Description and crystal structure of vajdakite, [(Mo$^{6+}$O$_2$(H$_2$O)$_2$As$_3^2$O$_5$)$\cdot$H$_2$O—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, kařkite, 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$_2$(H$_2$O)$_2$As$_3^2$O$_5$)$\cdot$H$_2$O. The mineral is monoclinic, P$2_1$/c, a = 7.0515(6), b = 12.0908(9), c = 12.2190(14) Å, $\beta$ = 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(l)(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 $\gamma$ c = 12°; elongation is positive. Its birefringence is 0.28, with $2V_{calc}$ = 35.1°, $n_a$ = 1.757(2), $n_g$ = 1.778(2), and $n_c$ = 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 (MoK$_\alpha$ radiation) and refined using 1787 unique reflections to R = 0.0455, Rw = 0.1143. There are two 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$_2$O) octahedra. The two vertex-sharing, triangular AsO$_3$ groups form an (As$_2$O$_5$)$^{2-}$ 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.

INTRODUCTION

The city of Jáchymov (St. Joachimsthal) is located on the southern slope of the Krušné hory Mts. (Erzgebirge), approximately 20 km north of Karlovy Vary, NW Bohemia, Czech Republic (Fig. 1). In this area, Mo anomalies associated with Ag + As + Co + Ni ± Bi and U mineralizations of the Geschieber vein of the Svornost mine have been studied in the framework of the project “Secondary minerals from the Jáchymov ore district,” which was supported by the Grant Agency of the Czech Republic. That study confirmed the occurrence of a new, natural Mo-bearing compound that we named vajdakite, which has been investigated in detail, including solution and refinement of its crystal structure (Ondruš et al. 1997a, 1997b, 1997c).

Holotype material has been deposited in the mineralogical collection of the National Museum, Prague, Czech Republic (the acquisition number P1p 19/98). The new mineral and its name have been approved by the Commission on New Minerals and Mineral Names of the IMA in 1999 (98-031). The name is in honor of mineralogist Josef Vajdak (born 1930, Montana, U.S.A.), who drew our attention to this species, for his signifi-

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