(010) disorder, partial Si,Al ordering, and Ca distribution in triclinic (C1) epistilbite

PING YANG and THOMAS ARMBRUSTER

Laboratorium für chemische und mineralogische Kristallographie, Universität Bern, Freiestrasse 3, CH-3012 Bern, Switzerland

Abstract: The crystal structure of epistilbite, Na0.3K0.2Ca2.7Al6.2Si17.9O48·16 H2O, from Gibelsbach, Fiesch (Valais, Switzerland) was refined from X-ray single-crystal data at 100 K and 293 K in space group C1 (100 K: a = 9.051(3), b = 17.689(6), c = 10.152(7) Å, α = 89.93(4), β =124.35(4), γ = 89.95(3)°; 293 K: a = 9.083(1), b = 17.738(3), c = 10.209(1) Å, α = 89.95(1), β = 124.58(1), γ = 90.00(1)°). In contrast to previous studies where the space groups C2 or C2/m were assumed, reflection intensities clearly suggest triclinic symmetry. The reason for the symmetry lowering from monoclinic C2 to triclinic C1 is partial Si,Al ordering accompanied by a preferred distribution of the channel cations close to the underbonded oxygen atoms of the tetrahedral framework. The hitherto enigmatic occurrence of two domain variants (A, B) formed by different tetrahedral configurations could be modelled by (010) disorder caused by a local mirror plane.

Key-words: epistilbite, zeolite, Si,Al-ordering, disorder, crystal structure.

Introduction

Rose (1826) described epistilbite as a new zeolite mineral from Iceland and the Faroe Islands. A review of occurrences, chemistry and cell dimensions of epistilbite was presented by Galli & Rinaldi (1974). These authors concluded that epistilbite occurs primarily as a low-temperature alteration product of basic igneous rocks. The chemistry of this zeolite is always close to Ca3Al6Si18O48·16 H2O which allows only for a narrow variation of the monoclinic cell parameters. The morphology of this mineral is characterized by (100) twins on c-elongated prismatic crystals (Gottardi & Galli, 1985). Structural investigations were performed by Kerr (1964), Merlino (1965), and Perotta (1967) assuming C2/m symmetry. Slaughter & Kane (1969) attributed also C2/m symmetry to epistilbite with the exception of three framework oxygen atoms and one water molecule which were assumed to possess C2 symmetry. Alberti et al. (1985) established the acentric space group C2 for epistilbite (Theigharhorn, Iceland) which is in agreement with the observed piezoelectricity (Bond, 1943; Ventriglia, 1953). Alberti et al. (1985) found two tetrahedral configurations in epistilbite similar to those previously described for dachiardite (Vezzalini, 1984). Both epistilbite configurations have C2 symmetry but occur with different frequency (82 % and 18 %, respectively), thus the existence of a domain structure was suggested. The presence of these acentric domains was interpreted as a tendency to avoid T-O-T angles of 180°. Epistilbite possesses only one-dimensional channels, confined by eight-membered tetrahedral rings, running parallel to the c-axis. Two neighbouring channels are connected with each other (parallel to the a-axis) by a ten-membered ring of tetrahedra. The channels host Ca and H2O molecules.

Twinning and symmetry of epistilbite were