Structural and Electrical Investigation of New Melilite Compound $\text{K}_{0.86}\text{Na}_{1.14}\text{CoP}_2\text{O}_7$

Riadh Marzouki^{1,2,*}, Youssef Ben Smida³, Abderrahmen Guesmi², Samuel Georges⁴,
Ismat H. Ali¹, Stefan Adams⁵, Mohamed Faouzi Zid²

¹ Chemistry Department, College of Science, King Khaled University, Abha 61413, Saudi Arabia.

² Laboratory of Materials, Crystallochemistry and Applied Thermodynamics, Faculty of Sciences of Tunis, University of Tunis El Manar, Tunisia.

³ National Center of Materials Sciences Research, Technopole Borj Cedria, 8027 Soliman, Tunisia.

⁴ CNRS, LEPMI, F-38000 Grenoble, France.

⁵ Department of Materials Science and Engineering, Faculty of Engineering, National University of Singapore, Singapore.

*E-mail: riadh.marzouki@hotmail.fr

doi: 10.20964/2018.12.75

Received: 11 September 2018 / Accepted: 2 October 2018 / Published: 5 November 2018

A new sodium-potassium cobalt diphosphate, $\text{K}_{0.86}\text{Na}_{1.14}\text{CoP}_2\text{O}_7$, is synthesized by solid state reaction method and characterized by X-ray diffraction (XRD) and impedance spectroscopy. The resulting structural model is supported by bond-valence-sum analysis (BVS) and charge distribution validations (CHARDIT) tools. The mixed pyrophosphate crystallizes in the tetragonal system, space group $\text{P4}_2/\text{mmn}$ with $a=7.808(3)$ Å, $c=10.757(3)$ Å. The structure is described as a 2D anionic framework with alkali cations sandwiched between layers. As mechanical grinder, ball-milling was used in order to reduce average particle size of the prepared powder. The optimal sintering temperature of the ceramic is 560°C, leading to a relative density of 83%. Their microstructure is characterized by scanning electron microscopy (SEM). The conductivity measurements of the obtained ceramic are studied over a temperature range from 360°C to 480°C. It shows that $\text{K}_{0.86}\text{Na}_{1.14}\text{CoP}_2\text{O}_7$ material is a low ionic conductor with a conductivity of $\sigma=8.26\times10^{-7}$ S.cm⁻¹ at 390°C and an activation energy of 1.34 eV. The bond valence site energy (BVSE) model is used to identify the conduction pathways for the monovalent cations, allowing a better correlation between the electrical and the structural data.

Keywords: Crystal structure; relative density; microstructure; impedance spectroscopy; conduction pathways.

[FULL TEXT](#)

© 2018 The Authors. Published by ESG (www.electrochemsci.org). This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).