Enhancement of red emission and site analysis in Eu^{2+} doped new-type structure $Ba_3CaK(PO_4)_3$ for plant growth white LEDs

Jinmeng Xiang, Jiming Zheng, Ziwei Zhou, Hao Suo, Xiaoqi Zhao, Xianju Zhou, Niumiao Zhang, Maxim S. Molokeev, Chongfeng Guo

PII: S1385-8947(18)31754-6
DOI: https://doi.org/10.1016/j.cej.2018.09.036
Reference: CEJ 19875

To appear in: *Chemical Engineering Journal*

Received Date: 12 June 2018
Revised Date: 4 September 2018
Accepted Date: 6 September 2018

Please cite this article as: J. Xiang, J. Zheng, Z. Zhou, H. Suo, X. Zhao, X. Zhou, N. Zhang, M.S. Molokeev, C. Guo, Enhancement of red emission and site analysis in Eu^{2+} doped new-type structure $Ba_3CaK(PO_4)_3$ for plant growth white LEDs, *Chemical Engineering Journal* (2018), doi: https://doi.org/10.1016/j.cej.2018.09.036

Enhancement of Red Emission and Site Analysis in Eu^{2+} Doped New-Type Structure $Ba_3CaK(PO_4)_3$ for Plant Growth White LEDs

Jinmeng Xiang[†], Jiming Zheng[†], Ziwei Zhou[†], Hao Suo[†], Xiaoqi Zhao[†], Xianju Zhou[#], Niumiao Zhang[†], Maxim S. Molokeev[‡, Δ, ⊥*] and Chongfeng Guo[†*]

[†] *National Key Laboratory of Photoelectric Technology and Functional Materials in Shaanxi Province, National Photoelectric Technology and Functional Materials & Application of Science and Technology International Cooperation Base, Institute of Photonics & Photon-Technology and Department of Physics, Northwest University, Xi'an 710069, China*

[#] *School of Science, Chongqing University of Posts and Telecommunications, Chongqing, 400065, P. R. China*

[‡] *Laboratory of Crystal Physics, Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Krasnoyarsk 660036, Russia*

[Δ] *Siberian Federal University, Krasnoyarsk, 660041, Russia*

[⊥] *Department of Physics, Far Eastern State Transport University, Khabarovsk, 680021 Russia*

Corresponding authors

**E-mail: guocf@nwu.edu.cn (Prof. Guo)*

msmolokeev@mail.ru (Prof. Molokeev)

Abstract

A novel compound $Ba_3CaK(PO_4)_3$ (BCKP) with new-type structure was synthesized and its structure was determined by X-ray diffraction Rietveld refinement, in which crystal structure consists of $Ba1O_9$, $Ba2O_{12}$, $Ba3O_9$, CaO_8 and KO_{10} polyhedra, that's five cationic sites. As a phosphor host, Eu^{2+} doped BCKP emits cold white light with about 90% quantum efficiency (QE) through entering different cationic sites. Based on the results of refinement, three Eu^{2+} luminescence centers in sites Ca, Ba2 and K were clearly assigned in Eu^{2+} solely doped BCKP by the time-resolved emission spectra (TRES), Van Uitert equation, but the emissions of Eu^{2+} at Ba1 and Ba3 sites are not easy to be determined for the same coordination number (CN). According to their different spatial distribution of the coordinated atoms, the *first-principles calculation* was used to compute the *d* orbital splitting energy of Eu^{2+} ions in Ba1 and Ba3 sites to accurately distinguish the ambiguous luminescence centers. In order to meet the requirement of plant growth