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Siwaqaite, $Ca_6Al_2(CrO_4)_3(OH)_{12}\cdot 26H_2O$, a new mineral of the ettringite group from the pyrometamorphic Daba-Siwaqa complex, Jordan

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Abstract

A new mineral, siwaqaite, ideally $Ca_6Al_2(CrO_4)_3(OH)_{12}\cdot 26H_2O$ [$P31c$, Z = 2, a = 11.3640(2) Å, c = 21.4485(2) Å, V = 2398.78(9) Å^3], a member of the ettringite group, was discovered in thin veins and small cavities within the spurrite marble at the North Siwaqa complex, Lisdan-Siwaqa Fault, Hashem region, Jordan. This complex belongs to the widespread pyrometamorphic rock of the Hatrurim Complex. The spurrite marble is mainly composed of calcite, fluorapatite, and brownmillerite. Siwaqaite occurs with calcite and minerals of the baryte-hashemite series. It forms hexagonal prismatic crystals up to 250 μm in size, but most common are grain aggregates. Siwaqaite exhibits a canary yellow color and a yellowish-gray streak. The mineral is transparent and has a vitreous luster. It shows perfect cleavage on $(10\bar{1}0)$. Parting or twinning is not observed. The calculated density of siwaqaite is 1.819 g/cm^3. Siwaqaite is optically uniaxial (–) with ω = 1.512(2), ε = 1.502(2) (589 nm), and non-pleochroic. The empirical formula of the holotype siwaqaite calculated on the basis of 8 framework cations and 26 water molecules is $Ca_{6.01}(Al_{1.87}Si_{0.12})_{\Sigma 1.99}[(CrO_4)_{1.71}(SO_4)_{1.13}(SeO_4)_{0.40}]_{\Sigma 3.24}(OH)_{11.63}\cdot 26H_2O$. X-ray diffraction (XRD), Raman, and infrared spectroscopy confirm the presence of OH^- groups and H_2O molecules and absence of $(CO_3)^{2-}$ groups. The crystal structure of this Cr^{6+}-analog of ettringite was solved by direct methods using single-crystal synchrotron XRD data. The structure was refined to an agreement index R_1 = 4.54%. The crystal structure of siwaqaite consists of $\{Ca_6[Al(OH)_6]_2\cdot 24H_2O\}^{6+}$ columns with the inter-column space (channels) occupied by $(CrO_4)^{2-}$, $(SO_4)^{2-}$, $(SeO_4)^{2-}$, and $(SO_3)^{2-}$ groups and H_2O molecules. The tetrahedrally coordinated site occupied by different anion groups is subjected to disordering and rotation of these tetrahedra within the structure. The temperature of siwaqaite formation is not higher than ~70–80 °C, as is evident from the mineral association and as inferred from the formation conditions of the natural and synthetic members of the ettringite group minerals, which are stable at conditions of T < 120 °C and pH = 9.5–13. The name siwaqaite is derived from the name of the holotype locality—Siwaqa area, where the mineral was found.

Keywords: Siwaqaite, new mineral, ettringite group, crystal structure, Raman, FTIR, Daba-Siwaqa, Jordan