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Hardystonite from Franklin Furnace: A natural modulated melilite

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ABSTRACT

Natural hardystonite, $(Ca_{1.85}Na_{0.14}Pb_{0.01})(Zn_{0.85}Al_{0.07}Mg_{0.03}Mn^{3+}_{0.04}Fe^{3+}_{0.02})Si_{2.00}O_{7.00}$, from the type locality was reinvestigated with single crystal X-ray diffraction, microprobe analysis, and electron diffraction. The average structure, space group $P\bar{4}2_1m$, a = 7.800(1) Å, c = 5.000(1) Å, was refined to R = 1.91% using 331 independent reflections. Hardystonite exhibits an incommensurate modulated structure. As in synthetic melilite-type compounds, modulation is two-dimensional, with tartan-like appearance; modulation vectors are $\mathbf{q_1} = \alpha(\mathbf{a_1}^* + \mathbf{a_2}^*)$ and $\mathbf{q_2} = \alpha(-\mathbf{a_1}^* + \mathbf{a_2}^*)$. A modulation wavelength λ = 19.0(4) Å was estimated by centering satellite reflections using a single-crystal diffractometer. TEM-EDX investigations proved the chemical composition of the sample to be slightly inhomogeneous, with stronger and sharper satellites in the regions where the composition approaches the $Ca_2ZnSi_2O_7$ end-member. Geometrical parameters as well as anisotropic displacement ellipsoids of hardystonite are consistent with those of the other melilite-type compounds having a modulated character.