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Dehydration of the natural zeolite goosecreekite $CaAl_2Si_6O_{16}{\cdot}5H_2O$ upon stepwise heating: A single-crystal and powder X-ray study

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ABSTRACT

The zeolite mineral goosecreekite $CaAl_2Si_6O_{16}{\cdot}5H_2O$ has been structurally investigated between 25 and 600 °C to monitor structural modifications upon partial dehydration. Temperature-dependent in situ powder and single-crystal X-ray techniques were combined with TG/DTA experiments. Goosecreekite has a porous framework structure with well-ordered Si,Al distribution. In its natural form extraframework Ca is seven-coordinated. Up to ca. 100 °C, 1 H_2O molecule is expelled reducing the Ca coordination from 7 to 6 accompanied by very minor changes of the tetrahedral framework. Depending on humidity and equilibration time a second structural change begins between 150 and 250 °C due to loss of additional 2.8 H_2O pfu. The space group $P2_1$ is maintained but the c axis doubles and the structure is highly twinned. This new phase may be interpreted with a disordered model having two different framework topologies: one with the original T-O-T linkage and a second one with broken T-O-T links. Starting at ca. 300 °C, another 1.2 H_2O are lost and this new orthorhombic, strongly contracted phase of $P2_12_12_1$ symmetry has five-coordinated Ca. The X-ray powder signal of the orthorhombic phase persists up to 600 °C, but the structure becomes increasingly X-ray amorphous until complete destruction at 675 °C. A single crystal ($P2_1$ phase with doubled c axis) partly dehydrated at 200 °C recovers the structure of natural goosecreekite under ambient conditions. Similar rehydration occurs after one month under ambient humidity for a powder sample of the orthorhombic $P2_12_12_1$ phase produced by heating of goosecreekite to 325 °C.

Keywords: Zeolite, goosecreekite, dehydration, crystallography