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 the 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

\[
x = \frac{(r + 1 - l)}{2} \\
y = \frac{\sqrt{3}}{2} \cdot t + \frac{\sqrt{3}}{6} \cdot f \\
z = \frac{\sqrt{6}}{3} \cdot f
\]

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; Armiénti 1986; Maaløe and Abbott 2005; Armiénti 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; Armiénti 1986; Torres-Roldan et al. 2000; Ho et al. 2006; Armiénti and Longo 2011). Such applications are run on programing language platforms such as FORTRAN, BASIC, and JAVA.

This paper describes a different solution of the 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 without using a programing language; it can be drawn and manipulated within a spreadsheet application (e.g., Microsoft Excel).

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 \( t, l, r, \) and \( f \) (here, \( t + l + r + f = 1 \)). The side length of the equilateral triangle is set to 1. The apex L conform to the origin of the X-Y orthogonal coordinate system. In this case, the coordinates \((x, y)\) of vertices T, L, and R are \((0.5, \sqrt{3}/2), (0, 0), \) and \((0, 1)\), respectively.

Since the \( x \)-coordinate of \( P \) is a center between L’ and R’ in Figure 1, then,

\[
x = \frac{(r + 1 - l)}{2}. \quad (1a)
\]

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

\[
y = \frac{\sqrt{3}}{2} \cdot t. \quad (1b)
\]

The triangular diagram can be constructed using a frame line \((0.5, \sqrt{3}/2)+(0, 0)+(0, 1)\) 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.

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