

MS14-P36 | THE CRYSTAL STRUCTURE OF KONINCKITE

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The name koninckite designates a phosphate mineral discovered in Richelle (Belgium) by G. Cesàro, who carefully examined the chemical composition and defined the formula $\text{Fe}^{3+}(\text{PO}_4)\cdot 3\text{H}_2\text{O}$. The mineral forms pale brownish spheroidal aggregates constituted by tiny needle-like crystals; due to this fibrous habit, the crystal structure was very difficult to solve from single-crystal X-ray diffraction data. Recently, the structure of koninckite from Kociha, Slovakia, was solved by using synchrotron powder X-ray diffraction data (space group $P4_12_12$, $a = 11.9800(5)$ and $c = 14.618(1)$ Å); the H atoms were localized from DFT calculations. A re-investigation of samples from the type locality allowed us to find good quality isolated crystals of koninckite, which were used to obtain single-crystal X-ray diffraction data. The structure was solved in space group $P4_12_12$ ($a = 11.9852(2)$ and $c = 14.6239(3)$ Å), to a R_1 factor of 0.0375. The asymmetric unit contains 2 Fe, 2 P, 14 O and 12 H atoms; Fe atoms are coordinated by 4 O atoms and 2 water molecules, forming fairly regular octahedral sites. These octahedra are connected to tetrahedral PO_4 sites by corner-sharing, and the resulting heteropolyhedral framework shows large channels running along the c axis. The channels contain two water molecules; according to their site multiplicities, the formula of the mineral is revised as $\text{Fe}^{3+}(\text{PO}_4)\cdot 2.75\text{H}_2\text{O}$. Hydrogen-bonding scheme of the structure is discussed in detail.