

The Crystal Structure of Koninckite

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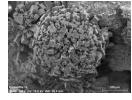


Introduction

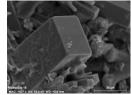
- Koninckite was discovered in Richelle (Belgium) by G. Cesàro en 1884, and studied by Van Tassel in 1968.
- Forms pale brownish spheroidal aggregates measuring less then 0.5 mm in diameter, and associated with Richellite.
- Crystal structure is difficult to solve from single-crystal Xray diffraction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

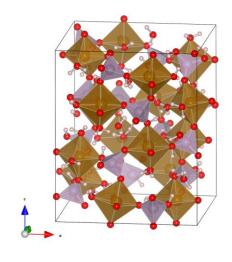








Crystal structure



	a¶Å)	11.9800(5)2	11.9852(2)	
	b(A)	11.9800(5)2	11.9852(2)2	
	c [[Å)	14.6180(1)2	14.6239(3)2	
	<i>V</i> Q ų)ℤ	2097.90(2)2	2100.67(7)2	
	S.G.🛮	P41212	P41212	
	Z	82	162	
	2	Plášil@t al.@ (2015)@	This study 2	
		0		
8				
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8			
	4 %		
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Fe1-022	2.064(3)2	Fe2-0102	1.	.99!
Fe1-042	2.019(3)2	Fe2-0112	2.	.113
Fe1-052	1.988(3)2	P3-012	1.	.514
Fe1-02	1.981(3)2	P3-02	1.	.552
Fe1-092	1.927(3)2	P3-092	1.	.52
Fe1-0122	2.087(4)2	P3-0102	1.	.548
Fe2-012	1.891(3)2	P4-04?	1.	.53:
Fe2-032	2.075(3)2	P4-052	1.	.54
Fe2-072	1.996(3)2	P4-072	1.	.541
Fe2-082	1.946(3)2	P4-082	1.	.54

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 PO₄ sites by corner-sharing.
- Heteropolyhedral framework of alternating Fe(O,H₂O)₆ octahedra and PO₄ 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 H₂O molecule, the chemical formula of the mineral is Fe(PO₄).2.75H₂O (Z = 16).