

On the nature of tincalconite

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ABSTRACT

An examination of synthetic crystalline material by single crystal X-ray diffractometry reveals a unit-cell dimension that was previously ascribed to tincalconite. However, the best fit to the reflection data obtained at 291(2) K is obtained with composition $\text{Na}_6[\text{B}_4\text{O}_5(\text{OH})_4]_3 \cdot 8\text{H}_2\text{O}$. This formula is different from the $\text{Na}_2[\text{B}_4\text{O}_5(\text{OH})_4] \cdot 3\text{H}_2\text{O}$ previously assigned to tincalconite from an earlier crystallographic study. Additionally, our model fits best with non-crystallographic measurements and agrees with the analysis from a more recent low temperature crystallographic analysis. Tincalconite is best formulated as $\text{Na}_6[\text{B}_4\text{O}_5(\text{OH})_4]_3 \cdot 8\text{H}_2\text{O}$. It is trigonal, $R32$, $a = 11.1402$ (11), $c = 21.207$ (3) Å, $Z = 3$, $R = 0.020$ for 512 $F_o > 4\sigma(F_o)$ and 0.021 for all 529 data at 291(2) K.