Edgrewite Ca₉(SiO₄)₄F₂-hydroxyledgrewite Ca₉(SiO₄)₄(OH)₂, a new series of calcium humite-group minerals from altered xenoliths in the ignimbrite of Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia

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ABSTRACT

Members of the edgrewite $Ca_9(SiO_4)_4F_2$ -hydroxyledgrewite $Ca_9(SiO_4)_4(OH)_2$ series, structural analogues of clinohumite-hydroxylclinohumite series, $Mg_9(SiO_4)_4(F,OH)_2$, were discovered in xenoliths of carbonate-silicate rock altered to skarn within ignimbrites of the Upper Chegem volcanic structure, Kabardino-Balkaria, Northern Caucasus, Russia. The new minerals occur sparingly in zones containing bultfonteinite, hillebrandite, jennite, and chegemite, as well as rare relics of larnite and rondorfite enclosed in a matrix of hydroxylellestadite. Edgrewite and hydroxyledgrewite are largely altered to jennite in places with admixed zeophyllite and trabzonite, and are preserved as elongate relics mostly 0.1–0.4 mm long in the central part of atoll-like pseudomorphs. The new minerals form a solid-solution series $Ca_9(SiO_4)_4(F,OH)_2$, in which the content of the edgrewite end-member $Ca_9(SiO_4)_4F_2$ ranges from 74% (F = 3.64 wt%) to 31% (F = 1.52 wt%).

Structure refinement of crystals containing 51% and 37% of the edgrewite end-member gave, respectively, $R_1 = 3.03\%$, space group $P2_1/b11$ (no. 14), Z = 2, a = 5.06870(10), b = 11.35790(10), c = 15.4004(2) Å, $\alpha = 100.5980(10)^\circ$, V = 871.47(3) Å³; and $R_1 = 1.61\%$, space group $P2_1/b11$ (no. 14), Z = 2, a = 5.06720(10), b = 11.35450(10), c = 15.3941(2) Å, $\alpha = 100.5870(10)^\circ$, and V = 870.63(2) Å³.

Minerals of the edgrewite-hydroxyledgrewite series are colorless, optically biaxial (+), $2V_{\text{meas}} = 80(5)^\circ$; $2V_{\text{calc}} = 78.7^\circ$; dispersion r > v, medium; orientation: Z = a, $X \land c = 12(2)^\circ$; edgrewite: $\alpha = 1.621(2)$, $\beta = 1.625(2)$, $\gamma = 1.631(2)$; hydroxyledgrewite: $\alpha = 1.625(2)$, $\beta = 1.629(2)$, $\gamma = 1.635(2)$ (589 nm). The micro-hardness VHN₅₀ = 352–366 kg/mm² corresponds to the Mohs scale of 5.5–6. 5. FTIR spectra of edgrewite and hydroxyledgrewite show resolved bands at (edgrewite/hydroxyledgrewite, cm⁻¹): 3558 and 3551 and 3543/3554, absent/3486, 1075/1075, 996/996, 980/982, 934/933, 917/918, 904/903, 890/884, 864/864, 842/842, 818/820. Raman spectra are characterized by the following bands (edgrewite/hydroxyledgrewite, cm⁻¹) at: 921/923, 889/890, 839/840, and 815/814 (SiO₄ stretching), at: 556/559, 527/527, 423/419, 406/404, and 394/394 (SiO₄ bending), 309/295, 269/256, and 163/166 (CaO₆). In the OH stretching region three bands are noted at 3554, 3547, and 3540 cm⁻¹ for edgrewite and two – 3550 and 3475 cm⁻¹ for hydroxyledgrewite confirming the corresponding IR spectra. The major difference in Raman and IR spectra of edgrewite and hydroxyledgrewite is the presence of two resolved peaks in the OH stretching region at ca. 3550 and 3480 cm⁻¹ for hydroxyledgrewite.

Keywords: New mineral, edgrewite, hydroxyledgrewite, humite, structure, Raman, FTIR, Russia