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Crystal chemistry and hydrogen bonding of rustumite $Ca_{10}(Si_2O_7)_2(SiO_4)(OH)_2Cl_2$ with variable OH, Cl, F

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Rustumite $Ca_{10}(Si_2O_7)_2(SiO_4)(OH)_2Cl_2$, space group $C2/c$, a ≈7.6, b ≈ 18.5, c ≈ 15.5 Å, β ≈ 104° has first been reported from contact-metamorphosed Jurassic limestone at Kilchoan, on the Northwest coast of Scotland (Agrell 1965). Together with dellaite $Ca_6(Si_2O_7)(SiO_4)(OH)_2$, it is one of two rare ortho- di-silicates, sharing the same Ca/Si ratio and variable Cl content, which can not be routinely distinguished by electron microprobe investigations (Armbruster et al. 2011). Cl contents are between 0 – 5.2 wt.% for dellaite (Armbruster et al. 2011) and 3.22 – 7.38 wt.% for rustumite (this study).

Three samples of the skarn mineral rustumite with variable OH, Cl, F content were investigated by electron microprobe, single-crystal X-ray structure refinements, and Raman spectroscopy: (1) low chlorine rustumite $(Ca_{10}(Si_2O_7)_2(SiO_4)(OH)_{2.60}F_{0.12}Cl_{1.28})$ from skarns associated with the Rize batholith near Ikizedere, Turkey; (2) F-bearing rustumite $(Ca_{10}(Si_2O_7)_2(SiO_4)(OH)_{1.17}F_{0.87}Cl_{1.96})$ from xenoliths in ignimbrites of the Upper Chegem Caldera, Northern Caucasus, Russia, and (3) low-Cl, F-bearing rustumite $(Ca_{10}(Si_2O_7)_2[(SiO_4)_{0.88}(H_4O_4)_{0.12}](OH)_{2.09}F_{1.07}Cl_{0.84})$ from altered merwinite skarns of the Birkhin massif, Baikal Lake area, Eastern Siberia, Russia. Rustumite from Birkhin massif is characterized by a significant hydrogarnet-like substitution at the orthosilicate group, leading to specific atomic displacements. The crystal structures including hydrogen positions have been refined from single-crystal X-ray data. Depletion in Cl and replacement by OH is associated with smaller unit cell dimensions. The substitution of OH by F leads to shorter hydrogen bonds HO-H•••F instead of HO-H•••OH. Raman spectra for all samples have been measured and confirm slight strengthening of the hydrogen bonds with uptake of F.

Rustumite is occasionally associated with dellaite. However, a paragenesis of two minerals with the same Ca/Si ratio and similar Cl content is rather unlikely.

Agrell, S.O. (1965) Min. Mag., 34, 1-15, Armbruster, T. et al. (2011) Min. Mag., 75, 379–394.