The crystal structure of jagoite

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Abstract

The crystal structure of jagoite \((a = 8.528(8), c = 33.33(3)\text{Å})\) was solved and refined in space group \(P6_2\) \(c\) to \(R_1 = 0.057\).

The structure is characterized by the presence of double and single tetrahedral layers connected by a sheet of iron and lead cations. Other lead cations as well as chloride anions are located inside the double layer. The single layer is characterized by an incomplete net of tetrahedra: the absent tetrahedron at the origin is replaced by the Fe(1) octahedron. The double layer is made up of two tetrahedral sheets, each of them built up of six membered rings of tetrahedra and \(\text{PbO}_3\) \(\psi\)-tetrahedra.

The chemical data give rise to the following crystal chemical formula:

\[
\langle \text{Pb}^{2+}_{12}\text{Na}_{1.30}\text{K}_{0.33}\text{Ca}_{0.71}\rangle\text{Pb}^{2+}_{12}(\text{Fe}^{3+}_{0.99}\text{Ti}_{0.09}\text{Mg}_{1.06}\text{Mn}_{0.94}\text{Ca}_{0.08})
\langle \text{Pb}^{2+}_{4}\text{Si}_{3.07}\text{Be}_{0.37}\text{Al}_{0.66}\text{Fe}^{3+}_{5.3}\rangle\text{O}_{29.81}(\text{OH})_{1.28}\text{Cl}_{6.18}\.
\]

The corresponding idealized crystal chemical formula is

\[
\text{VI}_x\text{Pb}^{2+}_{x+\text{VI}}\text{M}_{4}(\text{Si}_2\text{T}_2)/\langle \text{Pb}^{2+}_{x+\text{VI}}\text{Si}_{3}\text{T}_4\rangle\text{O}_{0.78}(\text{OH},\text{Cl})_6.
\]

The chemical and structural data suggest ordering of silicon and iron in tetrahedral sites and of iron, magnesium, and manganese in octahedral sites. Possible ordering schemes, in space group \(P31c\), are proposed.

Introduction

Jagoite is a rare lead and iron silicate, which was described from Långban, Sweden, by Blix et al. (1957). On the basis of its physical properties and chemical composition they suggested that jagoite is a sheet silicate with unit cell content

\[
\langle \text{Pb},\text{Ca},\text{Mn},\text{Na},\text{K}_{x}\rangle_{x}(\text{Fe}^{3+},\text{Al},\text{Mg})_{x}
\langle \text{Si},\text{Al},\text{Be}_{x}\rangle_{x}\text{O}_{4x}(\text{OH},\text{Cl})_x.
\]

The absence of adequate data concerning its crystal chemistry and its classification among the silicate minerals led us to undertake a crystal structure analysis.

Experimental

The specimen of jagoite from Långban used in this study (NMNH #113302) was kindly given us by Dr. J. S. White of the Smithsonian Institution.

Whereas Blix et al. (1957) reported that jagoite is trigonal with Laue group 3, no systematic extinctions, and lattice parameters \(a = 8.65(3)\) and \(c = 33.5(1)\text{Å}\), many crystals we examined displayed the Laue symmetry \(6/mmm\) and systematic extinctions in \(hkl\) for \(l = 2n + 1\). This indicated \(P6_3/mmc\), \(P6_{3}mc\) and \(P6\) \(2c\) as possible space groups for jagoite. It is worthwhile to recall that Blix et al. (1957) reported that the "quality of the photographs was rather poor on account of the easiness with which the plates of jagoite are deformed." Actually, we too observed the easy deformability of jagoite crystals; notwithstanding, we obtained very fine diffraction patterns by carefully picking very tiny crystals.

From the many crystals we examined, a small platelet (nearly \(0.17 \times 0.14 \times 0.53\) mm\(^3\)) was chosen for intensity data collection. The lattice parameters, refined by least squares fitting of 18 medium range \(\theta\) values, were \(a = 8.528(8), c = 33.33(3)\text{Å},\) measured by a Philips PW1100 single crystal diffractometer, using graphite monochromatized MoK\(\alpha\) radiation (\(\lambda = 0.7107\)Å). A total of 3376 reflections were collected by the same diffractometer and the same radiation.