

Semi-ordered crystalline structure of the Santa Olalla vermiculite inferred from X-ray powder diffraction

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ABSTRACT

A sample of Mg-vermiculite from Santa Olalla (Spain) was studied by X-ray powder diffraction, electron microprobe, and thermo-gravimetry. The 3D structure is described as a disordered stack of two types of 2D building blocks, which are made up of one talc-type layer and one interlayer space containing hydrated Mg²⁺ cations. We have succeeded in the refinement of both the atomic positions and occupancies of exchangeable cations and water molecules in the interlayer space of this vermiculite using the program package DIFFaX+. The position of the Mg²⁺ cations is the only difference between the two layers. Besides the water molecules associated to the octahedrally coordinated Mg²⁺, we also located water molecules in the interlayer space. The structural analysis confirms that vermiculite is a semi-ordered crystalline material characterized by the existence of a large density of defects due to random $\sim\pm b/3$ translations along the crystalline [010] direction. In this way, this structure can no longer be described by means of a unit cell repeated in 3D space. Instead, long-range order is only recognized in the *a-b* plane. The 3D structure is described by means of a recursive method.

Keywords: Mg-vermiculite, stacking faults, X-ray diffraction, DIFFaX+