American Mineralogist, Volume 92, pages 1038–1047, 2007

Thermal expansion of deuterated hopeite, $Zn_3(PO_4)_2 \cdot 4D_2O$

Paul F. Schofield,[1,*] Kevin S. Knight,[1,2] Mark E. Hodson,[1,3] and Anna M. Lanfranco[1,†]

[1]Department of Mineralogy, Natural History Museum, Cromwell Road, London SW7 5BD, U.K.
[2]ISIS Science Division, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, U.K.
[3]Department of Soil Science, School of Human and Environmental Sciences, The University of Reading, Whiteknights, Reading, RG6 6DW, U.K.

Abstract

The lattice parameters extracted from Lebail analysis of neutron powder diffraction data collected between 2 and 300 K have been used to calculate the temperature evolution of the thermal expansion tensor for hopeite, $Zn_3(PO_4)_2 \cdot 2H_2O$, *Pnma*, $Z = 4$ with $a = 10.6065(4)$ Å, $b = 18.2977(4)$ Å, $c = 5.0257(2)$ Å at 275 K. The *a* lattice parameter shows a negative thermal expansion, the *b* lattice parameter appears to saturate at 275 K while the *c* lattice parameter has a more typical positive thermal expansion. At 275 K, the magnitudes of the thermal expansion coefficients are $\alpha_a = -1.1(4) \times 10^{-5}$ K^{-1}, $\alpha_b = 2.4(9) \times 10^{-6}$ K^{-1} and $\alpha_c = 3.6(2) \times 10^{-5}$ K^{-1}. Under the conditions of these experiments, hopeite begins to dehydrate to the dihydrate between 300 and 325 K, and between 480 and 500 K the monohydrate is formed. The thermal expansion of the dihydrate has been calculated between 335 and 480 and at 480 K the magnitudes of the thermal expansion coefficients are $\alpha_a = 1(2) \times 10^{-5}$ K^{-1}, $\alpha_b = 4(1) \times 10^{-6}$ K^{-1}, $\alpha_c = 4(2) \times 10^{-5}$ K^{-1}, $\alpha_\beta = 1(1) \times 10^{-5}$ K^{-1}, and $\alpha_V = 2(2) \times 10^{-5}$ K^{-1}. The thermal expansion of hopeite is described in terms of its crystal structure and possible dehydration mechanisms for the α and β modifications of hopeite are discussed.

Keywords: Hopeite, thermal expansion, dehydration, neutron diffraction