

The structure of metahohmannite, $\text{Fe}_2^{3+}[\text{O}(\text{SO}_4)_2] \cdot 4\text{H}_2\text{O}$, by in situ synchrotron powder diffraction

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ABSTRACT

Metahohmannite, $\text{Fe}_2^{3+}[\text{O}(\text{SO}_4)_2] \cdot 4\text{H}_2\text{O}$, is a hydrated sulfate of ferric iron that occurs in sulfate deposits in the desert areas of Northern Chile. The compound used for this study was obtained as a dehydration product of hohmannite, $\text{Fe}_2^{3+}[\text{O}(\text{SO}_4)_2] \cdot (4+4)\text{H}_2\text{O}$. Intensities for the structure analysis were collected from a powdered sample using in situ synchrotron X-ray powder diffraction at ESRF (Grenoble, France). The structure was solved ab initio by profile deconvolution and the application of standard Patterson and difference Fourier maps. The structure was refined to $R_p = 5.46\%$ using the Rietveld method. Metahohmannite crystallizes in the triclinic system, space group $P\bar{1}$ with unit-cell parameters $a = 7.3484(5) \text{ \AA}$, $b = 9.7710(6) \text{ \AA}$, $c = 7.1521(5) \text{ \AA}$, $\alpha = 91.684(5)^\circ$, $\beta = 98.523(5)^\circ$, $\gamma = 86.390(5)^\circ$, and $Z = 2$. The structure consists of four Fe^{3+} octahedra and four sulfate tetrahedra, which share vertices and edges to form a complex building block of $\text{Fe}_4^{3+}[\text{O}_2(\text{SO}_4)_4] \cdot 8\text{H}_2\text{O}$ composition. Such blocks are connected to form chains running parallel to the c axis. A complicated system of hydrogen bonds connects adjacent chains into a three-dimensional network. Finally, the crystal structures of metahohmannite, hohmannite, and amarantite are compared and the geometrical features discussed in detail.