

High pressure phase transition in datolite

Liudmila A. Gorelova¹, Anna S. Pakhomova², Sergey V. Krivovichev¹, Leonid S. Dubrovinsky³, Georgios Aprilis³

¹St. Petersburg State University, Department Of Crystallography, St. Petersburg, Russian Federation, ²Deutsches Elektronen-Synchrotron (DESY), Petra III, Hamburg, Germany, ³University of Bayreuth, Bayerisches Geoinstitut, Bayreuth, Germany
E-mail: gorelova.ljudmila@gmail.com

Datolite, CaBSiO₄(OH), belongs to the gadolinite group of minerals with its crystal structure based upon [BSiO₄(OH)]₂-layers formed by four- and eight-membered rings of corner-sharing SiO₄ and BO₄ tetrahedra [1]. Despite their diversity in nature (there are thirteen gadolinite-group minerals [2]), their behaviour under extreme conditions is poorly studied. In particular, for datolite, its Raman-spectroscopy study performed up to 250 °C and up to 5 GPa under non-hydrostatic conditions revealed the occurrence of two phase transitions, which, however, have never been fully characterized [3].

Behavior of datolite under high-pressure conditions was studied using in situ single-crystal X-ray diffraction in a diamond anvil cell at the Extreme Conditions Beamline P02.2 of PETRA III (DESY, Hamburg) using the wavelength of 0.2896 Å. For the study, we have used crystals of natural datolite from the Avam river (Krasnoyarsk Krai, Russia) with size of 0.010×0.010×0.005 mm³. Experiment was performed at ambient temperature in the pressure range from 2 to 43 GPa with the pressure step no more than 6 GPa (12 pressure points in total).

The phase transition was observed in the pressure range 27–33 GPa. The crystal structure of datolite measured at 33 GPa contains Si atoms coordinated by five oxygen atoms to form a trigonal bipyramid SiO₅. As a result of phase transition, two SiO₄ tetrahedra across the eight-membered ring of the borosilicate layer approach each other and form dimers of edge-sharing SiO₅ bipyramids. As a consequence, the eight-membered ring transforms into a pair of five-membered rings. It is noteworthy that the structure symmetry (P21/c) remains unchanged.

Compression behavior of both modifications of datolite under high pressure is sharply anisotropic: maximal compressibility is along the b-axis, i.e. along one of the direction within the plane of the layer. The minimal compression is between the layers that is in agreement with its thermal expansion anisotropy.

This study was supported by the Russian Foundation for Basic Research.

[1] Ito T., Mori H. (1953) Acta Cryst. 6, 24–32.

[2] Bacik P. et al. (2017) Eur. J. Mineral., accepted.

[3] Goryainov S.V. et al. (2015) J. Raman Spectrosc. 46, 177–181.

Keywords: [high-pressure transition](#), [datolite](#), [fivefold coordinated silicon](#)