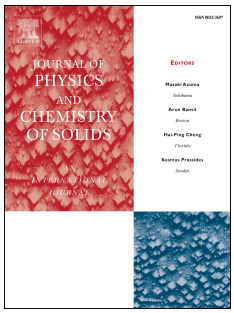
Accepted Manuscript



Synthesis and physicochemical characterizations of a new valence-mixed pyrophosphate: $Cu_{0.5}Zn_{0.5}Fe_2(P_2O_7)_2$

H. Lamsaf, A. Oulmekki, E.H. Elghadraoui, R. Fausto, B.F.O. Costa

PII: S0022-3697(17)31929-7

DOI: 10.1016/j.jpcs.2018.03.040

Reference: PCS 8510

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 10 October 2017

Revised Date: 1 March 2018

Accepted Date: 30 March 2018

Please cite this article as: H. Lamsaf, A. Oulmekki, E.H. Elghadraoui, R. Fausto, B.F.O. Costa, Synthesis and physicochemical characterizations of a new valence-mixed pyrophosphate: $Cu_{0.5}Zn_{0.5}Fe_2(P_2O_7)_2$, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.03.040.

Synthesis and Physicochemical Characterizations of a New Valence-Mixed Pyrophosphate: $Cu_{0.5}Zn_{0.5}Fe_2(P_2O_7)_2$

H. Lamsaf, [1,2] *A. Oulmekki,*[1] *E. H. Elghadraoui,*[1] *R. Fausto,*[2] *B. F. O. Costa*[3]

[1] Chemistry Laboratory of Condensed Matter (LCMC), Faculty of Science and Technology Fez, University ofSidi Mohammed Ben Abdellah, BP. 2202 Morocco.

[2] CQC, Department of Chemistry, University of Coimbra, P-3004-535 Coimbra, Portugal.

[3]CFisUC, Department of Physics, University of Coimbra, P-3004-516 Coimbra, Portugal.

Abstract: A new valence-mixed iron(III)-zinc(II)-copper(II) pyrophosphate, $Cu^{2+}_{0.5}Zn^{2+}_{0.5}Fe^{3+}_2(P_2O_7^{4-})_2$, has been synthesized by a dry-way method and structurally characterized by several techniques. The powder diffraction pattern of the new material shows that the pyrophosphate is isostructural with the iron(III)-iron(II) pyrophosphate $Fe^{2+}Fe^{3+}_2(P_2O_7^{4-})_2$, crystallizing in an orthorhombic arrangement in the *Pnma* space group. $Cu^{2+}Fe^{3+}_2(P_2O_7^{4-})_2$ was formed as a secondary phase, as determined both by X-ray diffraction and Mössbauer spectroscopy. Mössbauer spectroscopy and magnetometry measurements showed that $Cu_{0.5}Zn_{0.5}Fe_2(P_2O_7)_2$ is paramagnetic at room temperature and the iron ions are in octahedral coordination. Néel temperature is about 3 K. Infrared and Raman spectroscopies were also used in this study to characterize the new pyrophosphate.

Keywords: Mixed iron(III)-zinc(II)-copper(II) pyrophosphate; X-ray diffraction (XRD); Infrared, Raman and Mössbauer spectroscopies; Vibrating sample magnetometry (VSM).

1. Introduction

Sedimentary phosphates are a source of natural wealth of great importance, both economically and in terms of the development of scientific and technological research in Morocco.

Many previous studies focused on the industrial applications of phosphates, including pyrophosphates, especially because of their importance in the catalysis sector **[1,2]** and demonstrated ability for encapsulation of nuclear wastes **[3].** Phosphates are characterized by the PO_4^{3-} group (pyrophosphates by the $P_2O_7^{4-}$ group), which is the basic structural unit for the construction of the different phosphate-based materials.