American Mineralogist, Volume 90, pages 1655–1660, 2005

Zoltaiite, a new barium-vanadium nesosubsilicate mineral from British Columbia: Description and crystal structure

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ABSTRACT

Zoltaiite, ideal formula $BaV_2^{4+}V_{12}^{3+}Si_2O_{27}$, space group $P\bar{3}$, $a = 7.601(1)$, $c = 9.219(1)$ Å, $V = 461.34(1)$ Å^3, $Z = 1$, is a new mineral found on the eastern edge of the Shuswap metamorphic complex of British Columbia, Canada. It is a metamorphic mineral formed under greenschist-facies *P-T* conditions as part of an assemblage that includes quartz, celsian, apatite, sphalerite, pyrrhotite, galena, and pyrite. Zoltaiite has a Mohs hardness of 6–7, no cleavage, an anhedral to semi-prismatic habit, and a calculated density of 4.83 g/cm^3. It is opaque with reflectance and color similar to those of sphalerite. The strongest eight lines of the X-ray powder diffraction pattern [*d* in Å (*I*) (*hkl*)] are 3.103(78)(021), 2.934(89)(2$\bar{1}$2), 2.785(67)(013), 2.679(48)(022), 2.403(50)(211), 2.190(100)(212), 1.934(53)(213), and 1.438(63)(140). The empirical formula, derived from electron-microprobe analysis and the crystal structure, is $Ba_{1.05}(Ti_{1.31}V_{0.69}^{4+})_{\Sigma 2.00}(V_{11.06}^{3+}Fe_{0.49}^{3+}Cr_{0.34})_{\Sigma 11.89}Si_{2.06}O_{27}$ based on O = 27. The crystal structure was solved by direct methods and refined on the basis of F_0^2 using all unique reflections measured with Mo$K\alpha$ X-radiation on a CCD-equipped diffractometer. The final *R* factor was 3.2%, calculated using 659 unique observed reflections. The unit cell contains four layers of two types parallel to (001): X, an octahedral and tetrahedral sheet, and Y, an octahedral plus barium sheet; both layers are doubled through inversion centers resulting in the sequence XXYY... Two consecutive equivalent layers are interconnected through shared octahedral edges, whereas consecutive non-equivalent layers are linked through shared corners. The high calculated density is consistent with the dense packing of the structure.