The crystal structure of tuscanite

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Abstract

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\[ \text{[K}_{0.6} \text{Si}_{0.4} \text{(H}_2 \text{O)}_{1.3}] \text{(Cu}_{0.1} \text{Zn}_{0.9} \text{Na}_{0.1} \text{Fe}_{2.10} \text{Mg}_{0.11}) \text{(Si}_{6.34} \text{Al}_{3.66} \text{Ti}_{0.22}) \text{(SO}_{4} \text{)}_{2.24} \text{(CO}_{3} \text{)}_{1.36} \text{(OH)}_{0.50} \text{(H}_2 \text{O)}_{0.11}] \]

space group \( P2_1/\alpha \), \( a = 24.03(2) \), \( b = 5.11(1) \), \( c = 10.88(2) \), \( \alpha = 106.94(9)^\circ \), was determined by direct methods using diffractometric data. Anisotropic thermal refinement led to a final \( R \) value of 0.034 (\( R_w \) = 0.038). The crystal structure is characterized by the presence of double layers of (Si,Al) tetrahedra; the double layer can be described, as in latiumite, as made up by five-membered rings, nearly parallel to (010), but whereas in latiumite each tetrahedron in the ring points upward, in tuscanite three tetrahedra in every ring point upward and two downward. These layers are connected by calcium and sulphate ions, as in latiumite; whereas in latiumite successive layers are related by unit translation, in tuscanite they are related by a glide plane. The substitutions of (CO$_3$OH) and (H$_2$O) for SO$_4$ are proposed and discussed.

Introduction

Tuscanite was discovered by Orlandi et al. (1977) in some ejected blocks found in a pumice deposit in Pitigliano, Tuscany, Italy. They pointed out the close relationships between tuscanite and latiumite, a sheet silicate described by Tilley and Henry (1953) and whose crystal structure was studied by Cunnillo et al. (1973). Orlandi et al. (1977) noted the similarity of the X-ray powder diffraction patterns of tuscanite and latiumite; in fact, the unit cell of tuscanite is very similar to that of latiumite, from which it is obtainable by doubling the \( a \) parameter. We easily made the hypothesis that tuscanite and latiumite differ only in the stacking sequence, namely unit translation in latiumite and glide plane in tuscanite, of the same structural unit. To understand the precise structural relationships between the two minerals, namely whether the relation is polytypic or polymorphic, and to discover possible differences, we undertook the present structural analysis. A preliminary report on the main features of the crystal structure of tuscanite was presented at the 1975 meeting of Società Italiana di Mineralogia e Petrologia.

Experimental

A small \((0.15 \times 0.12 \times 0.27\,\text{mm})\) tabular crystal of tuscanite from Pitigliano was used for the X-ray structure analysis. Unit-cell data of our specimen, determined by the Philips PW-1100 single-crystal automatic diffractometer, are \( a = 24.03(2) \), \( b = 5.11(1) \), \( c = 10.88(2) \), \( \alpha = 106.94(9)^\circ \), space group \( P2_1/\alpha \), in good agreement with the values found by Orlandi et al. (1977) by least-squares fitting of powder data. Intensity data were collected by the same diffractometer, using graphite-monochromatized MoK\(\alpha\) radiation \((\lambda = 0.7107\,\text{A})\). \(\omega\) scan, integration width \(1.2^\circ\), 3724 independent reflections were collected from \(2^\circ\) to \(30^\circ\); the corresponding values of \(F_{\text{obs}}\) and \(s(F_{\text{obs}})\) were obtained by the procedure of Davies and Gatehouse (1973); no absorption correction was made owing to the small dimensions of the crystal \((a = 19.7\,\text{cm})\); also, no extinction correction was applied. 2420 reflections were classified as "observed, ..."