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Eliminating closure in mineral formulae with specific application to amphiboles

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Abstract

Competition among atomic or molecular species for occupancy of crystallographic sites exaggerates correlations among chemical elements in suites of mineral chemical data, a phenomenon known as closure. Such exaggerated correlations can lead to incorrect conclusions about ionic substitution mechanisms and the petrological forces that drive them. Expressing mineral compositions in terms of a single additive component and molar concentrations of exchange components, eliminates the effects of closure. Statistical analysis of data so transformed can, in some instances, lead to conclusions distinct from analysis of the same data expressed in terms of ionic abundances. The chemical variability of fictive and naturally occurring amphiboles serves to illustrate the potential difficulties brought about by closure and the benefits of its elimination.