American Mineralogist, Volume 95, pages 1413–1421, 2010

Crystal chemistry and low-temperature behavior of datolite: A single-crystal X-ray diffraction study

Romano Rinaldi,[1] G. Diego Gatta,[2,3,*] and Ross J. Angel[4]

[1]Dipartimento di Scienze della Terra, Università degli Studi di Perugia, Piazza Università 1, I-06100 Perugia, Italy
[2]Dipartimento di Scienze della Terra, Università degli Studi di Milano, Via Botticelli 23, I-20133 Milano, Italy
[3]CNR-Istituto per la Dinamica dei Processi Ambientali, Via Mario Bianco 9, 1-20131 Milano, Italy
[4]Crystallography Laboratory, Department of Geosciences, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24060, U.S.A.

Abstract

The crystal chemistry of six natural datolites from different localities was investigated by electron microprobe analysis in the wavelength dispersive mode and single-crystal X-ray diffraction. The chemical analyses show no significant site substitution. The single-crystal structure refinements confirm the structural model of datolite previously reported (with $a \sim 4.83$, $b \sim 7.61$, $c \sim 9.63$ Å, and $\beta \sim 90.15°$, space group $P2_1/c$). Intra-polyhedral bond distances and angles show common features in all samples at room T: (1) the Si-tetrahedron is strongly deformed, with Si-O distances ranging between ~1.57 and ~1.66 Å and O-Si-O angles ranging between ~105.4 and ~115.3°; (2) the B-tetrahedron is almost regular; (3) the Ca-polyhedron is significantly distorted, with bond distances ranging between ~2.28 and ~2.67 Å; (4) only one independent H-site occurs and its refined position suggests a bifurcated hydrogen bonding scheme with O5 as donor and O4 and O2 as acceptors [with O5-H ~ 0.8 Å and (1) O5···O4 ~ 2.99 Å, H···O4 ~ 2.33 Å, and O5-H···O4 ~ 140°, and (2) O5···O2 ~ 2.96 Å, H···O2 ~ 2.36 Å, and O5-H···O2 ~ 131°]. Low-temperature diffraction measurements between 300 and 100 K show that the thermal expansion of datolite is mainly governed by the axial response along [100] and [010], whereas the c-axis length is almost unchanged in this temperature interval. The volume thermal expansion coefficient ($\alpha_V = V^{-1}\partial V/\partial T$) between 100 and 280 K is $\alpha_V = 1.5(2)\cdot 10^{-5}$ K^{-1}. The higher thermal expansion of the a-axis is due to the layered nature of the structure of datolite: the Ca-O bond distances are the most compressible and expandable, and govern the contraction, upon cooling, along the direction perpendicular to the polyhedral layers. The tetrahedral layer is significantly more rigid and no changes of the tetrahedral tilts are observed from 300 to 100 K.

Keywords: Datolite, crystal structure, crystal chemistry, low temperature, single-crystal X-ray diffraction