Raman investigation of potential new mineral - Fe³⁺-analogue of wadalite from calcareous-silicate xenoliths of the Upper Chegem caldera, Northern Caucasus, Russia

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A new Fe³⁺-analogue of wadalite was discovered in altered calcareous-silicate xenoliths in ignimbrites of Upper Chegem volcanic caldera, Kabardino-Balkaria, North Caucasus, Russia [1,2]. Fe³⁺-analogue wadalite was found in altered larnite-rondorfite skarns, associated with larnite, cuspidine, wadalite, rondorfite, lakargiite, srebrodolskite, reinhardbraunsite, chegemite, hydroxylellestadite, perovskite, dovyrenite, tazheranite, kerimasite, andradite, hillebrandite, awfillite, ettringite group minerals, hydrogrossular [1]. Both high-temperature phases and low-temperature alteration products are associated with Fe³⁺-analogue wadalite [1,3]. It forms fine, numerous crystals, up to 5 μ m, together with srebrodolskite in the external zones of rondorfite crystals and usually they are associated with larnite inclusions crystals. Larger crystals, up to 10 μ m, form rare inclusions within partially altered larnite grains and are limited to surface of rondorfite as inclusions. Based on microprobe analyses, the calculated empirical formula for Fe³⁺-analogue of wadalite is Ca_{12.222}(Fe³⁺_{9.407}Al_{1.259}Si_{2.963} Ti⁴⁺_{0.112} Mg_{0.037})_{\Sigma13.778}O_{31.889}Cl_{5.038}.

In the present study the Fe³⁺-analogue wadalite $Ca_{12}(Fe^{3+}{}_{10}Si_4)_{\Sigma 14}O_{32}Cl_6$ spectrum was compared with the spectra of mayenite $Ca_{12}Al_{14}O_{33}$ and wadalite $Ca_{12}(Al_{10}Si_4)_{\Sigma 14}O_{32}Cl_6$. The main bands on Feanalogue wadalite spectrum are as follows (cm⁻¹): 927, 787, 700, 466, 414, 325, 309, 256, 182. A band shift on Fe³⁺-analogue wadalite spectrum to lower frequencies relative to wadalite and mayenite spectra is observed. The main band on mayenite spectrum is 777 cm⁻¹ and it is responsible for the $[AlO_4]^{5-}$ stretching vibrations. Intensive bands near 700-710 cm⁻¹, responding stretching vibrations of $[Fe^{3+}O_4]^{5-}$, appear on spectra of mayenite and wadalite. One intensive band near 700 cm⁻¹ (stretching vibrations of $[Fe^{3+}O_4]^{5-}$) keeps on Fe-analogue wadalite spectrum. In the high-wavenumber region responsible for OH vibrations there are no bands for Fe³⁺-analogue wadalite, which are characteristic for mayenite and wadalite containing both OH-groups and H₂O.

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