

## Chiavennite revisited: A temperature dependent *in situ* single crystal X-ray diffraction study

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Chiavennite ( $\text{CaMnBeSi}_5\text{O}_{13}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ ,  $Z = 4$ ) is a rare Be-bearing zeolite mineral with an interrupted framework of four-connected  $[\text{SiO}_4]$  and three-connected  $[\text{BeO}_4]$  tetrahedra. A sample from the type locality in the Rhetic Alps of Italy has been re-investigated at room temperature in order to clarify the space group ambiguity discussed in the literature [1] and to explore the system of hydrogen bonds. In addition, the thermal stability of this zeolite was tracked by *in situ* single-crystal X-ray diffraction between 25 °C and 425 °C. In spite of the pseudo-orthorhombic cell dimension, the new data indicate that at room temperature chiavennite is truly monoclinic  $P2_1/c$  ( $\beta \approx 90^\circ$ ) and twinned as recently shown for the new mineral ferrochiavennite [2]. The temperature-dependent dehydration experiments under dry conditions showed that chiavennite continuously released water up to at least 425 °C without topological modification. The loss of more than one  $\text{H}_2\text{O}$  molecule at 250 °C, decreases the Ca coordination from eight- to seven-fold. After release of the first  $\text{H}_2\text{O}$  molecule, and strong dynamic disorder of the remaining  $\text{H}_2\text{O}$ , chiavennite evolves into orthorhombic symmetry of space group  $Pbcn$ . The continuous monoclinic-orthorhombic transition from space group  $P2_1/c$  to  $Pbcn$  upon dehydration is attributed to softening of the system of hydrogen bonds with extraframework  $\text{H}_2\text{O}$  as donor and oxygen at the cavity walls as acceptor.

[1] Tazzoli, V., Domeneghetti, M. C., Mazzi, F., Cannillo, E. (1995), *European Journal of Mineralogist* **7**, 1339-1344.

[2] Grice, J. D., Kristiansen, R., Friis, H., Rowe, R., Poirier, G. G., Selbekk, R. S., Cooper, M. A., Larsen, A.O. (2013), *Canadian Mineralogist* **51**, 285-296.