Na_{1.82}K_{0.38}Rb_{0.80}Fe₃(AsO₄)₄: Synthesis, crystal structure and alkali conduction pathways simulation

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A new iron arsenate Na_{1.82}K_{0.38}Rb_{0.80}Fe₃(AsO₄)₄ (**1**), with layer structure has been synthesized by solid-state method and studied by X-ray diffraction. It crystallizes in orthorhombic space group Cmce with lattice parameters a=10.8710(9)Å, b=20.882(2)Å, c=6.5163(7)Å, V= 1479.3(2)Å³ and Z = 4. The final agreement factors are R = 0.039 and wR = 0.109. The X-ray single-crystal structure reveals a layered structure. Each layer is made of AsO₄ tetrahedra and FeO₆ octahedra sharing corners and edges. The Rb⁺ and K⁺ reside between the undulating iron arsenate slabs, whereas the smaller Na⁺ cations are located in the cavities of the anionic framework. The structural model was validated by bond valence sum (BVS), distortion indices (DI) and charge distribution (CD) methods. Pathways migration simulation of alkali cations was studied by extended BVS models (BVSP and BVEL).

Keywords: Iron arsenate, Crystal structure, Bond valence analysis, Pathways simulation, Ionic conductor.

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