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On the existence of a Na-deficient monoclinic trinepheline with composition $Na_{7.85}Al_{7.85}Si_{8.15}O_{32}$

Predrag Vulić,* Volker Kahlenberg, and Jürgen Konzett

Institute for Mineralogy and Petrography, University of Innsbruck, Innrain 52, A-6020 Innsbruck, Austria

Abstract

The crystal structure of a new synthetic $Na_{8-r}Al_{8-r}Si_{8+r}O_{32}$ ($r = 0.15$) modification has been solved by direct methods and refined to an R index of 0.0289 for 11 643 independent reflections and 764 parameters. The compound is monoclinic with space group symmetry $P112_1$, $a = 9.9897(6)$ Å, $b = 9.9622(6)$ Å, $c = 24.979(2)$ Å, and $\gamma = 119.788(4)°$. The twinning of three individuals related by rotation around the **c** direction for 120° was accounted for in the calculation. The phase was named monoclinic trinepheline because the length of its c lattice parameter is 3× the length of the c parameter in nepheline, whereas the a parameter is almost the same in both structures, similarly to a previously investigated trinepheline of hexagonal symmetry. Actually, the present compound represents an intermediate state between these two phases. The characteristic of the crystal structure are layers of six-membered rings built up of regularly alternating AlO_4 and SiO_4 tetrahedra. The layers are perpendicular to [001] and are connected through apical O atoms. The resulting spatial network contains channels in which the Na cations are situated. The structure of monoclinic trinepheline can be described as a consecutive stacking of basic nepheline like modules (containing two tetrahedral sheets) and one sheet corresponding to those observed in the hexagonal trinepheline structure. The topology of the new compound corresponds to that of tridymite. The coordination sequences are identical for all T atoms in the asymmetric unit: 4-12-25-44-67-96-130-170-214-264. The vertex symbols for the tetrahedral centers are $6_2 \cdot 6_2 \cdot 6_2 \cdot 6_2 \cdot 6_2 \cdot 6_2$. The framework density of the structure is equal to 22.2 T atoms/1000 $Å^3$.

Keywords: Monoclinic trinepheline, $Na_{7.85}Al_{7.85}Si_{8.15}O_{32}$, flux method, nepheline