Charleshatchettite, CaNb₄O₁₀(OH)₂·8H₂O, a new mineral from Mont Saint-Hilaire, Québec, Canada: Description, crystal-structure determination, and origin

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ABSTRACT

Charleshatchettite, CaNb₄O₁₀(OH)₂·8H₂O, 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, anciyte-(Ce), and siderite. Charleshatchettite is inferred to be biaxial (−) with α′ = ~1.72(2) and γ′ = ~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), Al₂O₃ 0.13 (b.d.–0.49), SiO₂ 1.04 (0.49–1.88), TiO₂ 3.64 (2.45–5.05), Nb₂O₅ 68.07 (64.83–71.01), and H₂O (calc) 22.96, total 104.04 wt% gives the average empirical formula: (Ca₁.00Mg₀.04)Σ1.04(Nb₃.62Ti₀.32Si₀.12Al₀.02)Σ4.08O₁₀(OH)₂·8H₂O (based on 20 anions). This is similar to that of hochelagaite (CaNb₂O₇·nH₂O), 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 β = 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(H₂O)₄ 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 crystal-chemical related to Sandia Octahedral Molecular Sieves [SOMS; Na₂Nb₂M₄O₁₄(OH)₆·3H₂O 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

INTRODUCTION

Franconite-group minerals (FGM) are alkali-niobate hydrates that develop as late-stage, low-T minerals in agpaitic environments including Mont-Saint-Hilaire (Horváth and Gault 1990), the Saint-Amable sill (Horváth et al. 1998), the Khibiny massif (Pekov and Podlesnyi 2004), the Vuoriyarvi alkaline-ultrabasic massif (Belovitskaya and Pekov 2004), and the Vishnevogorsk alkali complex (Nikandrov 1990). Current members of the FGM include franconite [Na(Nb₂O₅)(OH)₃H₂O], hochelagaite (CaNb₂O₇·nH₂O; Jambor et al. 1986), and ternovite (MgNb₂O₇·nH₂O; Subbotin et al. 1997). The crystal structures and chemical formulas of these minerals are in general, difficult to resolve, primarily owing to their occurrence in thin (<5 μm) blades, but also because these typically develop into more complex, radiating spheres wherein more than one species may be present. Despite obvious challenges, progress has been made in unraveling the crystal-chemical structures of the FGM, mainly due to advances having been made in single-crystal X-ray diffraction methods. For example, the crystal structure of franconite was solved by Haring and McDonald (2014) who showed the mineral is strongly layered with sheets of Nb(O,OH)₆ polyhedra alternating with sheets NaO₃H₂O polyhedra, these being joined by weak H-bonds along [100], and provided a refined chemical formula Na(Nb₂O₃)(OH)·3H₂O. The crystal structures of hochelagaite and ternovite still remain unsolved but a combination of data from PXRD and Raman/FTIR spectroscopy suggest they are all closely related.

As part of a broader study aimed at better understanding the development of late-stage niobate minerals from agpaitic environments, an investigation of a previously undescribed species believed to be related to minerals of the FGM, was undertaken. This mineral, which serves as the subject of this report, was likely first observed in specimens (n = 5) collected by Elys and Les Horváth in 1978. It was not recognized as a potentially new species until 1985, based on material (n = 2) collected in...