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Crystal structures of K-cymrite and kokchetavite from single-crystal X-ray diffraction

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Abstract

We determined for the first time the crystal structures of high-pressure K-cymrite ($KAlSi_3O_8 \cdot H_2O$) and its dehydrated form kokchetavite ($KAlSi_3O_8$) using single-crystal X-ray diffraction. The K-cymrite structure has been successfully refined in the hexagonal space group *P*6/*mmm* [a = 5.3361(3) Å, c = 7.7081(7) Å, V = 190.08(3) Å^3, $R1$ = 0.036 for 127 unique observed reflections], which is in agreement with previous models from powder X-ray diffraction. In contrast, kokchetavite shows superstructural reflections, suggesting a different unit cell and a space group of *P*6/*mcc* [a = 10.5757(3) Å, c = 15.6404(6) Å, V = 1514.94(10) Å^3, $R1$ = 0.068 for 1455 unique observed reflections]. Upon dehydration, single-crystal grains of K-cymrite transform into single-crystal grains of kokchetavite. The latter questions a previous interpretation of kokchetavite crystals in mineral inclusions as a product of direct crystallization from fluid/melt. The Raman spectrum of K-cymrite shows a strong polarization dependence, which is important in identification of the mineral inclusions.

Keywords: K-cymrite, kokchetavite, single-crystal X-ray diffraction, Raman spectroscopy