Schreyerite, V₂Ti₃O₉: New occurrence and crystal structure

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ABSTRACT

A new occurrence of schreyerite, V₂Ti₃O₉, has recently been found in metamorphic rocks of the Sludyanka complex at the southern shore of Lake Baikal, Russia. In contrast to previously known schreyerite lamellae, which are intergrown with rutile, crystals from the Sludyanka complex occur as isolated single crystals associated with titanite, allowing single-crystal X-ray diffraction experiments. The chemical composition was determined with an electron microprobe giving the composition (V_{1.785}Cr_{0.157}Fe_{0.036})(Ti_{2.536}V_{0.468})O₉. A peculiarity of this schreyerite sample is the partial substitution of V⁴⁺ for Ti⁴⁺. The crystal structure was determined by single-crystal X-ray diffraction and was refined in the monoclinic space group C2/c [a = 17.102(2), b = 5.0253(5), c = 7.0579(8) Å, β = 106.636(10)°] to R₁ = 2.84%. The structure is in agreement with the qualitative model of Grey et al. (1973) determined on the basis of electron diffraction and X-ray powder data for synthetic (Fe,Cr)₂Ti₃O₉. Reinvestigation of schreyerite from the type locality indicates that this sample has cell dimensions and symmetry corresponding to the Sludyanka sample. The structure of schreyerite may be considered as a 1:1 polysome composed of slabs of berdesinskiite, V₂TiO₅, and Ti₂O₄ (a high-pressure phase of TiO₂ with α -PbO₂ structure).

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