The Crystal Structure of Koninckite

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## Introduction

- Koninckite was discovered in Richelle (Belgium) by G. Cesàro en 1884, and studied by Van Tassel in 1968.
- Forms pale brownish spheroidal aggregates measuring less then 0.5 mm in diameter, and associated with Richellite.
- Crystal structure is difficult to solve from single-crystal Xray diffraction due to the fibrous habit.
- Plášil et al. (2015) solved the structure of Koninckite from Kociha, Slovakia, by using synchrotron powder Xray diffraction data.
- New investigation on Koninckite from the type locality, Richelle, allowed to find good quality isolated crystal, used to obtain single-crystal diffraction data.



## Structure of Koninckite

- Asymmetric unit contains $2 \mathrm{Fe}, 2 \mathrm{P}, 14 \mathrm{O}$ and 12 H atoms.
- Fe are coordinated by 4 O atoms and 2 water molecules, forming fairly regular octahedral sites connected to tetrahedral $\mathrm{PO}_{4}$ sites by corner-sharing.
- Heteropolyhedral framework of alternating $\mathrm{Fe}\left(\mathrm{O}, \mathrm{H}_{2} \mathrm{O}\right)_{6}$ octahedra and $\mathrm{PO}_{4}$ tetrahedra.
- Channels parallel to the $c$ axis, which contain water molecules.

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## Conclusions

- The results are similar to Plášil et al. (2015).
- Accurate localization of hydrogen atoms.
- Due to the lower multiplicity of one $\mathrm{H}_{2} \mathrm{O}$ molecule, the chemical formula of the mineral is $\mathrm{Fe}\left(\mathrm{PO}_{4}\right) \cdot 2 \cdot 75 \mathrm{H}_{2} \mathrm{O}(\mathrm{Z}=16)$.


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