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AMFORM, a new mass-based model for the calculation of the unit formula of amphiboles from electron microprobe analyses

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Abstract

In this work, we have studied the relationships between mass concentration and unit formula of amphibole using 114 carefully selected high-quality experimental data, obtained by electron microprobe (EMP) + single-crystal X-ray structure refinement (SREF) ± secondary-ion mass spectrometry (SIMS) analyses, of natural and synthetic Li-free monoclinic species belonging to the Ca and Na-Ca subgroups, and 75 Li-free and Mn-free *C*2/*m* end-members including oxo analogs of Ca amphiboles. Theoretical considerations and crystal-chemical driven regression analysis allowed us to obtain several equations that can be used to: (1) calculate from EMP analyses amphibole unit-formulas consistent with SREF±SIMS data, (2) discard unreliable EMP analyses, and (3) estimate $^{W}O^{2-}$ and Fe^{3+} contents in Li-free *C*2/*m* amphiboles with relatively low Cl contents (≤1 wt%). The AMFORM approach mostly relies on the fact that while the cation mass in Cl-poor amphiboles increases with the content of heavy elements, its anion mass maintains a nearly constant value, i.e., 22O + 2(OH,F,O), resulting in a very well-defined polynomial correlation between the molecular mass and the cation mass per gram ($R^2 = 0.998$).

The precision of estimating the amphibole formula [e.g., ^{T}Si ± 0.02, ^{C}Al ± 0.02, $^{A}(Ca+Na+K)$ ± 0.04 apfu] is 2–4 times higher than when using methods published following the last IMA recommended scheme (2012). It is worth noting that most methods using IMA1997 recommendations (e.g., PROBE-AMPH) give errors that are about twice those of IMA2012-based methods. A linear relation between $^{W}O^{2-}$ and the sum of $^{C}(Ti, Fe^{3+})$ and $^{A}(Na+K)$ contents, useful to estimate the iron oxidation state of highly oxidized amphiboles typical of post-magmatic processes, is also proposed. A step by step procedure (Appendix[1] 1) and a user-friendly spreadsheet (AMFORM.xlsx, provided as supplementary material[1]) allowing one to calculate amphibole unit-formulas from EMP analyses are presented. This work opens new perspectives on the unit-formula calculation of other minerals containing OH and structural vacancies (e.g., micas).

Keywords: Li-free amphiboles, oxo component, cation mass, amphibole oxidation, amphibole deprotonation, SREF, SIMS, Mössbauer spectroscopy