

ACTINIDES IN GEOLOGY, ENERGY, AND THE ENVIRONMENT

Ichnusaite, $\text{Th}(\text{MoO}_4)_2 \cdot 3\text{H}_2\text{O}$, the first natural thorium molybdate: Occurrence, description, and crystal structure†

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ABSTRACT

The new mineral species ichnusaite, $\text{Th}(\text{MoO}_4)_2 \cdot 3\text{H}_2\text{O}$, has been discovered in the Mo-Bi mineralization of Su Seinargiu, Sarroch, Cagliari, Sardinia, Italy. It occurs as colorless thin {100} tabular crystals, up to 200 μm in length, associated with muscovite, xenotime-(Y), and nuragheite, $\text{Th}(\text{MoO}_4)_2 \cdot \text{H}_2\text{O}$. Luster is pearly adamantine. Ichnusaite is brittle, with a perfect {100} cleavage. Owing to the very small quantity of available material and its intimate association with nuragheite, density and optical properties could not be measured. Electron microprobe analysis gave (mean of 4 spot analyses in wt%): MoO_3 47.86(1.43), ThO_2 43.40(79), total 91.26(87). On the basis of 8 O atoms per formula unit and assuming 3 H_2O groups, in agreement with the crystal structure data, the chemical formula of ichnusaite is $\text{Th}_{0.99}\text{Mo}_{2.01}\text{O}_8 \cdot 3\text{H}_2\text{O}$. Main diffraction lines, corresponding to multiple hkl indices, are [$d(\text{\AA})$, relative visual intensity]: 5.66 (m), 3.930 (m), 3.479 (s), 3.257 (s), 3.074 (m). Ichnusaite is monoclinic, space group $P2_1/c$, with $a = 9.6797(12)$, $b = 10.3771(13)$, $c = 9.3782(12)$ \AA , $\beta = 90.00(1)^\circ$, $V = 942.0(2)$ \AA^3 , $Z = 4$. The crystal structure has been solved and refined to a final $R_1 = 0.051$ on the basis of 2008 observed reflections [with $F_o > 4\sigma(F_o)$]. It consists of electroneutral $[\text{Th}(\text{MoO}_4)_2(\text{H}_2\text{O})_2]^0$ (100) sheets of polymerized $\text{ThO}_7(\text{H}_2\text{O})_2$ and MoO_4 polyhedra; successive sheets, stacked along [100], are connected through hydrogen bonds. Ichnusaite brings new understanding about the crystal chemistry of actinide molybdates, that may form during the alteration of spent nuclear fuel and influence the release of radionuclides under repository conditions.

Keywords: Ichnusaite, new mineral species, molybdate, thorium, crystal structure, Su Seinargiu, Sardinia, Italy