

Abstract Submitted
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Structural modifications in the $\text{Rb}_x\text{Cs}_{1-x}\text{H}_2\text{PO}_4$ ($0 \leq x \leq 1$) superprotonic conductor series: a single-crystal x-ray diffraction and impedance spectroscopy study. ALAN GOOS, ANDRES JOSE ENCERRADO MANRIQUEZ, HEBER MARTINEZ, ALEX PRICE, CRISTIAN BOTEZ, None — We have used single-crystal x-ray diffraction to investigate the structural modifications induced by Rb-doping of the superprotonic conductor CsH_2PO_4 . Our data collected on the $\text{Rb}_x\text{Cs}_{1-x}\text{H}_2\text{PO}_4$ ($0 \leq x \leq 1$) series shows that the monoclinic $\text{P}21/m$ CsH_2PO_4 modification persists upon Rb-doping up to $x = 0.8$. We found that $\text{Rb}_{0.8}\text{Cs}_{0.2}\text{H}_2\text{PO}_4$ exhibits a previously unreported $\text{P}21/c$ monoclinic structure, where the mirror plane is lost and disorder is present in the PO_4 tetrahedra even at room temperature. Higher levels of x display a tetragonal $\text{I-}42d$ unit cell isomorphic with the known structure of RbH_2PO_4 . The temperature dependence of the proton conductivity determined from impedance spectroscopy data collected within the 160C - 250C range is also markedly different at high Rb-doping levels, $x \geq 0.8$. Finally, we found that $\text{Rb}_{0.9}\text{Cs}_{0.1}\text{H}_2\text{PO}_4$ undergoes a transition from its room-temperature tetragonal $\text{I-}42d$ phase to an intermediate-temperature monoclinic $\text{P}21/m$ modification at a significantly lower temperature ($\sim 80\text{ C}$) than its RbH_2PO_4 counterpart ($\sim 120\text{ C}$).

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None

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