

## **Kumtyubeite $\text{Ca}_5(\text{SiO}_4)_2\text{F}_2$ —A new calcium mineral of the humite group from Northern Caucasus, Kabardino-Balkaria, Russia**

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### **ABSTRACT**

Kumtyubeite,  $\text{Ca}_5(\text{SiO}_4)_2\text{F}_2$ —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  $\text{Ca}_5(\text{Si}_{1.99}\text{Ti}_{0.01})_{\Sigma 2}\text{O}_8(\text{F}_{1.39}\text{OH}_{0.61})_{\Sigma 2}$ . Single-crystal X-ray data were collected for a grain of  $\text{Ca}_5(\text{SiO}_4)_2(\text{F}_{1.3}\text{OH}_{0.7})$  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,  $\beta = 108.8625(7)^\circ$ ,  $V = 484.352(13)$  Å<sup>3</sup>. For direct comparison, the structure of reinhardbraunsite  $\text{Ca}_5(\text{SiO}_4)_2(\text{OH}_{1.3}\text{F}_{0.7})$  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,  $\beta = 108.7698(9)^\circ$ ,  $V = 488.114(14)$  Å<sup>3</sup>. The following main absorption bands were observed in kumtyubeite FTIR spectra ( $\text{cm}^{-1}$ ): 427, 507, 530, 561, 638, 779, 865, 934, 1113, and 3551. Raman spectra are characterized by the following strong bands ( $\text{cm}^{-1}$ ) at: 281, 323, 397 ( $\nu_2$ ), 547 ( $\nu_4$ ), 822 ( $\nu_1$ ), 849 ( $\nu_1$ ), 901 ( $\nu_3$ ), 925 ( $\nu_3$ ), 3553 ( $\nu_{\text{OH}}$ ). Kumtyubeite with compositions between  $\text{Ca}_5(\text{SiO}_4)_2\text{F}_2$  and  $\text{Ca}_5(\text{SiO}_4)_2(\text{OH}_{1.0}\text{F}_{1.0})$  has only the hydrogen bond  $\text{O5-H1}\cdots\text{F5}'$ , whereas reinhardbraunsite with compositions between  $\text{Ca}_5(\text{SiO}_4)_2(\text{OH}_{1.0}\text{F}_{1.0})$  and  $\text{Ca}_5(\text{SiO}_4)_2(\text{OH})_2$  has the following hydrogen bonds:  $\text{O5-H1}\cdots\text{F5}'$ ,  $\text{O5-H1}\cdots\text{O5}'$ , and  $\text{O5-H2}\cdots\text{O2}$ .

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