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The crystal structure of thornasite, $Na_{12}Th_3[Si_8O_{19}]_4(H_2O)_{18}$: A novel interrupted silicate framework

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ABSTRACT

The crystal structure of thornasite, $Na_{12}Th_3[Si_8O_{19}]_4(H_2O)_{18}$, $Z = 6$, rhombohedral, $a = 29.124(1)$, $c = 17.2602(9)$ Å, $V = 12{,}679.2(9)$ Å^3, space group $R\bar{3}c$, has been solved by direct methods, and refined to an agreement index ($R1$) of 5.7% calculated, based on 2266 unique observed reflections collected using Mo$K\alpha$ X-radiation and a CCD-based detector. The structure consists of a new interrupted silicate framework with composition $[Si_8O_{19}]^{6-}$. The framework density is 15.4 atoms per 1000 Å^3, which is typical for microporous aluminosilicate materials. The framework density, together with the presence of a three-dimensional network of channels in the structure, permit thornasite to be designated as a new member of the zeolite structure family. The framework consists of cubic cages and distorted six-membered rings linked via common edges. The circuit symbol is $(4^3 14^3)(4^3 6^2 14)_3(6.10.12)_3(6_2 10)_6$. Interruptions of the framework are caused by the presence of Th^{4+} cations that are coordinated by eight O atoms. Na^+ cations and H_2O groups are located in channels through the structure. The theoretical parent framework for thornasite may be constructed by the insertion of two additional Si atoms in place of one Th atom. The theoretical framework density is 18.0 atoms per 1000 Å^3; the circuit symbol is $(4^3 10^3)(4^3 6^2 10)_6(4^3 6^2 8)_3(4^3 6.8.10)_3(4^2 6^2 8.10)_3(4^1 6^3 8.10)_3$.