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Kumtyubeite $Ca_5(SiO_4)_2F_2$—A new calcium mineral of the humite group from Northern Caucasus, Kabardino-Balkaria, Russia

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Abstract

Kumtyubeite, $Ca_5(SiO_4)_2F_2$—the fluorine analog of reinhardbraunsite with a chondrodite-type structure—is a rock-forming mineral found in skarn carbonate-xenoliths in ignimbrites of the Upper Chegem volcanic structure, Kabardino-Balkaria, Northern Caucasus, Russia. The new mineral occurs in spurrite-rondorfite-ellestadite zones of skarn. The empirical formula of kumtyubeite from the holotype sample is $Ca_5(Si_{1.99}Ti_{0.01})_{\Sigma 2}O_8(F_{1.39}OH_{0.61})_{\Sigma 2}$. Single-crystal X-ray data were collected for a grain of $Ca_5(SiO_4)_2(F_{1.3}OH_{0.7})$ composition, and the structure refinement, including a partially occupied H position, converged to $R = 1.56\%$: monoclinic, space group $P2_1/a$, $Z = 2$, $a = 11.44637(18)$, $b = 5.05135(8)$, $c = 8.85234(13)$ Å, $\beta = 108.8625(7)°$, $V = 484.352(13)$ Å^3. For direct comparison, the structure of reinhardbraunsite $Ca_5(SiO_4)_2(OH_{1.3}F_{0.7})$ from the same locality has also been refined to $R = 1.9\%$, and both symmetry independent, partially occupied H sites were determined: space group $P2_1/a$, $Z = 2$, $a = 11.4542(2)$, $b = 5.06180(10)$, $c = 8.89170(10)$ Å, $\beta = 108.7698(9)°$, $V = 488.114(14)$ Å^3. The following main absorption bands were observed in kumtyubeite FTIR spectra (cm^{-1}): 427, 507, 530, 561, 638, 779, 865, 934, 1113, and 3551. Raman spectra are characterized by the following strong bands (cm^{-1}) at: 281, 323, 397 (ν_2), 547 (ν_4), 822 (ν_1), 849 (ν_1), 901 (ν_3), 925 (ν_3), 3553 (ν_{OH}). Kumtyubeite with compositions between $Ca_5(SiO_4)_2F_2$ and $Ca_5(SiO_4)_2(OH_{1.0}F_{1.0})$ has only the hydrogen bond O5-H1···F5′, whereas reinhardbraunsite with compositions between $Ca_5(SiO_4)_2(OH_{1.0}F_{1.0})$ and $Ca_5(SiO_4)_2(OH)_2$ has the following hydrogen bonds: O5-H1···F5′, O5-H1···O5′, and O5-H2···O2.

Keywords: Kumtyubeite, new mineral, reinhardbraunsite, crystal structure, chondrodite, composition, Raman, FTIR, Northern Caucasus, Russia