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IJG > Vol.2 No.3, August 2011

OPEN ACCESS

Three-Dimensional Representation of Geochemical Data from a Multidimensional Compositional Space

PDF (Size: 566KB) PP. 231-239 DOI : 10.4236/ijg.2011.23025

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ABSTRACT

Systems described by a wide set of variables, like rock compositions, may be often modeled by a reduced set of components, like minerals, that can be represented in diagrams in two or three dimensions. This paper deals with an original algorithm that allows the representation of compositional data in tetrahedral diagrams, provided that they can be recast on the basis of four end members. The algorithm is based on the orthogonal projection of a given point belonging to R^n to the 3D-space through four R^n points representing the compositions of suitable end members. The algorithm is applied to the assessment of mass balance problems (in weight% or molar basis) as well as to the identification of the geochemical imprint revealed by isotope ratios in igneous rock suites. The fields of possible applications are by far wider, encompassing all problems of comprehensive data representation from a multidimensional space to a bi-dimensional plot.

KEYWORDS

Principal Component Analysis, Phase Diagrams, Rendering, Geochemistry

Cite this paper

P. Armienti and P. Longo, "Three-Dimensional Representation of Geochemical Data from a Multidimensional Compositional Space," *International Journal of Geosciences*, Vol. 2 No. 3, 2011, pp. 231-239. doi: 10.4236/ijg.2011.23025.

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