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Nuragheite, $Th(MoO_4)_2 \cdot H_2O$, the second natural thorium molybdate and its relationships to ichnusaite and synthetic $Th(MoO_4)_2$†

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Abstract

The new mineral species nuragheite, $Th(MoO_4)_2 \cdot H_2O$, 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 ichnusaite, $Th(MoO_4)_2 \cdot 3H_2O$. Luster is pearly to adamantine; nuragheite is brittle, with a perfect (100) cleavage. Owing to the very small amount of available material and its intimate association with ichnusaite, density and optical properties were not measured. Electron microprobe analysis gave (wt% = mean of six spot analyses): MoO_3 49.38, ThO_2 45.39, H_2O_{calc} 3.09, total 97.86. On the basis of eight O atoms per formula unit and assuming one H_2O group, in agreement with the crystal structure data, the chemical formula of nuragheite is $Th_{1.00}Mo_{2.00}O_8 \cdot H_2O$. Main diffraction lines, corresponding to multiple *hkl* indices, are [*d* in Å (relative visual intensity)]: 5.28 (m), 5.20 (m), 5.04 (m), 4.756 (m), 3.688 (m), 3.546 (vs), 3.177 (s), 3.024 (m). The crystal structure study gives a monoclinic unit cell, space group $P2_1/c$, with $a = 7.358(2)$, $b = 10.544(3)$, $c = 9.489(2)$ Å, $\beta = 91.88(2)°$, $V = 735.8(2)$ Å^3, $Z = 4$. The crystal structure has been solved and refined to a final $R_1 = 0.078$ on the basis of 1342 "observed" reflections [$F_o > 4\sigma(F_o)$]. It consists of (100) layers formed by ninefold-coordinated Th-centered polyhedra and Mo-centered tetrahedra. Its crystal structure is discussed in relation to that of ichnusaite and that of synthetic orthorhombic $Th(MoO_4)_2$. The relationship between the progressive loss of water in the interlayer and the layer topology passing from ichnusaite through nuragheite to synthetic $(ThMoO_4)_2$ is examined. Nuragheite, the second thorium molybdate reported so far in nature, adds new data to the understanding of the crystal chemistry of actinide molybdates potentially forming during the alteration of spent nuclear fuel and influencing the release of radionuclides under repository conditions.

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