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LETTER

The crystal structure of bartelkeite, with a revised chemical formula, $PbFeGe^{VI}(Ge_2^{IV}O_7)(OH)_2 \cdot H_2O$, isotypic with high-pressure $P2_1/m$ lawsonite

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ABSTRACT

Bartelkeite from Tsumeb, Namibia, was originally described by Keller et al. (1981) with the chemical formula $PbFeGe_3O_8$. By means of electron microprobe analysis, single-crystal X-ray diffraction, and Raman spectroscopy, we examined this mineral from the type locality. Our results show that bartelkeite is monoclinic with space group $P2_1/m$, unit-cell parameters $a = 5.8279(2)$, $b = 13.6150(4)$, $c = 6.3097(2)$ Å, $\beta = 127.314(2)°$, and a revised ideal chemical formula $PbFeGe^{VI}Ge_2^{IV}O_7(OH)_2 \cdot H_2O$ ($Z = 2$). Most remarkably, bartelkeite is isostructural with the high-pressure $P2_1/m$ phase of lawsonite, $CaAl_2Si_2O_7(OH) \cdot H_2O$, which is only stable above 8.6 GPa and a potential host for H_2O in subducting slabs. Its structure consists of single chains of edge-sharing FeO_6 and $Ge1O_6$ octahedra parallel to the *c*-axis, cross-linked by $Ge2_2O_7$ tetrahedral dimers. The average <Ge-O> bond lengths for the GeO_6 and GeO_4 polyhedra are 1.889 and 1.744 Å, respectively. The Pb atoms and H_2O groups occupy large cavities within the framework. The hydrogen bonding scheme in bartelkeite is similar to that in lawsonite. Bartelkeite represents the first known mineral containing both 4- and 6-coordinated Ge atoms and may serve as an excellent analog for further exploration of the temperature-pressure-composition space of lawsonite.

Keywords: Bartelkeite, germanate, hydrous mineral, crystal structure, X-ray diffraction, Raman spectra