

The structure of braitschite, a calcium rare earth borate

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ABSTRACT

The crystal structure of braitschite, $\text{Ca}_{6.15}\text{Na}_{0.85}\text{RE}_{2.08}[\text{B}_6\text{O}_7(\text{OH})_3(\text{O},\text{OH})_3]_4(\text{H}_2\text{O})$, is reported here in space group $P6/m$ with unit-cell parameters $a = 12.1506(6)$, $c = 7.3678(4)$ Å, and $V = 942.03(8)$ Å³. Data were collected from a single crystal using a $\text{MoK}\alpha$ source and a CCD detector, solved by direct methods, and refined to an R factor of 2.81%. The mineral structure consists of hexaborate fundamental building blocks that polymerize along [001] and are bound by Ca^{2+} and REE^{3+} counterions. The framework forms hexagonal channels, which are occupied alternately by Ca^{2+} cations and water molecules. In an investigation of its thermal stability, braitschite maintains its crystallinity to a temperature of 400 °C, after which it undergoes decomposition. Using Rietveld refinements against powder X-ray diffraction data, we were able to track the loss of water molecules in channels and hydroxyl groups in the covalent B-O network with increasing temperature.

Keywords: Braitschite, borate, rare earth mineral, crystal structure