

The structure of nekoite,  $\text{Ca}_3\text{Si}_6\text{O}_{15} \cdot 7 \text{H}_2\text{O}$ , a new type of sheet silicate

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## Abstract

Nekoite,  $\text{Ca}_3\text{Si}_6\text{O}_{15} \cdot 7 \text{H}_2\text{O}$ , is a new type of sheet silicate. The sample studied, from Caxias do Sul, Rio Grande do Sul, Brazil, is triclinic, space group  $P1$ , with  $a = 7.588$ ,  $b = 9.793$ ,  $c = 7.339 \text{ \AA}$ ,  $\alpha = 111.77$ ,  $\beta = 103.50$ ,  $\gamma = 86.53^\circ$ ;  $Z = 1$ . The structure was solved through a combination of direct methods and the Patterson synthesis, and refined to a final  $R$  factor of 6.8 percent. The crystal structure consists of tetrahedral sheets interlayered with octahedral chains. The tetrahedral  $\text{Si}_6\text{O}_{15}$  sheets are obtained by interconnecting a "Dreierkette" so as to form alternating bands of 5- and 8-membered rings. Ca-octahedral chains, which crosslink the tetrahedral sheets, are formed by a double strand of octahedra, of which three out of four are occupied and the fourth is empty. Water molecules occupy the empty spaces between these chains. The balance of the electrostatic valences suggests that only oxygen atoms occupy the vertices of the tetrahedral sheet, while only water molecules occur outside the tetrahedral sheet.

## Introduction

Nekoite is a rare hydrated calcium silicate, first discovered at Crestmore, Riverside County, California by Eakle (1917), who identified it as okenite on the basis of its chemical composition and optical properties. Based on studies of the same mineral from Eakle's holotype, Gard and Taylor (1956) showed it to be a new species, and named it nekoite. Chalmers *et al.* (1962) and Nicol (1971) have reported further results on the chemical composition and dehydration of nekoite from Crestmore.

Vezzalini (1979) recently described a second occurrence of nekoite in the cavities of a basaltic rock from Caxias do Sul, Rio Grande do Sul, Brazil. Nekoite occurs as tufts of well-shaped vitreous prismatic needles, up to 5 mm long, lying on large transparent crystals of heulandite and apophyllite which coat the surface of the cavities. These thin flat prisms of nekoite are only exceptionally good single crystals. Normally they occur as thin laths, up to 0.4 mm wide and 0.003 mm thick, of two or more individuals, which in turn can be twinned.

The usually accepted composition is  $\text{Ca}_3\text{Si}_6\text{O}_{15} \cdot 8 \text{H}_2\text{O}$ . Chemical analyses of nekoite given in the literature are similar except for the water content, which varies from 6  $\text{H}_2\text{O}$  (Eakle, 1917) to 8  $\text{H}_2\text{O}$  (Gard and Taylor, 1955; Chalmers *et al.*, 1962).

A structural model for nekoite was proposed by Mamedov and Belov (1958), but has not been verified. Nicol (1971) announced the publication of the structure of nekoite which has not yet been published. The aim of our research is to determine the crystal structure of nekoite and to provide a better knowledge of its crystal chemistry.

## Experimental

An untwinned fragment of nekoite ( $0.28 \times 0.07 \times 0.02$  mm in size) was obtained from Vezzalini's specimen by cutting a twinned lath. Preliminary Weissenberg photographs confirmed the lattice parameters given by Vezzalini, which are reported along with other crystal data and experimental conditions in Table I. The unit cell orientation has been chosen according to the recommendations of the Commission on Crystallographic Data of the International Union of Crystallography (Kennard *et al.*, 1967). The orientation of the triclinic unit cell assumed by Nicol (1971) can be derived by means of the transformation matrix 010/001/100.

Diffraction intensities were measured in the  $\omega$ -scan mode with a Philips PW 1100 single-crystal automatic X-ray diffractometer (Centro di Cristallografia Strutturale del CNR, Pavia, Italy) and graphite-monochromatized  $\text{CuK}\alpha$  radiation at room temperature. For each reflection, repeated scans were made

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URS-CALC SURT# (0-C1)/SIG(U) 10  
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ADJUSTMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1  
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 SURTF (SUM(W\*(0-C1)\*E2)/(NU-NV)) IS 2.5025

NUMERATOR DENOMINATOR R  
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