Kumtyubeite Ca₅( SiO₄ )₂F₂:—A new calcium mineral of the humite group from Northern Caucasus, Kabardino-Balkaria, Russia

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ABSTRACT

Kumtyubeite, Ca₅( SiO₄ )₂F₂—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 Ca₅( SiO₄ )₂F₂O₂(OH)₂. Single-crystal X-ray data were collected for a grain of Ca₅( SiO₄ )₂F₂O₂(OH)₂ composition, and the structure refinement, including a partially occupied H position, converged to R = 1.56%: monoclinic, space group P2₁/a, Z = 2, a = 11.44637(18), b = 5.05135(8), c = 8.85234(13) Å, β = 108.8625(7)°, V = 484.352(13) Å³. For direct comparison, the structure of reinhardbraunsite Ca₅( SiO₄ )₄OH₁,F₃,2 has the same locality but a significantly refined cell: a = 11.4542(2), b = 5.06180(10), c = 8.9170(10) Å, β = 108.7698(9)°, V = 488.114(14) Å³. 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 main absorption bands (cm⁻¹): 427, 507, 530, 561, 638, 779, 865, 934, 1113, and 3551. Raman spectra are characterized by the following main absorption bands: 281, 323, 397, 427, 507, 530, 561, 638, 779, 865, 934, 1113, and 3551. Kumtyubeite with compositions between Ca₅( SiO₄ )₂F₂ and Ca₅( SiO₄ )₄OH₁,F₃,2 has only the hydrogen bond O5-H1···F5′, whereas reinhardbraunsite with compositions between Ca₅( SiO₄ )₄OH₁,F₃,2 and Ca₅( SiO₄ )₄OH₁ 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

INTRODUCTION

Kumtyubeite, Ca₅( SiO₄ )₂F₂, the calcium analog of chondrodite, was discovered in contact-metasomatic rocks formed by interaction of carbonate xenoliths with subvolcanic magma and volcanites of the Upper Chegem caldera structure, Kabardino-Balkaria, Northern Caucasus, Russia (Gazeev et al. 2006). Kumtyubeite is the fluorine analog of reinhardbraunsite, Ca₅( SiO₄ )₄OH₁,F₃,2. Reinhardbraunite (Karimova et al. 2008) and Ca₅( SiO₄ )₄OH₁,F₃,2 (IMA2008-38, Galuskin et al. in preparation), the Ca and hydroxyl analog of humite, were also discovered in the same xenoliths.

Minerals belonging to the humite group are characterized by the crystal-chemical formula n Aₙ( SiO₄ )ₙ₋₂( F,OH )₂, where A = Mg, Fe²⁺, Mn²⁺, Zn, Ca, and others with n = 1, 2, 3, or 4. The humite group of minerals, sensu stricto, comprises nesosilicates with cations in octahedral sites and additional (OH), F⁻ groups (Jones et al. 1969; Ribbe and Gibbs 1971). From a structural point of view (Thompson 1978), they are polysomes assembled of norbergite and olivine modules. Strunz and Nickel (2001) classify the corresponding minerals as norbergite-chondrodite group distinct from the ribbeite-leucophoenicite-jerrygibbsite group, which may also be derived by the same crystal-chemical formula given above but the M(O,OH)₂₃₄ chains are linked by dimers of edge-sharing SiO₄ tetrahedra with only one Si site of the dimer being statistically occupied.

Among minerals, hydroxyl analogs of the humite group seem to predominate. Only in case of Mg end-members does a complete polyomastic series of F-dominant phases exist: norbergite Mg₃( SiO₄ )₃(F,OH), chondrodite (Mg,Fe²⁺)(SiO₄)₃(F,OH), humite (Mg,Fe²⁺)(SiO₄)₃(F,OH), and clinohumite (Mg,Fe²⁺)(SiO₄)₃(F,OH), whereas only one hydroxyl analog of the Mg end-members is known: hydroxyl-clinohumite (Gekimyants et al. 1999). Within the chondrodite series three mineral species have been defined up to now: alleghanyite Mn₃( SiO₄ )₃(OH), chondrodite (Mg,Fe²⁺)(SiO₄)₃(F,OH),