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Crystal structure of $Na_3Fe(SO_4)_3$: A high-temperature product (~400 °C) of sideronatrite $[Na_2Fe(SO_4)_2OH{\cdot}3H_2O]$

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Abstract

The iron sulfate $Na_3Fe(SO_4)_3$ studied here has been obtained as a high-temperature (HT) product (~400 °C) from the thermal decomposition of sideronatrite from Sierra Gorda (Chile) having composition $Na_2Fe(SO_4)_2(OH){\cdot}3H_2O$. The structure determination was carried out using synchrotron X-ray powder diffraction. Structural data refined by the Rietveld method, up to $R_p = 11.95\%$, are: space group $R\bar{3}$, lattice parameters $a = b = 13.6231(1)$ Å and $c = 9.0698(1)$ Å, $V = 1457.76(2)$ Å^3, and $Z = 6$. The structure of $Na_3Fe(SO_4)_3$ can be described in terms of FeO_6 octahedra connected to sulfate tetrahedra by corner-sharing to form infinite chains $[Fe(SO_4)_3]_\infty$, running along **c**. These chains are joined together by Na atoms to build up a three-dimensional network of strong (Fe-O-S) and weak (Na-O) bonds. The topological relationships of $Na_3Fe(SO_4)_3$ to the structure of some analog minerals are also discussed.

Keywords: Iron sulfate, synchrotron, structure solution, Rietveld refinement