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Description and crystal structure of vajdakite, $[(Mo^{6+}O_2)_2(H_2O)_2As^{3+}_2O_5]\cdot H_2O$—A new mineral from Jáchymov, Czech Republic

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ABSTRACT

Vajdakite, a new mineral from Jáchymov, NW Bohemia, Czech Republic, forms minute acicular, gray-green crystals associated with arsenolite, scorodite, parascorodite, kaňkite, annabergite, köttigite, pyrite, marcasite, nickelskutterudite, and löllingite. Microprobe analysis gave (in wt%): As = 27.72, Mo = 35.39, O = 36.66, total = 99.77. The simplified chemical formula is $[(Mo^{6+}O_2)_2(H_2O)_2As^{3+}_2O_5]\cdot H_2O$. The mineral is monoclinic, $P2_1/c$, a = 7.0515(6), b = 12.0908(9), c = 12.2190(14) Å, β = 101.268(9)°, V = 1021.7(2) Å^3, Z = 4, D_{meas} = 3.50(2) g/cm^3, and D_{calc} = 3.509 g/cm^3. The strongest lines in the powder X-ray diffraction pattern d(I)(hkl) are: 6.046 (100)(020), 3.324 (59)(023), 6.915 (26)(100), 2.264 (19)(310), 3.457 (16)(200), 2.624 (15)(230), and 3.819 (10)(031). Vajdakite is optically positive, with X || b and Z $\wedge$ c = 12°; elongation is positive. Its birefrigence is 0.28, with $2V_{calc}$ = 35.1°, n_α = 1.757(2), n_β = 1.778(2), and n_γ = 2.04(1). The pleochroic scheme is X ~ Y = light greenish gray, and Z = yellowish gray. Crystal size varies between 0.1 to 0.5 mm. TG curve and IR spectra show that vajdakite contains two distinct types of water molecules. The crystal structure was solved by direct methods (Mo$K\alpha$ radiation) and refined using 1787 unique reflections to R = 0.0455, Rw = 0.1143. There are double chains built up by two individual chains with a sequence -O-As-O-Mo- interconnected by oxygen atoms from two triangular AsO_3 groups and two structurally non-equivalent $MoO_5(H_2O)$ octahedra. The two vertex-sharing, triangular AsO_3 groups form an $(As_2O_5)^{4-}$ diarsenite group. The first type of water molecule is not included in the coordination, but the second one is in octahedral coordination around Mo. The water molecules are linked by a complicated net of interlayer and intralayer hydrogen bonds.