American Mineralogist, Volume 94, pages 1005–1011, 2009

The crystal structure and hydrogen bonding of synthetic konyaite, $Na_2Mg(SO_4)_2 \cdot 5H_2O$

Evelyne M.S. Leduc,[1,*] Ronald C. Peterson,[1] and Ruiyao Wang[2]

[1]Department of Geological Sciences and Geological Engineering, Queen's University, Kingston, Ontario K7L 3N6, Canada
[2]Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada

Abstract

The crystal structure of synthetic konyaite, $Na_2Mg(SO_4)_2 \cdot 5H_2O$, $a = 5.7690(8)$, $b = 23.951(3)$, $c = 8.0460(11)$ Å, $\beta = 95.425(2)°$, $V = 1106.8(3)$ Å^3, space group $P2_1/c$, $Z = 4$, was solved using single-crystal X-ray diffraction. Hydrogen atom positions were determined and the structure solution was refined to $R_1 = 3.31\%$ and $wR_2 = 6.28\%$ for the 2167 measured independent reflections. Three distinct cation sites host the Mg and Na atoms in distorted octahedra and eight-coordinated polyhedra. The coordination polyhedra share edges to form compact sheets oriented perpendicular to *b* and linked to one another by hydrogen bonds. This results in a {010} tabular habit. A comparison of this structure is made to that of blödite [$Na_2Mg(SO_4)_2 \cdot 4H_2O$], the dehydration product of konyaite. Konyaite is discussed within the context of the Na_2O-MgO-SO_4-H_2O system. This study is part of ongoing investigations into the dehydration mechanisms and phase stability of this system.

Keywords: Konyaite, crystal structure, single-crystal X-ray diffraction, hydrogen bonding, blödite, dehydration, phase stability