Non-centrosymmetric $\text{Na}_7\text{Li}_{0.8}\text{K}_{0.2}\text{Co}_5(\text{As}_3\text{O}_{10})_2(\text{As}_2\text{O}_7)_2$: synthesis, structure and alkali ion-conduction pathways simulation

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doi: 10.20964/2020.05.38

Received: 5 November 2019 / Accepted: 15 February 2020 / Published: 10 April 2020

A novel di-triarsenate material $\text{Na}_7\text{Li}_{0.8}\text{K}_{0.2}\text{Co}_5(\text{As}_3\text{O}_{10})_2(\text{As}_2\text{O}_7)_2$ has been synthesized by solid state reaction route. The structural study determined by single crystal X-ray diffraction showed the non-centrosymmetry of the structure. It crystallizes in the monoclinic system of C2 space group with the unit cell parameters: $a=10.136(2)$ Å, $b=8.722(2)$ Å, $c=16.952(3)$ Å, $\beta=101.86$ (2)°, $V=1466.9(5)$ Å³ and $Z=2$. Structural analysis using Charge Distribution (CHARDI) and Bond-Valence Sum (BVS) calculations tools are envisaged to confirm the proposed structural model. The $[\text{Co}_2\text{O}_{10}\text{As}_3\text{O}_{10}]_\infty$ chains connected to triarsentae groups toughen by CoO_6 octahedra forms a 3D anionic framework showing different tunnels, where alkali ions are located. Bond Valence Site Energy (BVSE) computational model was used to simulate the alkali-ion migration pathways in the anionic framework of the studied material. It shows that the alkali ion-conduction is probably ensured by sodium cations with an activation energy $E_a=0.83$ eV. Only Na^+ ions migration is probably along [100] direction which diffuse through an infinite 1D pathway.

Keywords: Di-triarsenate, crystal structure, non-centrosymmetric, anionic framework, alkali-ion migration.

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