Tetrahedral plot diagram:

A geometrical solution for quaternary systems

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ABSTRACT

The transformation from a tetrahedral four-component system to an XYZ-orthogonal coordinate axis system has been solved using the geometry of a tetrahedron. If a four component mixing ratio is described as t, l, r, and f (here, $t + l + r + f = 1$), the transforming equations can be written as, $x = (r + 1 - l) / 2$, $y = \frac{\sqrt{3}}{2}t + \frac{\sqrt{3}}{6}f$, and $z = \frac{\sqrt{6}}{3}f$. A tetrahedral plot diagram can be easily constructed using the algorithms described in this paper. We present an implementation of these algorithms in a custom-designed Microsoft Excel spreadsheet, including adjustable viewing angles for the tetrahedral plot. This will be of general utility for petrological or mineralogical studies of quaternary systems.

Keywords: Tetrahedral diagram, triangular diagram, quaternary systems, phase diagram, three-dimension, trilinear coordinates, tetrahedron

INTRODUCTION

Tetrahedral diagrams are commonly used in petrology and mineralogy, for example, the Di-Fo-Ne-Qz diagram for basaltic rocks (Yoder and Tilley 1962), the An-Ab-Or-Qz diagram for granitic rocks (Winkler 1979), and four-component metamorphic phase diagrams (e.g., Thompson 1957; Spear 1993). The algorithm of transformation from a tetrahedral four-component system to an XYZ-orthogonal coordinate system has been addressed by several studies (e.g., Korzhinskii 1959; Mertie 1964; Arem 1971; Spear 1980; Armienti 1986; Maaløe et al. 2005; Armienti and Longo 2011). These authors solved the transformation by vector and/or linear algebra using computer programs. Computer applications for tetrahedral plots have also been presented by many authors (e.g., Spear et al. 1982; Armienti 1986; Torres-Roldan et al. 2000; Ho et al. 2006; Armienti and Longo 2011). Such applications are run on programing language platforms such as FORTRAN, BASIC, and JAVA.

This paper describes a different solution of transformation from a tetrahedral to an orthogonal coordinate system. It has been solved using the geometry of a tetrahedron, and by combining three simple equations. By this method, a tetrahedral diagram can be easily constructed, and without programing language; it can be designed with a spread sheet application (e.g. Microsoft Excel).

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COORDINATE TRANSFORMATION

Ternary system to orthogonal coordinate system

Although the main theme of this paper concerns tetrahedral diagrams, it is first necessary to explain a triangular diagram. The three components named here are Top (T), Left (L), and Right (R), respectively. The point of interest is referred to as P (Fig. 1), where the mixing ratios corresponding to P are expressed as t, l, and r (here, $t + l + r = 1$). The side length of the equilateral triangle is set to 1. The apex L conforms to the origin of the X-Y orthogonal coordinate system. In this case, the coordinates (x, y) of vertices T, L, and R are (0.5, $\frac{\sqrt{3}}{2}$), (0, 0), and (0, 1), respectively.

Since the x-coordinate of P is a center between L' and R' in Figure 1, then,

$$x = (r + 1 - l) / 2 \quad (1a)$$

The y-coordinate of P can be calculated by the height ratio of the equilateral triangle, namely;

$$y = \frac{\sqrt{3}}{2}t \quad (1b)$$

The triangular diagram can be constructed using a frame line (0.5, $\frac{\sqrt{3}}{2}$) - (0, 0) - (0, 1) and plot data (x, y). According to equations 1a and 1b, if the $t + l + r = 1$ condition is met, a negative component is also allowable. For example (t, l, r) = (-0.1, 0.5, 0.6) is also true. In this case, the point plots outside of the triangle. For example, in AFM diagram (Thompson 1957), the composition of biotite, projected from muscovite, plots outside the triangle.

An example of a triangular diagram constructed using Microsoft Excel can be downloaded as a supplementary electronic file[1].

Quaternary system to orthogonal coordinate system

The Z-axis extends from the origin of the X-Y orthogonal coordinate system (Fig. 2). The four components are named here as Top (T), Left (L), Right (R), and Front (F), respectively. Let TLRF be a regular tetrahedron. The base triangle TLR is same as that of the triangular diagram (Fig. 1). The point of interest is again named P, where the mixing ratio of P is described as t, l, r, and f (here, $t + l + r + f = 1$). The side length of the equilateral triangle is set to 1. The apex L conforms to the origin of the X-Y-Z orthogonal coordinate system. The coordinates (x, y, z) of vertices T, L, R, and F are $(0.5, \frac{\sqrt{3}}{2}, 0)$, $(0, 0, 0)$, $(1, 0, 0)$, $(0.5, \frac{\sqrt{3}}{6}, \frac{\sqrt{6}}{3})$, respectively, as dictated by the geometrical feature of a regular tetrahedron (Fig. 2; see also Fig. A1 of appendix[1]).

First, the relationship between the coordinate x and the components L and R is illustrated. P lies on the line F'T', which is the intersection of the r and l isopleth surfaces. Since the spatial figure T'L'R'F' is also a regular tetrahedron, the line F'T' is parallel to the YZ-plane. Because the *x* coordinate of P is the same as T', *x* is given by equation 1a,

$$x = (r + 1 - l) / 2 \tag{2a}$$

The second consideration concerns the relation of *y* and T. The surface FLR, which is the $t = 0$ plane, is not parallel with XZ-plane. Since the *y*-coordinate of apex F is $\frac{\sqrt{3}}{6}$, the *y*-coordinate of P is, adding $\frac{\sqrt{3}}{6}f$ to equation 1b, gives -

$$y = \frac{\sqrt{3}}{2}t + \frac{\sqrt{3}}{6}f \tag{2b}$$

The third consideration is the relationship between *z* and F. The $f = 0$ plane is same as the XY-plane. Since the height of a regular tetrahedron is $\frac{\sqrt{6}}{3}$, then

$$z = \frac{\sqrt{6}}{3}f \tag{2c}$$

In the XYZ orthogonal coordinate system, the tetrahedron frame can be constructed using a line (0.5, $\frac{\sqrt{3}}{2}$, 0) - (0, 0, 0) - (1, 0, 0) - (0.5, $\frac{\sqrt{3}}{6}$, $\frac{\sqrt{6}}{3}$). The plot data (*x*, *y*, *z*) can be calculated by equations 2a, 2b, and 2c (Fig. 2). According to these equations, the same as described for the triangle diagram, if the $t + l + r + f = 1$ condition is met, a negative component is also allowable. For example (*t*, *l*, *r*, *f*) = (-0.1, 0.5, 0.6, 0) is also true. In this case, the point plots outside of the tetrahedron.

IMPLICATIONS

A tetrahedral diagram to enable visualization of four component systems can be easily constructed using the algorithms described in this paper. After the transformation from a tetrahedral to an orthogonal coordinate system, the tetrahedral diagram can be rotated in 3D space using Euler angle equations. Both parallel and perspective projections from 3D to 2D can be calculated. These projections, and tetrahedral diagrams with user-specified viewing angles, can be drawn using a spreadsheet application (e.g. Microsoft Excel), without the need for specialized programming language. An example Microsoft Excel file is available as a supplemental electronic file[1]. Additional information concerning the derivation and rotation of tetrahedral diagrams using the approach described above is presented in an appendix[1].

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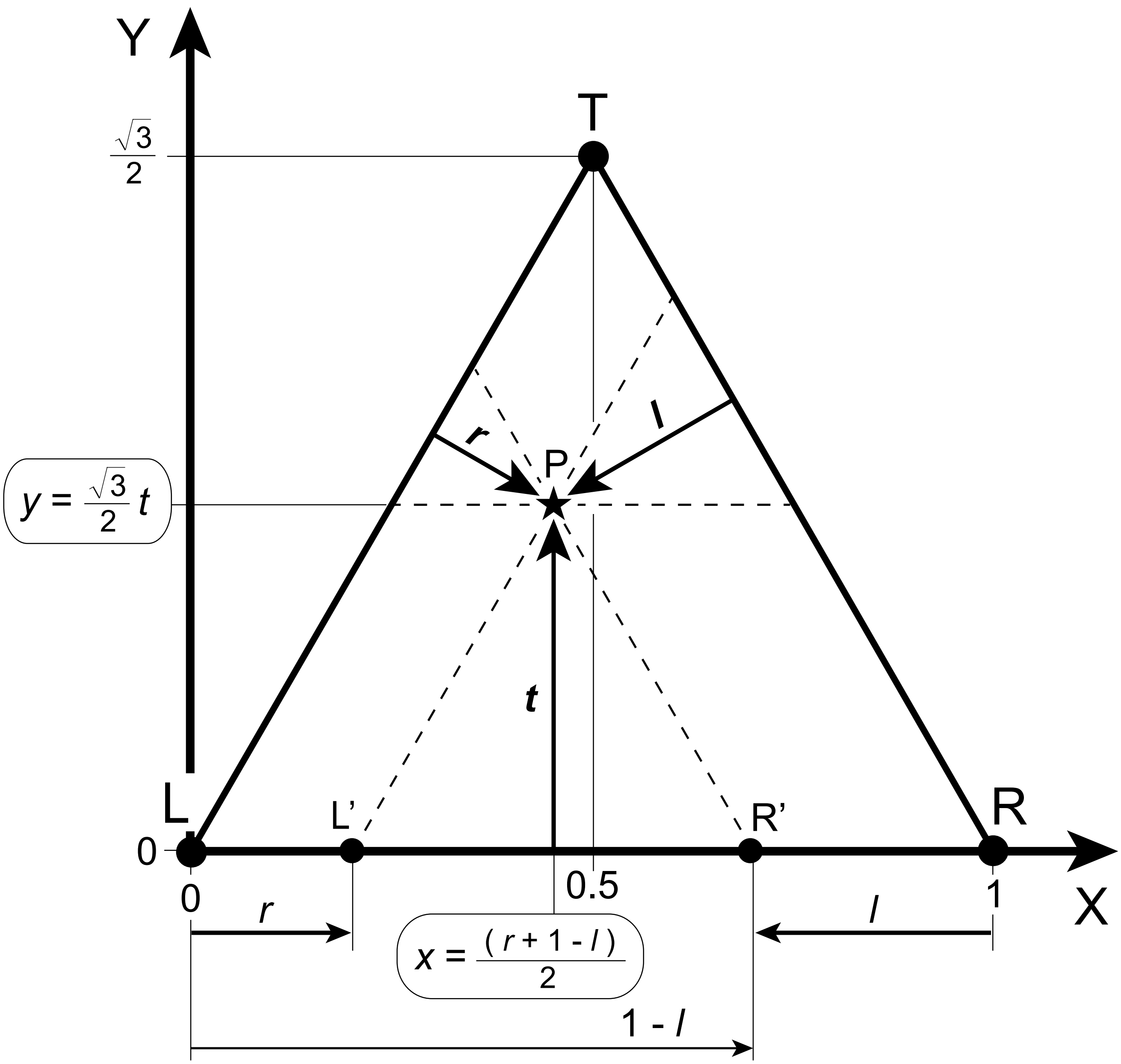
Footnote to tetrahedral plot diagram

[1] Deposit item AM-XX-XXX, an Appendix and a Microsoft Excel file. Deposit items are stored on the MSA web site and available via the American Mineralogist Table of Contents. Locate the article in the table of contents at GSW (ammin.geoscienceworld.org) or MSA (www.minsocam.org), and then click on the link to the Deposit Item.

Figure Captions

Figure 1. Geometrical relationships between the ternary system (triangular diagram) and the XY-orthogonal coordinate axis system.

Figure 2. Geometrical relationships between the quaternary system (tetrahedral diagram) and the XYZ-orthogonal coordinate axis system.


Y
T
$\frac{\sqrt{3}}{2}$
r
l
P
$y = \frac{\sqrt{3}}{2} t$
t
L
L'
R'
R
0
0
0.5
1
X
r
l
$x = \frac{(r + 1 - l)}{2}$
1 - l

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