

Sideronatrite, $\text{Na}_2\text{Fe}(\text{SO}_4)_2(\text{OH})\cdot 3\text{H}_2\text{O}$: Crystal structure of the orthorhombic polytype and OD character analysis

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ABSTRACT

Sideronatrite, $\text{Na}_2\text{Fe}(\text{SO}_4)_2(\text{OH})\cdot 3\text{H}_2\text{O}$, is a secondary hydrated sulfate occurring in desert areas as the result of pyrite alteration. It is one of the environmental indicators of soil-water processes operating in specific landscapes, and, as a consequence, an important marker of acid mine drainage pollution. Sideronatrite has been demonstrated from its peculiar diffraction pattern to belong to a family of OD structures formed by equivalent layers.

In this work, a crystal with weak diffuse streaks proved to be suitable for a single-crystal X-ray diffraction study. The crystal structure was solved by direct methods and refined by full matrix least-squares ($R = 7.4\%$ and $R_w = 8.0\%$) in the space group $P2_12_12_1$ with $a = 7.265(2)$, $b = 20.522(6)$, $c = 7.120(2)$ Å, $V = 1061.5(5)$ Å³, and $Z = 4$, using 798 reflections with $I > 3.0 \sigma(I)$.

Sideronatrite is characterized by infinite $[\text{Fe}^{3+}(\text{SO}_4)_2(\text{OH})]^{2-}$ octahedral-tetrahedral chains of the type $[\text{M}(\text{TO}_4)_2\phi]$ running parallel to the c axis. These chains are cross-linked by a columnar system of corner-sharing, Na-distorted octahedra along c to form corrugated sheets parallel to the (010) plane. Adjacent sheets are hydrogen-bonded through water molecules coordinated by Na atoms. The present results allow a complete description of the OD character of the structure, with the derivation of the OD groupoid and MDO polytypes.

Finally, chemical and structural relationships are taken into account to explain the possible paragenetic sequence concerning several sulfates associated with sideronatrite.

Keywords: Sideronatrite, structure solution, OD character, polytypism