



Memorandum

Datum: 5.3.2015
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An: siehe Verteiler
cc:

Einladung zu einem ausserordentlichen LES Palaver

Ich lade Sie herzlich ein.

Referentin: Dr. Georgia Cametti
Mineralogical Crystallography, Institute of Geological Sciences, University of Bern

Thema: Thermal stability of natural zeolites: *in situ* single-crystal X-ray investigation of scolecite and chiavennite

Zeit: Freitag, 20. März 2015, 10:00 – 11:00 Uhr

Ort: Sitzungszimmer OFLA/209

Abstract

The understanding of zeolite behavior upon heating is of particular importance since the sorptive and catalytic properties are enhanced in the dehydrated state. It has been suggested that extraframework Ca ions play a special role. After loss of coordinating water molecules, Ca may attract framework oxygen to form new bonds, originating local strain, and promoting phase transitions.

Scolecite ($\text{CaAl}_2\text{Si}_3\text{O}_{10}\cdot 3\text{H}_2\text{O}$, $Z = 8$) dehydration mechanism has been investigated between 25 and 300°C by *in situ* single-crystal X-ray diffraction at 30(5) % RH. Results are compatible with previous spectroscopic and thermal analyses, describing dehydration as a two-step process: scolecite ($3\text{H}_2\text{O}$) – metascolecite ($2\text{H}_2\text{O}$) – X-ray amorphous anhydrous phase. The new data with located hydrogen positions allowed analyzing the driving forces for the scolecite-metascolecite transition. A second set of *in situ* experiments under dry nitrogen conditions, led to the phase sequence: scolecite – metascolecite – x2-phase – x1-phase – amorphization. The crystal structures of the x2- and x1-phase have been solved. Both structures represent strongly compacted and distorted varieties of the NAT framework type.

Chiavennite ($\text{CaMnBeSi}_5\text{O}_{13}(\text{OH})_2\cdot 2\text{H}_2\text{O}$, $Z = 4$) is a rare Be-bearing natural zeolite with an interrupted framework of four-connected $[\text{SiO}_4]$ and three-connected $[\text{BeO}_4]$ tetrahedra. The crystal structure has been re-investigated at room temperature in order to clarify the space group ambiguity. The new data showed the structure to be monoclinic twinned $P2_1/c$ and not orthorhombic $Pbcn$ as previously suggested. In addition, the temperature – dependent behavior of this zeolite was tracked by *in situ* single crystal X-ray diffraction between 25°C and 425°C. The experiments showed that chiavennite continuously released water up to at least 425°C, without any significant structural modification. The loss of more than one H_2O molecule at 250°C, does not affect the Ca coordination. However, after the release of the first water molecule, chiavennite approaches orthorhombic space group $Pbcn$.

Freundliche Grüsse

S.V. Churakov