Mössbauer spectroscopic study of synthetic leucophosphite, KFe₂(PO₄)₂(OH)·2H₂O

V.G. DE RESENDE,^{1,*} G.M. DA COSTA,² E. DE GRAVE,¹ AND A. VAN ALBOOM^{1,3}

¹Department of Subatomic and Radiation Physics, University of Ghent, B-9000 Gent, Belgium ²Chemistry Department, Federal University of Ouro Preto, 35400-000, Ouro Preto (MG), Brazil ³Faculty of Applied Engineering Sciences, University College Ghent, B-9000 Gent, Belgium

ABSTRACT

A Mössbauer study of synthetic leucophosphite, KFe₂(PO₄)₂(OH)·2H₂O is reported. The sample was prepared by the reaction of synthetic goethite (α -FeOOH) with a K-phosphate solution of pH 2 at 373 K for 20 days. The obtained cell parameters are a = 9.771(1), b = 9.675(2), c = 9.747(2) Å, $\beta = 102.45(1)^\circ$. The Mössbauer spectra from 295 K down to 40 K show the existence of two Fe³⁺ doublets with $\Delta E_{Q1} \approx 0.62$ mm/s and $\Delta E_{Q2} \approx 0.91$ mm/s (at 80 K), respectively, whereas for lower temperatures the spectra are composed of two sextets with $H_{hf1} \approx 48.3$ T and $H_{hf2} \approx 48.8$ T at 4.2 K. The magnetic transition temperature was determined to be 36 K from a Mössbauer thermoscan experiment. The magnetic ordering is presumed to be antiferromagnetic. The temperature variations of the hyperfine fields cannot be explained by the simple molecular field approximation. Using a model that takes into account the exchange magnetostriction associated to a non-second-order transition, an excellent reproduction of the $H_{hf}T$ curves was obtained.

Keywords: Leucophosphite, Mössbauer spectroscopy, magnetic ordering