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New insights into the crystal chemistry of epididymite and eudidymite from Malosa, Malawi: A single-crystal neutron diffraction study

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Abstract

The crystal chemistry of two dimorphic hydrated sodium beryllium silicates, epididymite [a = 12.7334(4), b = 13.6298(5), c = 7.3467(3) Å, V = 1275.04 Å^3, space group *Pnma*)] and eudidymite [a = 12.6188(10), b = 7.3781(5), c = 13.9940(9) Å, β = 103.762(5)°, V = 1265.47 Å^3, space group $C2/c$] from Malosa, Malawi, has been reinvestigated by means of energy dispersive X-ray spectroscopy, thermo-gravimetric analysis, inductively coupled plasma-optical emission spectroscopy and single-crystal neutron diffraction. Two anisotropic structure refinements have been performed with final agreement index R_1 = 0.0317 for 137 refined parameters and 2261 unique reflections with $F_o > 4\sigma(F_o)$ for epididymite, and R_1 = 0.0478 for 136 refined parameters and 1732 unique reflections with $F_o > 4\sigma(F_o)$ for eudidymite. The analysis of the difference-Fourier maps of the nuclear density of the two dimorphs confirms the presence of extra-framework water molecules in both, and not hydroxyl groups as wrongly reported in previous studies and in several crystal-structure databases. The correct chemical formula of edipidymite and eudidymite is $Na_2Be_2Si_6O_{15}\cdot H_2O$ (Z = 4). The configuration of the water molecules and the hydrogen bonds are fully described for both the dimorphs. The chemical analyses show that a small, but significant, amount of Al and Fe (most likely substituting for Si in the tetrahedral sites) and K (substituting for Na as an extra-framework cation) occurs in both dimorphs.

Keywords: Epididymite, eudidymite, crystal chemistry, single-crystal neutron diffraction, hydrogen bonding