

## 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  $\text{PO}_4$  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.