CRYSTAL CHEMISTRY OF LOW SYMMETRY VESUVIANITES FROM KHARMANKULSIY AND MONETNAYA DACHA MINES (URALS, RUSSIA)

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Introduction

Vesuvianite is a complex mineral with a range of crystal chemical phenomena arising due to so-called 'rod polytypism' [1-3]. Its general formula looks like $X_{x+y}^{z} \{Y_{x}^{z}Z_{y}^{z}\} O_{z}(OH,P)$, where $X$, $Y$, $Z$ = Ca, Na, K (are centred with no centred coordinate), $Y$ = Mg, Al, Fe$^{2+}$, Fe$^{3+}$, Mn, Cr, FeO (has octahedral coordination); $Z$ = Mg, Al (has tetrahedral coordination). In the structures of high vesuvianites (space group P4/nnc), rods are disordered, whereas in the structures of low vesuvianites (space groups P4/n and P4nmc), there is an ordered arrangement of rods.

Fig. 1 (a) Projection of the vesuvianite structure down [100]; (b) projection of the vesuvianite structure down [100] (Total occupation positions $x$ and $y$ are equal 1).

"High" and "low" vesuvianite

P4/nnc  P4/n

Disordered "high" vesuvianites (sp. gr. P4/n) crystallize at temperatures 200-600 °C.

Ordered "low" vesuvianites (sp. gr. P4/n and P4nmc) crystallize at temperatures 300-500 °C.

Diffraction of "high" and "low" vesuvianites

Three types of olivine reflections were distinguished: (1) hkl with h + k = 2n + 1; (2) hkl with k = 2n + 1, l = 2n + 1; (7h) hkl with l = 2n + 1. Type 1 violates the n glide plane perpendicular to the hkl axes, types 2a violates the n glide plane in (2n), and type 2b violates the n glide plane in (2n + 1). Occurrence of type 2 reflections indicates space groups P4/n and P4nmc and suggests P4nmc. Observation of reflections of type 2b indicates the existence of a C4v symmetry.

Samples were taken from collections of Mineralogical Museum of St. Petersburg State University.

Fig. 2 Reconstruction of reciprocal space 110 for sample from Monetnaya Dacha.

Infrared spectra

Infrared spectra of vesuvianite were collected using Bruker Vertex 70 FTIR spectrometer at room temperature. Interpretation of the IR spectrum obtained was done on the basis of the methodology developed by Kurakina et al. (7). In the IR spectrum, two absorption bands at 438 and 476 cm$^{-1}$ belong to the 0 shearing deformation vibrations of the Si-O bonds. The bands at 986, 881, 818, 864 and 1016 cm$^{-1}$ may be attributed to asymmetric stretching vibrations of the Si-O-Si and Si-O-Si bonds. The bands in the range 1316-1265 cm$^{-1}$ correspond to regions of the hydroxyl vibrations. In terms of the group-theoretical analysis for the space group P4/n, the spectrum of the absorption bands in the range 3600-450 cm$^{-1}$ corresponds to the symmetry of the tetrahedral C2 vibrations. Therefore, IR data correspond to the 16P'4 vesuvianite, which is in agreement with the results of structural refinement. For sample from Monetnaya Dacha we have some differences only in 0 cm$^{-1}$ and 80 cm$^{-1}$ deformation vibrations 605 and 572 cm$^{-1}$ and shift of vibrations in the hydroxyl region and this data (3) is in an agreement with the model of its orientation for P4/mnc vesuvianite.