

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

**ALEXANDR V. ROMANENKO^{1,2,*}, SERGEY V. RASHCHENKO^{1,2}, ALEXANDER G. SOKOL^{1,†},
ANDREY V. KORSAKOV¹, YURI V. SERYOTKIN^{1,2}, KONSTANTIN V. GLAZYRIN³, AND KIRA MUSIYACHENKO^{1,4}**

¹Sobolev Institute of Geology and Mineralogy SB RAS, 3 Koptyuga Avenue, 630090 Novosibirsk, Russia

²Novosibirsk State University, 2 Pirogova Street, 630090 Novosibirsk, Russia

³Photon Science, Deutsches Elektronen-Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany

⁴Department of Earth and Environmental Sciences, University of Pavia, Via A. Ferrata, 1 27100 Pavia, Italy

ABSTRACT

We determined for the first time the crystal structures of high-pressure K-cymrite ($\text{KAlSi}_3\text{O}_8 \cdot \text{H}_2\text{O}$) 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 $P6/mmm$ [$a = 5.3361(3) \text{ \AA}$, $c = 7.7081(7) \text{ \AA}$, $V = 190.08(3) \text{ \AA}^3$, $R1 = 0.036$ 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 $P6/mcc$ [$a = 10.5757(3) \text{ \AA}$, $c = 15.6404(6) \text{ \AA}$, $V = 1514.94(10) \text{ \AA}^3$, $R1 = 0.068$ 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