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Towards a revisitation of vesuvianite-group nomenclature: The crystal structure of Ti-rich vesuvianite from Alchuri, Shigar Valley, Pakistan

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Abstract

© 2016 International Union of Crystallography. Vesuvianite containing 5.85 wt% TiO₂ from an Alpine-cleft-type assemblage outcropped near Alchuri, Shigar Valley, Northern Areas, Pakistan, has been investigated by means of electron microprobe analyses, gas-chromatographic analysis of H₂O, X-ray powder diffraction, single-crystal X-ray structure refinement, ²⁷Al NMR, ⁵⁷Fe Mössbauer spectroscopy, IR spectroscopy and optical measurements. Tetragonal unit-cell parameters are: $a = 15.5326(2)$, $c = 11.8040(2)$ Å, space group P4/nnc. The structure was refined to final $R1 = 0.031$, $wR2 = 0.057$ for 11247 I > 2σ(I). A general crystal-chemical formula of studied sample can be written as follows ($Z = 2$): [8-9](Ca_{17.1}Na_{0.9}) [8]Ca_{1.0}[5](Fe₂₊ 0.44Fe₃₊ 0.34Mg_{0.22}) [6](Al_{3.59}Mg_{0.41}) [6](Al_{4.03}Ti_{2.20}Fe₃₊+1.37Fe₂₊ 0.40) (Si₁₈O₆₈) [(OH)_{5.84}O_{2.83}F_{1.33}]. The octahedral site Y2 is Al-dominant and does not contain transition elements. Another octahedral site Y3 is also Al-dominant and contains Fe₂₊, Fe₃₊ and Ti. The site Y1 is split into Y1a and Y1b predominantly occupied by Fe₂₊ and Fe₃₊, respectively. The role of the Y1 site in the diversity of vesuvianite-group minerals is discussed.

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Keywords

27 Al NMR NMR spectroscopy, crystal chemistry, IR spectroscopy, Mössbauer spectroscopy, vesuvianite