

# The Crystal Structure of Koninckite

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### Introduction

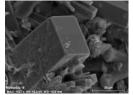
- Koninckite was discovered in Richelle (Belgium) by G. Cesàro en 1884, and studied by Van Tassel in 1968.
- Forms pale brownish spheroidal aggregates measuring less then 0.5 mm in diameter, and associated with Richellite.
- Crystal structure is difficult to solve from single-crystal Xray diffraction 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.

## **Morphology**

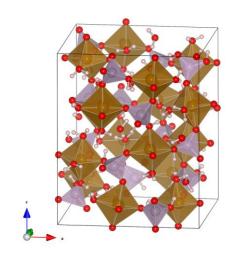








#### **Crystal structure**



	a (Å)	11.9800(5)	11.9852(2)					
	b(Å)	11.9800(5)	11.9852(2)					
	c (Å)	14.6180(1)	14.6239(3)					
	V (Å3)	2097.90(2)	2100.67(7)					
	S.G.	P41212	P41212					
	Z	8	16					
		Plášil <i>et al.</i> (2015)	This study					
			0					
9		0 0						
			0					

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	0.0	

Fe1-02	2.064(3)	Fe2-010	1.99	95
Fe1-04	2.019(3)	Fe2-011	<b>2</b> .11	13
Fe1-05	1.988(3)	P3-01	<b>1</b> .51	14
Fe1-0	1.981(3)	P3-0	<b>1</b> .55	52
Fe1-09	1.927(3)	P3-09	1.52	25
Fe1-012	2.087(4)	P3-010	<b>1</b> .54	18
Fe2-01	1.891(3)	P4-04	<b>1</b> .53	33
Fe2-03	2.075(3)	P4-05	<b>1</b> .54	10
Fe2-07	1.996(3)	P4-07	1.54	ł1
Fe2-08	1.946(3)	P4-08	<b>1</b> .54	13

#### **Structure of Koninckite**

- Asymmetric unit contains 2 Fe, 2 P, 14 O and 12H atoms.
- Fe are coordinated by 4 O atoms and 2 water molecules, forming fairly regular octahedral sites connected to tetrahedral PO<sub>4</sub> sites by corner-sharing.
- Heteropolyhedral framework of alternating Fe(O,H<sub>2</sub>O)<sub>6</sub> octahedra and PO<sub>4</sub> 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 H<sub>2</sub>O molecule, the chemical formula of the mineral is Fe(PO<sub>4</sub>).2.75H<sub>2</sub>O (Z = 16).