

Single crystal X-ray refinement of pyrophyllite- $1Tc$

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Abstract

The crystal structure of pyrophyllite from Ibitiara, Bahia, Brazil has been refined by least-squares from single crystal X-ray data to an unweighted R value of 0.060 and a weighted R value of 0.070. The Ibitiara pyrophyllite is a $1Tc$ polytype having space group symmetry of $C\bar{1}$. Average bond lengths are Al-O 1.912, Si(1)-O 1.617, and Si(2)-O 1.618 Å. The tetrahedral rotation angle (α) is 10.2°, the octahedral flattening angle (ψ) is 57.1° and the tetrahedral thickness angle (τ) is 109.4°. The results agree closely with the structural determination from X-ray powder data of Wardle and Brindley (1972).

Formulae to calculate the apical oxygen separation are derived in order to determine the magnitude of the effects of four geometric parameters: (a) the tetrahedral rotation angle, (b) the octahedral flattening angle, (c) the deviation of the apical oxygen from a mean $O_{\text{Apical}} - O_{\text{basal}}$ angle and (d) the corrugation parameter, Δz . Of these, the corrugation is more effective in adjusting the distance between apical oxygens to provide linkage between the tetrahedral and octahedral sheets and to allow readjustments around the larger vacant site.

Introduction

Earlier work on pyrophyllite has shown it to exist in three polytypic forms: a two layer monoclinic ($2M$), a one layer triclinic ($1Tc$) and a disordered form (Gruner, 1934; Zvyagin, *et al.*, 1969; and Brindley and Wardle, 1970). Rayner and Brown (1965) studied a partially disordered pyrophyllite- $2M$ single crystal for lack of better material. Later, powder data were analyzed from the one layer form by Wardle and Brindley (1970) to establish the ideal structure and then to refine the results partially. These results confirmed the earlier model of Zvyagin, *et al.* (1969). Due to the difficulty in obtaining well-crystallized material and the fine-grained nature of pyrophyllite, a detailed single crystal study has not been possible previously.

A single crystal X-ray refinement of the structure of pyrophyllite- $1Tc$ has been undertaken using material from a recently discovered extensive deposit near Ibitiara, Bahia, Brazil. The crystals appear to be hydrothermal in origin; a thin section of the matrix material shows crystallization of pyrophyllite occur-

ring in vugs, veins, and other openings. Crystals range in size up to 5 cm. Although a detailed study of this deposit has not been made, pyrophyllite- $1Tc$ has been shown by synthesis work to form at 375°C and above, whereas the $2M$ variety forms at lower temperature (Eberl, 1979).

Experimental

The crystal chosen for analysis measured originally $5 \times 1 \times 1$ cm and was elongate parallel to the a axis. Portions were stained reddish brown from iron oxides, but large sections were pearly white to pale yellow. Material was cleaved from the white/yellow portions and then cut to size with a razor blade. These crystals were quite sensitive to solvents such as acetone and would partially split along cleavage upon drying. Furthermore, slight pressure caused the platelets to bend. Seventy sections were examined by the precession method and one, approximately rectangular in shape and $0.6 \times 0.5 \times 0.05$ mm in size, was chosen for further study. This crystal, mounted so that the b^* axis was parallel to the fiber length, was glued along the fiber for support. The composition of a nearby crystal was determined by wet chem-

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