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Chemical formula of biotite deduced on the base of EMPA-WDS data:Crystal chemistry and genetic significance

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Micas are one of common rock-forming minerals in igneous and metamorphic rocks, and the structure has a general formula of $IM_{2-3}<>_{1-0}T_4O_{10}A_2$, where I is an interlayer cation(e.g.K,Na,Rb,Ca);M is an octahedral layer cation(e.g.Li,Fe(2+,3+),Mg,Mn(2+,3+),Al is a vacancy in the octahedral layer;T is a tetrahedral layer cation(Be,Al,B,Fe^{3+},Si);O is oxygen;and A is an anion not bonded to T(OH,F,Cl,O,S). Because of the complicated chemical composition, micas often have vacancies except T site, and examination of the crystal chemistry of mica is essential to determine the chemical formula. If the chemical data are available, commonly constructed by the procedure adopted by Rimsaite(1970), and so on. However, there is no previous study on the chemical formula of biotite deduced on the basis of only EMPA-WDS data. The present work focuses on the procedure to determine the chemical formulas of biotite, the representative of micas, on the basis of only EMPA-WDS data, and on discussing the crystal chemistry and the genetic significance.

The used samples are biotites from Tanakami granite, Shiga Prefecture, and those from the transition zone of pegmatite in its granite. Chemical analyses were performed using the JEOL-8530 electron microprobe equipped with five wavelength-dispersion spectrometers (WDS) at the Chemical Analysis Division, University of Tsukuba. The chemical formulas were obtained using the following procedure.

(1)The difference between the measured total $<$100 wt% and the ideal weight (100 wt%) was assumed as H_2O content, and the formula was calculated on the basis of 12(O,OH,F,Cl).

(2)If the procedure (1) resulted in the total anion charge $>$22, you use the following procedure:

(a)M site $<$3

The calculate formulas of (1) were used.

(b)M site $>$3

Combination of the result of (1) (all iron is calculated as Fe^{2+}) with that of all iron calculated as Fe^{3+} leads to the approach of the M site occupancy to 3 as full as possible.

(3)If total of the anion charge calculated was $<$22 after the procedure (1), an idealized anion group must be assumed, and the formula should be based on 22 positive charges (The content of OH was determined as (OH+F+Cl)=2). Then, this was combined with the calculated result based on the assumption of Fe^{3+}, following the approach of the total wt% to 100% as full as possible.

Based on this procedure, the representative calculated chemical formula of the biotites from Tanakami granite is $(K_{0.865}Na_{0.007}<>_{0.128})($ Though this formula has large vacancies at I site and M site, there are limited vacancies in I and M sites of the biotite crystal structure (Fleet & Howie, 2003). It is considered that undetectable elements or molecules with EMPA, such as Li and H_3O^+, affected the result with some error. The representative chemical formula of the biotites from transition zone of a pegmatite in Tanakami granite is $(K_{0.937}Na_{0.003}<>_{0.060})(Al_{0.349}Fe^{2+}{}_{2.000}Mg_{0.436}Mn_{0.041}Ti_{0.127}<>_{0.047})Si_{2.902}Al_{1.098}O_{10.353}F_{0.424}Cl_{0.020}(OH)_{1.203}$. Comparing these two formulas, the biotite from transition zone of the pegmatite is more enriched in Si and F than that from the host granite.

The validity of the present formulation procedure is examined by applying biotites from the pegmatite and metapelitic granulite of Kerala Khondalite Belt, southeast India (Cesare et al. 2008). In Cesare et al.(2008), in addition to EMPA, Mossbauer spectroscopy(Fe^{2+}-Fe^{3+} ratio) and SIMS(H_2O content) were performed. When the chemical formula of biotites from the pegmatite of Kerala Khondalite Belt calculated based on all analysis is compared with that of the chemical formula calculated from the present procedure, the difference in vacancy is calculated to be 0.198 and 0.146 at the I site and the M site, respectively.

Keywords: biotite, chemical formula, EMPA, anion charge, classification, genetic place