The crystal structures of the four known CsCoPO₄ polymorphs have been reported by P. Henry [1] and H. Kawaji [2]. The structures were determined using synchrotron (phase 1-4) and neutron powder diffraction (phase 3) methods. Although the reported structures are correct and are in good agreement with known structural analogues, for example, CsZnPO₄, isotropic displacement parameters of some atoms seem to be questionable. For example, Biso of P1 of the phase 4 exhibits very low value of 0.3(1) Å². In order to understand the nature of low displacement parameters and to obtain more precise structural information for CsCoPO₄ polymorphs, a single crystal diffraction study has been performed. The compound undergoes three phase transitions at following temperatures: 280, 210, 30°C. It adopts two orthorhombic compounds (phase 2), and two monoclinic phases, space group Pn (phase 1) and P2₁/a (phase 3) and P1 2₁ (phase 4). New structural data of all four polymorphs with anisotropically refined displacement parameters will be presented and compared with known powder diffraction data. KEYWORDS Phosphates, Polymorphism, Crystal structure, Structure solution, Single-crystal diffraction


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Keywords: Phosphates, Polymorphism, Crystal structure, Structure solution, Single-crystal diffraction

References