic laws, and "legal" ones do not. The essential requirement of a legal chemographic diagram is that the equilibrium state of the system be uniquely determined (or determinable) by specifying pressure, temperature, and the proportions of the components represented in the diagram. If the diagram is a projection, then the phases or components from which the projection is made must either be present, pure, or have their chemical potentials fixed at a constant value over the whole of the diagram.

Projections as "Mappings" or "Transformations"

The construction of a legal projection can be thought of as consisting of two steps. First, all compositions of interest are "mapped" or transformed from their usual basis of oxide proportions to a new coordinate system, or basis, consisting of the compositions that will serve as points of projection or as points lying in the plane to receive the projection. This change of components must be possible because although thermodynamics gives us no help on the choice of components to represent a system, it does at least tell us how many components we need and, further, that no composition selected as a component can be a linear combination of any of the other components. Within these broad limits we are free to choose any components we deem appropriate. The choice of appropriate new components or basis vectors is governed by the restrictions of the projection we require. The second step consists of eliminating the projection points from every phase and normalizing the remainder.

For example, in the AFM diagram, projection is first made from SiO₂ and H₂O on the assumption that quartz is always present and H₂O is either present or has its chemical potential externally controlled at a fixed value. The projection consists, analytically, of writing out a table giving the composition of every phase and end-member to be projected, with the oxide proportions as rows and the minerals as columns, crossing out the rows corresponding to SiO₂ and H₂O, and normalizing the remaining columns to constant sum. The resulting table of numbers gives the coordinates of the compositions of every phase in terms of the subsystem Al₂O₃-FeO-MgO-K₂O. Further projection from muscovite requires either graphical construction or re-writing all the remaining minerals in terms of a new basis that includes muscovite as one of the rows and then crossing out that row and normalizing the remaining three-element columns to constant sum.

To make the foregoing more concrete, consider the following operations. First, let M^{ox} be the matrix of pelitic mineral compositions written in terms of oxide proportions. This matrix is given in the upper part of Table 1. In the lower part of Table 1 is given the same information on mineral compositions, except that the matrix has been "mapped" or transformed into a new coordinate system having as coordinate axes (or components), kyanite, quartz, muscovite, H_2O , FeO, and MgO. The transformed mineral matrix is labelled M^v in Table 1.

The mapping of $M^{\circ x}$ into M^{\vee} having been accomplished in Table 1, we may now perform the second step, projecting all minerals from quartz, muscovite, and H₂O simultaneously. This corresponds to crossing out the second, third, and fourth rows of M^{\vee} (Table 1) and normalizing the remaining columns that have positive sums to a constant sum, taken here as 4.0 for simplicity.¹ This projected matrix, designated as M^{\vee} (Q,Ms,W), is given in Table 2. Study of this matrix will show that the numbers are equal to 4 times the coordinates for the minerals in the AFM projection, and these are plotted in Figure 1.

Stepping back briefly to the operation of mapping M^{ox} into M^v (Ky,Q,Ms,W,FeO,MgO) it can be shown that M^v is the image of M^{ox} under a transformation *E*. That is,

$$M^{\mathbf{v}} = E M^{\mathrm{ox}},$$

¹ It is conventional to normalize to a sum of 1.0, in which case the coordinates can be regarded as mole fractions. There is nothing sacrosanct about this sum, however, and any number may be used, selected so as to simplify the arithmetic. Whatever choice is made makes no difference to the topology of the figure. Columns of negative sum are considered later.

TABLE 1. Pelitic Mineral Matrices

| | Ку | Q | Ms | W | A1 | Py | Ann | Ph1 | St | 0r | La | ь | Ch ₁ | Ch ₂ | Ch_3 | Ch4 | Ctd | Cď | |
|------------------|----|---|----|---|----|----|-----|-----|----|----|----|----------------|-----------------|-----------------|-----------------|-----------------|-----|----|------------------|
| Si0, | [1 | 1 | 6 | 0 | 3 | 3 | 6 | 6 | 8 | 6 | 7 | 7 | 8 | 8 | 4 | 4 | 2 | 5] | |
| A1_00_ | 1 | 0 | 3 | 0 | 1 | 1 | 1 | 1 | 9 | 1 | 1 | 1 | 0 | 0 | 4 | 4 | 2 | 2 | |
| Z 3 Fe0 | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 4 | 0 | 0 | 0 | 12 | 0 | 0 | 8 | 2 | 0 | _ wox |
| MgO | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 0 | 0 | 0 | 0 | 12 | 8 | 0 | 0 | 2 | - 11 |
| K.0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | |
| н ₂ 0 | 0 | 0 | 2 | I | 0 | 0 | 2 | 2 | 2 | 0 | 1 | 2 | 8 | 8 | 8 | 8 | 2 | 0 | |
| | Ky | Q | Ms | W | A1 | Рy | Ann | Ph1 | St | 0r | La | ^L b | ^{Ch} 1 | Ch ₂ | Ch ₃ | Ch ₄ | Ctd | Cd | |
| Ky | [1 | 0 | 0 | 0 | 1 | 1 | -2 | -2 | 9 | -2 | -2 | -2 | 0 | 0 | 4 | 4 | 2 | 2] | |
| Q | 0 | 1 | 0 | 0 | 2 | 2 | 2 | 2 | -1 | 2 | 3 | 3 | 8 | 8 | 0 | 0 | 0 | 3 | - × ^V |
| MS | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | - 11 |
| W | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 2 | -2 | -1 | 0 | 8 | 8 | 8 | 8 | 2 | 0 | |
| FeQ | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 4 | 0 | 0 | 0 | 12 | 0 | 0 | 8 | 2 | 0 | |
| MgO | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 0 | 0 | 0 | 0 | 12 | 8 | 0 | 0 | 2 | |

PROJECTIONS OF EXTENSIVE PHASE RELATIONSHIPS

TABLE 2. Pelitic AFM Matrix and Transformation Matrix

| | Al | Ру | Ann | Ph1 | St | Or | La | L _b | Ch1 | Ch ₂ | Ch ₃ | Ch ₄ | Ctđ | Cđ | |
|-----|----|----|-----|-----|------|----|----|----------------|-----|-----------------|-----------------|-----------------|-----|----|---------------------|
| Ку | [1 | 1 | -2 | -2 | 2.77 | -2 | -2 | -2 | 0 | 0 | 1.333 | 1.333 | 2 | 2 | |
| Fe0 | 3 | 0 | 6 | 0 | 1.23 | 0 | 0 | 0 | 4 | 0 | 0 | 2.667 | 2 | 0 | = $M^{V}(Q, Ms, W)$ |
| Mg0 | 0 | 3 | 0 | 6 | 0 | 0 | 0 | 0 | 0 | 4 | 2.667 | 0 | 0 | 2 | |

Transformation Matrix,

| | 0 | 1 | 0 | 0 | -3 | 0 | | 1 | 1 | 6 | 0 | 0 | 0 |
|---------|---|----|---|---|----|---|----|---|---|---|---|---|---|
| | 1 | -1 | 0 | 0 | -3 | 0 | | 1 | 0 | 3 | 0 | 0 | 0 |
| (wox)-1 | 0 | 0 | 0 | 0 | 1 | 0 | ox | 0 | 0 | 0 | 0 | 1 | 0 |
| (()) = | 0 | 0 | 0 | 0 | -2 | 1 | V= | 0 | 0 | 0 | 0 | 0 | 1 |
| | 0 | 0 | 1 | 0 | 0 | 0 | | 0 | 0 | 1 | 0 | 0 | 0 |
| | 0 | 0 | 0 | 1 | 0 | 0 | | 0 | 0 | 2 | 1 | 0 | 0 |

and it can be shown in this case that

 $E = (V^{\text{ox}})^{-1}$ (See Table 2, and Appendix) In other words, the transformation is accomplished by pre-multiplication of M^{ox} by the transformation matrix E which has the effect of re-writing every mineral in terms of the new basis. It will further be seen, by reference to Table 2, that the matrix product

 $(v^{ox})^{-1}$

$$(V^{\mathrm{ox}})^{-1}V^{\mathrm{ox}} = I,$$

showing that the transformation matrix is simply the inverse of the matrix giving the new basis in terms of the old one (see Appendix). The new basis must naturally have the same dimension as the old one, and be non-singular. This simple result is perfectly general and can be used to transform any system to a new basis prior to the cancelling of rows that constitutes projection.

Advantages of Matrix Projections

There are at least four advantages to using the approach suggested here for the construction of projections.

- 1. The projection from any point(s) to any plane is simple and unambiguous.
- 2. The resulting projection is thermodynamically "legal" under the specific constraints that components or phases corresponding to eliminated rows have known fixed or buffered chemical potentials.

- 3. It is difficult to ignore the constraints that are necessary for the projection to be legal, thus misuse of the result is less likely.
- 4. It is unnecessary to rely on projections requiring some constraint other than those appropriate for one's own specific problem.

Such diagrams as Figure 1, or any others made by similar rules, are readily extended to include additional components. For example, if Fe^{3^+} is to be treated in the normal AFM projection, it is only necessary to have Fe^{3^+} determined in the minerals and to have the presence of magnetite as an additional phase. Projection from Fe_3O_4 in the same way as from muscovite, quartz, and H_2O will leave the resulting diagram looking similar but with Fe^{3^+} concentrations definite at each point. Similar treatment can be accorded Ti if either rutile or ilmenite is present.

Projection in the Negative Sense

Thompson (1957, p. 847) draws special attention to the AFM projection of K-feldspar, which lies not between the projection point, muscovite, and the projection plane, but on the other side of muscovite, away from the projection plane. He proposes that the projection of such points be done by extending tie lines from muscovite toward them in a negative sense, that is, towards the projection plane; he suggests that we refer to this process as projection in the negative sense. For K-feldspar



FIG. 1. The AFM projection of J. B. Thompson. Abbreviations: Ky = kyanite; St = staurolite; Ctd = chloritoid; Cd = cordierite; Ch = chlorite of four limiting compositions; Al = almandine; Py = pyrope; Ann = annite; Phl = phlogopite; Or = K-feldspar; L_a and L_b = assumed liquids near the Or-Q-H₂O "eutectic". The diagram in the upper left corner represents a possible topology at about 4 kilobars and around 700°C. K-feldspar and the model liquids do not plot in the figure, but tie-lines to them extend to minus infinity, away from the Ky-corner (note that they have only one non-zero coordinate in Table 2, and it is negative).

this results in a projected location coincident with that of kyanite. In the presence of quartz and under divariant conditions, muscovite and H_2O , kyanite and K-feldspar are not stable together, one projecting positively (kyanite) and the other negatively (K-feldspar). At the *A*-apex of the AFM diagram, therefore, a discontinuity occurs because all phases and phase regions from and including kyanite toward and past biotite projecting in the positive sense (+phases) and all phases from and including K-feldspar in the opposite direction projecting in the negative sense (-phases).

An important point to notice is that +phases and -phases do not appear on the same diagram. However, while -phases cannot be represented on a diagram showing the relative positions of +phases, tie lines connecting +phases and -phases can be shown. Such tie lines can be extended to infinity, because each such tie line passes through a point that projects indefinitely far from the origin of our coordinate system. If it is desired to explicitly plot the relative positions of the -phases, then a diagram showing ony -phases must be constructed.

The recognition of +phases and -phases in the matrix context presented in this paper is simple. Reference to Table 2 will help. The +phases all have positive sums of coefficients. That is to say, the column of numbers associated with each +phase has a positive sum, while the column for each -phase has a negative sum. In this case only Or, L_a and L_b are -phases, all the others projecting in the positive sense. In keeping with the requirement that we may not show +phases and -phases in the same diagram, Figure 1 does not plot Or, L_a , or L_b , but tie lines that can lead toward these compositions are shown, originating at the points representative of minerals that can be plotted.

It is vital to retain the distinction between +phases and -phases so as to be sure of not inadvertently putting the two kinds on the same diagram. For this reason the matrices of Table 2 and Table 3 retain the signs of all coefficients so that in any further projection the two kinds of phases can be kept separate. Normalization to constant sum should thus be carried out for only one class of phases at a time, and they should never be all normalized to the same *positive* constant sum, because we would then lose this vital distinction.

In practice, if too many important phases should project negatively, it is preferable to choose a new projection plane, parallel to the original but displaced so as to change the sign of projection of the offending phases. If it is desired to find the directions of the tie lines from +phases to -phases, one can normalize the columns of the -phases, to the same *positive* sum as the +phases and by construction extend tie lines from the +phases outward, extending *away* from the plotted positions of the -phases. The -phases themselves are not represented, and should then be removed from the projection.

Alternative Projections of the "Pelite System"

Consideration of the full set of minerals and components available in this system (M^{ox} in Table 1) will show that the new basis ($V^{\text{ox}} = (\text{Ky}, \text{Q}, \text{Ms},$

W,FeO,MgO) is not unique. While it is desirable to keep FeO and MgO in the basis to show the Fe/Mg ratio in the minerals, we could have chosen any four of the five phases—Ky, Q, Ms, W, Or—as components in addition to FeO and MgO. This provides four more possible bases for projection. Each of these, including the one just treated, can give rise to four distinct projections, giving a total of twenty different and equally valid views of the phase relations in this system, according to what minerals are present or what components are to be regarded as extensive or intensive.

The view of the system just constructed (Fig. 1) projecting from Q, Ms, W on Ky, FeO, MgO is thus only one of the following four possibilities:

Projection from Q,Ms,W onto Ky,FeO,MgO (AFM) Projection from Ky,Ms,W onto Q,FeO,MgO Projection from Ky,Q,W onto Ms,FeO,MgO Projection from Q,Ky,Ms onto W,FeO,MgO

As an example of the use of changing our view of the system, let us consider the last of these new possibilities, projecting from (Q,Ky,Ms) onto H₂O, FeO, MgO. This is achieved by striking out rows 1, 2, and 3 from M^v (Table 1) and normalizing² the remaining columns to constant sum. The result is plotted in Figure 2. The phase L_a is an assumed liquid composition possible in the system forming a ternary eutectic between Or, Q, and H₂O. Data from natural anatectic melts could be substituted if available.

Figure 2 is legal for rocks containing quartz, muscovite, and one of the Al_2SiO_5 polymorphs, plotted here as kyanite. Several useful results can be read directly from the diagram. First and most obvious, H_2O has changed its role from that of an intensive variable in Figure 1 to an extensive variable in Figure 2, where its abundance relative to FeO and MgO is now critical to the assemblage, rather than its externally controlled chemical potential. Further, only part of the diagram has H_2O as a phase, the remainder of the assemblages being



FIG. 2. Projection of the six-component "pelite" system onto the plane H_2O -FeO-MgO from points representing quartz, kyanite, and muscovite. Water is shown as an extensive parameter in this diagram in contrast to its role as an intensive variable in Figure 1. The diagram in the upper left corner corresponds to the similarly placed diagram of Figure 1, where Gar-St-Bi are stable with H_2O and Ms, but not with kyanite. In Figure 2, above, Gar-St-Bi are shown as stable with Q, Ms, and Ky, but not with H_2O . Viewed from this vantage point all minerals plot in the positive sense, being within the triangle W-F-M, with the exceptions of Or, La, which cannot be plotted. Tie-lines towards them can be plotted, however, and may be extended to infinity.

in the water-deficient region (Yoder, 1955) where water plays the same role as any other extensive constituent. Reactions that involve the evolution of H_2O are seen on such a diagram as changes of tie-lines that involve H_2O as one of the reacting phases. As a corollary, there are solid-solid reactions possible, visible on inspection, that do not involve H_2O . For example, the following solid-solid reactions could be written

Chlorite + Almandine = Staurolite + Biotite (\pm Q,Ky,Ms) Annite = Almandine (\pm Q,Ky,Ms) Cordierite = Biotite (\pm Q,Ky,Ms).

Other features of the diagram are that tie-lines towards K-feldspar and the model liquid L_a both extend towards minus infinity away from the H₂O

^a If, after eliminating rows, any phase has all negative coefficients, or a negative sum of coefficients, it has no legal representation in the projection with phases, being positioned "behind" the projection point instead of between the projection point and the plane of the projection. It is possible, however, that phases which do plot, either in the positive or negative sense, will have plottable tie-lines leading towards such unrepresentable minerals. See K-spar in AFM as an example.

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TABLE 3. Transformed Matrices

V^{OX} = (Ky,Q,Ms,Or,Fe0,Mg0)

| | | | | ſ | 1 | 1 | б | 6 | 0 | 0 | | | ſ | 0 | 1 | 0 | 0 | -1 | -1] | |
|-----|----|----|----|---|----|-----|------|-------|---------|------|-------|------|-----|----|-----------------|-----------------|-----------------|-------------------|-----|----|
| | | | | | 1 | 0 | 3 | 1 | 0 | 0 | | | | 1 | -1 | 0 | 0 | -5 | 1 | |
| | | | эx | | 0 | 0 | 0 | 0 | 1 | 0 | | .ox1 | | 0 | 0 | 0 | 0 | 0 | .5 | |
| | | V | = | | 0 | 0 | 0 | 0 | 0 | 1 | (V |) | - | 0 | 0 | 0 | 0 | 1 | 5 | |
| | | | | | 0 | 0 | 1 | 1 | 0 | 0 | | | | 0 | 0 | 1 | 0 | 0 | 0 | |
| | | | | | C | 0 | 2 | 0 | 0 | 0 | | | | 0 | 0 | 0 | 1 | 0 | 0 | |
| | | | | | | | | | | | | | | | | C1 | Ch | | Chd | 64 |
| | Ку | Q | M | S | Or | A1 | Ру | Anı | n Phl | . 5 | tΨ | La | L. | с | Ch ₁ | Ch 2 | cn. | 3 ^{cn} 4 | Cta | |
| Ку | 1 | 0 | 0 | | 0 | 1 | 1 | -2 | -2 | 7 | -1 | -1 | | •2 | -8 | -8 | -4 | -4 | 0 | 2 |
| Q | 0 | 1 | 0 | | 0 | 2 | 2 | 2 | 2 | 1 | 1 | 2 | | 3 | 16 | 16 | 8 | 8 | 2 | 3 |
| Ms | 0 | 0 | 1 | | 0 | 0 | 0 | 1 | 1 | 1 | .5 | .5 | | 1 | 4 | 4 | 4 | 4 | 1 | 0 |
| Or | 0 | 0 | 0 | | 1 | 0 | 0 | 0 | 0 | -1 | 5 | .5 | | 0 | -4 | -4 | -4 | -4 | -1 | 0 |
| Fe0 | 0 | 0 | 0 | | 0 | 3 | 0 | 6 | 0 | 4 | 0 | 0 | | 0 | 12 | 0 | 0 | 8 | 2 | 0 |
| MgO | 0 | 0 | 0 | | 0 | 0 | 3 | 0 | 6 | 0 | 0 | 0 | | 0 | 0 | 12 | 8 | 0 | 0 | 2 |
| | | | | | | vox | = (K | y,Q,(| Dr,W,Fe | 0,Mg | 0) | | | | | | | | | |
| | | | | 1 | 1 | 6 | 0 | 0 | 0 | | | | 0 | 1 | 0 | 0 | -1 | 0 | | |
| | | | | 1 | 0 | 1 | 0 | 0 | 0 | | | | 1 | -1 | 0 | 0 | ~5 | 0 | | |
| | v | ×= | | 0 | 0 | 0 | 0 | 1 | 0 | | (vox) | -1 = | 0 | 0 | 0 | 0 | 1 | 0 | | |
| | | | | 0 | 0 | 0 | 0 | 0 | 1 | | | | 0 | 0 | 0 | 0 | 0 | 1 | | |
| | | | | 0 | 0 | 1 | 0 | 0 | 0 | | | | 0 | 0 | 1 | 0 | 0 | 0 | | |
| | | | L | 0 | 0 | 0 | 1 | 0 | 0 | | | | 0 | 0 | 0 | 1 | 0 | 0] | | |
| | Ку | Q | 0r | W | A1 | Η | у | Ann | Phl | St | Ms | La | L b | Cł | 1 | Ch ₂ | Ch ₃ | Ch ₄ | Ctd | Cd |
| Ку | 1 | 0 | 0 | 0 | 1 | ļ | L. | 0 | 0 | 9 | 2 | 0 | 0 | C | ł | 0 | 4 | 4 | 2 | 2 |
| Q | 0 | 1 | 0 | 0 | 2 | ŝ | 2 | 0 | 0 | -1 | -2 | 1 | 1 | 8 | | 8 | 0 | 0 | 0 | 3 |
| Or | 0 | 0 | 1 | 0 | 0 | (| D | 1 | 1 | 0 | 1 | 1 | 1 | (|) | 0 | 0 | 0 | 0 | 0 |
| W | 0 | 0 | 0 | 1 | 0 | (| D | 2 | 2 | 2 | 2 | 1 | 2 | 8 | | 8 | 8 | 8 | 2 | o |
| Fe0 | 0 | 0 | 0 | 0 | 3 | (| D | 6 | 0 | 4 | 0 | 0 | 0 | 12 | | 0 | 0 | 8 | 2 | 0 |
| Mg0 | 0 | 0 | 0 | 0 | 0 | 3.7 | 3 | 0 | 6 | 0 | 0 | 0 | 0 | C |) | 12 | 8 | 0 | 0 | 2 |

corner. This indicates that either K-feldspar or L_a could coexist with garnet and biotite (+ Q,Ky,Ms) but not both L_a and K-feldspar. In addition, neither K-feldspar nor L_a are stable in the presence of H₂O when biotite and garnet coexist. Thus any liquids will be undersaturated with respect to H₂O. This suggests that partial melting or anatexis may occur without a vapor phase, or that, if one is present at first, it may be immediately consumed by the melt.

mineral matrices, together with the transformation matrices that accomplish the mapping. Each of these transformed matrices can be reduced to four different 3-component projections by the methods already given. Taken together, these four, with M^v (Table 1), define twenty different views of the pelite system, each with its own specific constraints.

Conclusions

Table 3 presents the other four transformed

Legal projections of extensive phase relations of

TABLE 3, Continued

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V<sup>OX</sup> = (Ky,Or,Ms,W,Fe0,Mg0)
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| | [1 | 6 | 6 | 0 | 0 | 0 | | 0 |
|-----------------|----|---|---|---|---|---|-------------------------------|---|
| | 1 | 1 | 3 | 0 | 0 | 0 | .55 0 0 -1.5 | 0 |
| v ^{ox} | 0 | 0 | 0 | 0 | 1 | 0 | $(y^{0}x)^{-1} =5 .5 0 0 2.5$ | 0 |
| V == | 0 | 0 | 0 | 0 | 0 | 1 | 1 -1 0 0 -5 | 1 |
| | 0 | 1 | 1 | 0 | 0 | 0 | 0 0 1 0 0 | 0 |
| | D | 0 | 2 | 1 | 0 | 0 | 0 0 0 1 0 | 0 |

| | Ку | Or | Ms | W | A1 | Ру | Ann | Ph1 | St | Q | La | Ъ | Ch ₁ | Ch ₂ | Ch ₃ | Ch ₄ | Ctd | Cd | |
|-----|----|----|----|---|----|----|-----|-----|----|----|-----|-----|-----------------|-----------------|-----------------|-----------------|-----|------|--|
| Ку | Гı | 0 | 0 | 0 | 3 | 3 | 0 | 0 | 8 | 1 | 1 | 1 | 8 | 8 | 4 | 4 | 2 | 5 | |
| Or | 0 | 1 | 0 | 0 | 1 | 1 | 1 | 1 | 5 | .5 | 1.5 | 1.5 | 4 | 4 | 0 | 0 | 0 | 1.5 | |
| Ms | 0 | 0 | 1 | 0 | -1 | -1 | 0 | 0 | .5 | 5 | 5 | 5 | -4 | -4 | 0 | 0 | 0 | -1.5 | |
| W | 0 | 0 | 0 | 1 | 2 | 2 | 2 | 2 | 1 | 1 | 2 | 3 | 16 | 16 | 8 | 8 | 2 | 3 | |
| Fe0 | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 4 | 0 | 0 | 0 | 0 | 12 | 0 | 8 | 2 | 0 | |
| Mg0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 0 | 0 | 0 | 12 | 0 | 8 | 0 | 0 | 2 | |

V^{OX} = (Or,Q,Ms,W,Fe0,Mg0)

| | | | | 6 | 1 | 6 0 | 0 | 0 | | | | 0 | 5 | 0 | 0 | 1.5 | 0 | | |
|-----|----------|----|----|---|----|-----|-----|-----|------|-----|----|---|----------|----|----------------|-----------------|-----|-----|----|
| | | | | 1 | 0 | 3 0 | 0 | 0 | | | | 1 | 0 | 0 | 0 | -6 | 0 | | |
| | | ox | | 0 | 0 | 0 0 | 1 | 0 | | ox. | -1 | 0 | .5 | 0 | 0 | 5 | 0 | | |
| | | V | 4 | 0 | 0 | 0 0 | 0 | 1 | (| V) | * | 0 | -1 | 0 | 0 | 1 | 1 | | |
| | | | | 1 | 0 | 1 0 | 0 | 0 | | | | 0 | 0 | 1 | 0 | 0 | 0 | | |
| | | | | 0 | 0 | 2 1 | 0 | 0 | | | | 0 | 0 | 0 | 1 | 0 | 0 | | |
| | 0r | Q | Ms | W | Al | Ру | Ann | Ph1 | St | Ку | La | Ъ | $^{Ch}1$ | CI | ^h 2 | Ch ₃ | Ch4 | Ctd | Cd |
| Or | 1 | 0 | 0 | 0 | 5 | 5 | 1 | 1 | -4.5 | 5 | 1 | 1 | 0 | | C | -2 | -2 | -1 | -1 |
| Q | 0 | 1 | 0 | 0 | 3 | 3 | 0 | 0 | 8 | 1 | 1 | 1 | 8 | ł | 8 | 4 | 4 | 2 | 5 |
| Ms | 0 | 0 | 1 | 0 | .5 | .5 | 0 | 0 | 4.5 | .5 | 0 | 0 | 0 | 1 | С | 2 | 2 | 1 | 1 |
| W | 0 | 0 | 0 | 1 | -1 | -1 | 2 | 2 | -7 | -1 | 1 | 2 | 8 | 1 | 3 | 4 | 4 | 1 | -2 |
| FeO | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 4 | 0 | 0 | 0 | 0 | 1 | 2 | 0 | 8 | 2 | 0 |
| MgO | lo | 0 | 0 | 0 | 0 | 3 | 0 | 6 | 0 | 0 | 0 | 0 | 12 | (| C | 8 | 0 | 0 | 2 |

mineralogic systems are most easily performed by a simple matrix multiplication, followed by elimination of rows representing points of projection (Kcomponents, Thompson, 1970), and normalization to constant sum. Phases having negative columnsums after row-elimination project in the negative sense (Thompson, 1957) and those having positive column-sums project in the positive sense. Projections explicitly representing the relative positions of phases that project in the positive sense cannot also represent the compositions of phases that project in the negative sense, but tie lines to minerals projecting negatively may be shown.

The transformation matrix is simply the inverse of the matrix of the new components given in terms of the old components.

Twenty useful and legal triangular projections of the six-component "pelite system" are possible, each with its own rules of projection and phase compatibilities. Similar projections can be made for any system provided there exist phases or components whose chemical potentials can be regarded as fixed for the purposes of comparing the rest of the assemblages.

Reliance upon diagrams devised for other problems than our specific problem is thus unnecessary, and it becomes as easy to generate a thoroughly appropriate diagram as it has been to adopt a readymade but often inappropriate one.

Appendix

Derivation of the Transformation Matrix

The required transformation can be represented as below, in which the notation is as in the text of the paper, with the additional symbols Ox^{ox} representing the original oxide basis in terms of oxides, Ox^v the oxides in terms of the new basis, A^{ox} and A^v the rest of the minerals expressed in terms of oxides and the new basis respectively. V^{ox} is the new basis written in terms of oxides. Then we can write a partitioned matrix as follows:



Now, either pre-multiplying by the correct transformation matrix, or equivalently, performing a series of elementary row operations, the above matrices can be changed to:



Clearly, the transformation matrix we require is one that transforms V^{ox} into I, or

$$EV^{ox} = I.$$

The only matrix that will accomplish this is the matrix $(V^{\text{ox}})^{-1}$ demonstrating that $E = (V^{\text{ox}})^{-1}$, which is what we set out to do.

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