Incorporation of sodium into the chlorite structure: the crystal structure of glagolevite, Na(Mg,Al)$_6$[Si$_3$AlO$_{10}$](OH$_2$,O)$_8$

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ABSTRACT

The crystal structure of glagolevite, Na(Mg,Al)$_6$[Si$_3$AlO$_{10}$](OH$_2$,O)$_8$, a new mineral from the Kovdor alkaline massif, Kola peninsula, Russia, has been solved and refined to $R_I = 0.117$, calculated from 1503 unique observed reflections ($F_I \geq 4\sigma F_I$), and to $R_I = 0.118$ for all 1550 unique reflections. The specimen contained several polytypes; the crystal studied yielded triclinic space group C1, $a = 5.3580\,\text{Å}$, $b = 9.2810\,\text{Å}$, $c = 14.5743\,\text{Å}$, $\alpha = 90.00\,\text{°}$, $\beta = 97.08\,\text{°}$, $\gamma = 90.00\,\text{°}$, $V = 719.2\,\text{Å}^3$. Glagolevite is the first mineral of the chlorite group that contains Na atoms located between the 1:2 layers and the interlayer octahedral sheets. The Na atoms are in sevenfold coordination. The Na(O,OH)$_2$ polyhedron is a trigonal prism with one of the triangular bases extended to a square. The tetrahedral sheets show disorder owing to polytype intergrowths. Tetrahedral site occupancies correlate with the occupancies of the Na sites. The polytypic composition of the crystal studied is estimated at 57% Iib-6, 31% Iib-2, and 12% Iib-4.

INTRODUCTION

Chlorite-group minerals are hydrous phyllosilicates with structures based upon alternating tetrahedral-octahedral 2:1 layers and interlayer hydroxide octahedral sheets. Bailey (1988) noted that, for common rock-forming chlorites, incorporation of large cations such as Na and Ca into sites located between the 2:1 layer and the interlayer sheet is unlikely. Dunn et al. (1987) described franklinfurnaceite, Ca$_4$Fe$_2$Mn$_3$(Mn$_{10}$Zn$_{18}$Si$_{10}$O$_{40}$)(OH)$_8$, a tri dioctahedral zincosilicate intermediate between chlorite and mica. Peacor et al. (1988) reported a crystal-structure determination for franklinfurnaceite, and demonstrated that the Ca atoms are in octahedral coordination between the 2:1 layers and the interlayer sheets. According to Peacor et al. (1988), this type of Ca incorporation into the chlorite structure is possible only if the structure type is Ilm, the interlayer sheet is dioctahedral, and if substitutions of substantial Al and/or Fe$^{3+}$ occur in the 2:1 layer. The Ca-bearing tri dioctahedral chlorite was also reported by Makarov (1971).

Recently, during mineralogical investigations of the Kovdor Phlogopite quarry, Kovdor massif, Kola peninsula, Russia, Seredkin et al. (2003) found a colorless platy mineral that forms, together with vesuvianite, large lenses within altered mellite rocks. The mineral has the chlorite structure but contains 4.40 wt% Na$_2$O. Its simplified formula is Na(Mg,Al)$_6$[Si$_3$AlO$_{10}$](OH$_2$,O)$_8$; the Na content corresponds to 0.76 atoms per formula unit (apfu). Comparison of unit-cell data derived from X-ray powder diffraction showed that this mineral is distinct from clinochlore, (Mg,Al)$_6$[Si$_3$AlO$_{10}$](OH)$_8$, as the c parameter of ∼14.6 Å is larger than that of clinochlore, which has c parameter ranging from 14.20 to 14.40 Å (Rule and Bailey 1987; Zheng and Bailey 1989; Joswig and Fuess 1990; Smyth et al. 1997; Guggenheim and Zhan 1999). This new species, and the name glagolevite, were approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association (CNMMN IMA) (Seredkin et al. 2003). Here we report the structure of glagolevite, which includes the first demonstration of Na in a chlorite structure between the 2:1 layer and the interlayer octahedral sheet. In contrast to franklinfurnaceite, glagolevite is a tri dioctahedral chlorite mineral.

EXPERIMENTAL METHODS

Many crystals of glagolevite were examined by single-crystal X-ray diffraction, but proved unsuitable for structural analysis owing to broad and ill-defined diffraction peaks, and the presence of substantial diffraction streaking. Eventually a specimen was obtained that contained a large but visually undistorted crystal of glagolevite. The crystal was carefully separated from the matrix and mounted on a Bruker three-circle diffractometer equipped with a Kα CCD (charge-coupled device) detector with a crystal-to-detector distance of 5.4 cm. Initial diffraction data contained various deleterious features, but the data collected was ultimately sufficient for solution and partial refinement of the structure. More than a hemisphere of data was collected using monochromated MoKα X-radiation and frames with 0.3° in 2θ. The unit-cell dimensions (Table 1) were refined on the basis of 564 strong reflections using least-squares techniques. The data were corrected for Lorentz, polarization, background, and absorption effects ($R_{wp} = 0.039$). Additional information pertinent to the data collection is given in Table 1. Scattering curves for neutral atoms, together with anomalous dispersion corrections, were taken from International Tables for X-ray Crystallography, Ibers and Hamilton (1974). The Bruker SHELXTL Version 5 system of programs was used for determination and