Okenite, Ca\textsubscript{10}Si\textsubscript{18}O\textsubscript{46}·18H\textsubscript{2}O: the first example of a chain and sheet silicate

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Abstract

The crystal structure of okenite, Ca\textsubscript{10}Si\textsubscript{18}O\textsubscript{46}·18H\textsubscript{2}O, was solved with triclinic space group \textit{P}1, \(a = 9.69, b = 7.28, c = 22.02\text{Å}, \alpha = 92.7^\circ, \beta = 100.1^\circ, \gamma = 110.9^\circ\). The structure is composed of the following structural units: (a) tetrahedral sheets \(S\), with composition \((\text{Si}_6\text{O}_{18})^{-6}\), characterized by five- and eight-membered rings of silicate tetrahedra, with five tetrahedra pointing in one direction and one tetrahedron pointing in the other direction; (b) three-repeat double chains \(C\), with composition \((\text{Si}_6\text{O}_{18})^{8}\) and characterized by four- and six-membered rings, made up by pairs of wollastonite chains, which point in opposite directions; (c) octahedral double chains \(O\), formed by two strands of octahedra. These structural units are connected by corner sharing to give the complex layer SO4, with composition \([\text{Ca}_8(\text{Si}_3\text{O}_{16})(\text{Si}_6\text{O}_{18})_2(\text{H}_2\text{O})_6]^{14}\). Such complex layers alternate in the structure with sheets \([\text{Ca}_2(\text{H}_2\text{O})_6\text{H}_2\text{Si}_3\text{O}_8]^{14}\). Weak supercell reflections revealed a larger unit cell with doubled \(a\) and \(b\) parameters in the unconventional space group \(\text{C}\).

Introduction

Okenite, a hydrated calcium silicate, has long been of interest to a large number of mineralogists and crystal chemists: its consistent association with gyrolite and zeolites in basalts seemed indicative of some structural relations among them. Of particular interest is the role of water molecules in the structure of okenite. The definition of which could lead to an understanding of the dehydration mechanism, according to Heller's X-ray studies (Gard and Taylor, 1956), leads topotactically to the formation of wollastonite.

Okenite was first described from Disko Island (Greenland) and was subsequently found in various other locations, such as Crestmore (California), Scaz Hill (Northern Ireland), Bordó (Faroer Islands), Bombay (India), usually in basalts. The most comprehensive account of its crystallographic properties was given by Gard and Taylor (1956) who studied a specimen from Bombay, India, consisting of fibrous aggregates. These authors studied okenite by electron diffraction, as single crystals of sufficient size for X-ray diffraction were not available.

The results indicated that the crystals were triclinic with \(a = 9.84, b = 7.20, c = 21.33\text{Å}, \alpha = 90.0^\circ, \beta = 103.9^\circ, \gamma = 111.5^\circ\). The fiber direction was [010], with repeated lamellar twinning across the cleavage plane [001]. On the basis of the cell volume and a chemical analysis by Christie (1925), Gard and Taylor (1956) proposed that the cell contents are Ca\textsubscript{4}Si\textsubscript{18}O\textsubscript{39}H\textsubscript{18}O\textsubscript{6} or Ca\textsubscript{4}Si\textsubscript{18}O\textsubscript{46}·18H\textsubscript{2}O.

Gard and Taylor (1956) also studied a mineral from Crestmore, California, which was previously characterized as okenite on the basis of its chemical composition and optical properties, and demonstrated that it was in fact a new species for which they proposed the name nekoite. Crystal structures for both minerals were hypothesized by Mamedov and Belov (1958) on the basis of the chemical composition and unit cell dimensions. The crystal structure of nekoite was recently solved by Alberti and Galli (1980) who showed that it was in many respects different from the structural model of Mamedov and Belov (1958).

The present work was undertaken to determine the crystal structure of okenite in order to further our understanding of the crystal chemistry of the hydrated calcium silicates.

Experimental

A specimen of okenite from Kolhapur District, Maharashtra State, India, donated by Prof. E. Passaglia, was used in this study. Careful examination of a large number of crystals from this specimen and testing by preliminary Weissenberg photographs resulted in the selection of crystals of sufficient quality for intensity measurement. By means of Weissenberg and precession photographs the lattice parameters were determined on a small fragment cut from a long lath-shaped crystal. The same crystal fragment was used to collect intensity data with a Philips PW 1100 single crystal diffactometer, after obtaining refined lattice parameters by least squares fitting of 20 medium range \(\theta\) values: \(a = 9.69(1), b = 7.28(1), c = 22.02(4)\text{Å}, \alpha = 92.7(2)^\circ, \beta = 100.1(3)^\circ, \gamma = 110.9(1)^\circ\).