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Charleshatchettite, $CaNb_4O_{10}(OH)_2 \cdot 8H_2O$, a new mineral from Mont Saint-Hilaire, Québec, Canada: Description, crystal-structure determination, and origin

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Abstract

Charleshatchettite, $CaNb_4O_{10}(OH)_2 \cdot 8H_2O$, is a new mineral related to franconite and hochelagaite, discovered on a fracture surface of a nepheline syenite at Mont Saint-Hilaire, Québec, Canada. The mineral occurs in white globules (~0.15–0.20 mm in diameter) composed of radiating crystals with individual crystals having average dimensions of ~0.002 × 0.010 × 0.040 mm. Crystals are euhedral, bladed (flattened on [100]), and are transparent to translucent. The mineral is associated with albite, quartz, muscovite, pyrrhotite, pyrite, ancylite-(Ce), and siderite. Charleshatchettite is inferred to be biaxial (–) with $\alpha' = \sim 1.72(2)$ and $\gamma' = \sim 1.82(2)$. Data from chemical analyses (SEM-EDS, $n = 8$): CaO 7.96 (7.04–8.63), MgO 0.24 (0.08–0.78), Al_2O_3 0.13 (b.d.–0.49), SiO_2 1.04 (0.49–1.88), TiO_2 3.64 (2.45–5.05), Nb_2O_5 68.07 (64.83–71.01), and H_2O (calc) 22.96, total 104.04 wt% gives the average empirical formula: $(Ca_{1.00}Mg_{0.04})_{\Sigma 1.04}(Nb_{3.62}Ti_{0.32}Si_{0.12}Al_{0.02})_{\Sigma 4.08}O_{10}(OH)_2 \cdot 8H_2O$ (based on 20 anions). This is similar to that of hochelagaite ($CaNb_4O_{11} \cdot nH_2O$), although the two are readily distinguished by their powder X-ray diffraction patterns. Results from single-crystal X-ray diffraction analysis give $a = 21.151(4)$, $b = 6.496(2)$, $c = 12.714(3)$ Å, and $\beta = 103.958(3)°$, space group $C2/c$ (no. 15). The crystal structure, refined to $R = 5.64\%$, contains 1 *Ca* site, 2 distorted octahedral Nb sites, and 10 O sites. It consists of clusters of four edge-sharing $Nb(O,OH)_6$ octahedra, linked through shared corners to adjacent clusters, forming layers of $Nb(O,OH)_6$ octahedra. These alternate along [100] with layers composed of $Ca(H_2O)_8$ polyhedra, the two being linked together by H-bonding. Charleshatchettite is a late-stage mineral, interpreted to have developed through the interaction of low-T (<150 °C) aqueous fluids with an alkali-, Nb-rich precursor under slightly reducing conditions and a highly alkaline pH. The precursor mineral(s) is unknown but is considered to have been Nb-dominant, relatively unstable under slightly reducing as well as alkaline conditions, and likely itself would have been a product of near-complete Nb/Ta fractionation due to the paucity of Ta in charleshatchettite. Charleshatchettite is crystallochemically related to Sandia Octahedral Molecular Sieves [SOMS; $Na_2Nb_{2-x}M_xO_{6-x}(OH)_x \cdot H_2O$ with M = Ti, Zr, Hf], a group of synthetic compounds with strong ion exchange capabilities.

Keywords: New mineral, charleshatchettite, Mont Saint-Hilaire, SOMS, hochelagaite, franconite, Nb/Ta fractionation, crystal structure