

RbCuFe(PO<sub>4</sub>)<sub>2</sub>

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{P}-\text{O}) = 0.006$  Å;  
 $R$  factor = 0.046;  $wR$  factor = 0.126; data-to-parameter ratio = 26.6.

A new iron phosphate, rubidium copper(II) iron(III) bis(phosphate), RbCuFe(PO<sub>4</sub>)<sub>2</sub>, has been synthesized as single crystals by the flux method. This compound is isostructural with KCuFe(PO<sub>4</sub>)<sub>2</sub> [Badri *et al.* (2011), *J. Solid State Chem.* **184**, 937–944]. Its structure is built up from Cu<sub>2</sub>O<sub>8</sub> units of edge-sharing CuO<sub>5</sub> polyhedra, interconnected by FeO<sub>6</sub> octahedra through common corners to form undulating chains that extend infinitely along the [011] and [01 $\bar{1}$ ] directions. The linkage of such chains is ensured by the PO<sub>4</sub> tetrahedra and the resulting three-dimensional framework forms quasi-elliptical tunnels parallel to the [101] direction in which the Rb<sup>+</sup> cations are located.

## Related literature

For the physical properties of iron phosphates, see: Elbouaani *et al.* (2002). For the structural chemistry of iron phosphates, see: Moore (1970); Gleitzer (1991). For rubidium iron phosphates, see: Hidouri *et al.* (2010). The title compound is isostructural with KCuFe(PO<sub>4</sub>)<sub>2</sub> (Badri *et al.*, 2011) and K(Fe,Mg)(PO<sub>4</sub>)<sub>2</sub> (Yatskin *et al.*, 2012). For P–O distances in monophosphate groups, see: Baur (1974). For ionic radii, see: Shannon (1976).

## Experimental

## Crystal data

RbCuFe(PO <sub>4</sub> ) <sub>2</sub>	$V = 658.3$ (2) Å <sup>3</sup>
$M_r = 394.80$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.054$ (1) Å	$\mu = 13.28$ mm <sup>-1</sup>
$b = 9.906$ (3) Å	$T = 293$ K
$c = 9.140$ (1) Å	$0.25 \times 0.21 \times 0.14$ mm
$\beta = 115.47$ (1)°	

## Data collection

Enraf–Nonius CAD4 diffractometer	1437 independent reflections
Absorption correction: part of the refinement model ( $\Delta F$ ) (SHELXLA; Sheldrick 2008)	1236 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.060$ , $T_{\max} = 0.119$	$R_{\text{int}} = 0.046$
1939 measured reflections	2 standard reflections every 120 min
	intensity decay: 1%

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$	54 parameters
$wR(F^2) = 0.126$	$\Delta\rho_{\max} = 3.25$ e Å <sup>-3</sup>
$S = 1.08$	$\Delta\rho_{\min} = -2.25$ e Å <sup>-3</sup>
1437 reflections	

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2226).

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## supporting information

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**RbCuFe(PO<sub>4</sub>)<sub>2</sub>****Abdessalem Badri, Mourad Hidouri and Mongi Ben Amara****S1. Comment**

Iron phosphates are the subject of growing interest because of their attractive physical properties (Elbouaanani *et al.*, 2002) as well as for their structural diversity (Moore, 1970; Gleitzer, 1991). Among the variety of iron monophosphates synthesized and characterized over the past three decades, only one rubidium-containing compound has been reported, namely Rb<sub>9</sub>Fe<sub>7</sub>(PO<sub>4</sub>)<sub>10</sub> (Hidouri *et al.*, 2010). In this paper, we report the structure of a new rubidium iron monophosphate RbCuFe(PO<sub>4</sub>)<sub>2</sub> synthesized during our investigation of the Rb<sub>3</sub>PO<sub>4</sub>—Cu<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>—FePO<sub>4</sub> quasi system.

Due to the poor quality of the crystal, anisotropic structure refinement systematically led to non-positive definite thermal parameters. For this reason, all the atoms were refined isotropically.

This compound is isostructural with KCuFe(PO<sub>4</sub>)<sub>2</sub> (Badri *et al.*, 2011) and K(Fe,Mg)(PO<sub>4</sub>)<sub>2</sub> (Yatskin *et al.*, 2012). The structure consists of a three-dimensional assemblage of Cu<sub>2</sub>O<sub>8</sub> units of edge-sharing CuO<sub>5</sub> trigonal bipyramids, linked to each other by FeO<sub>6</sub> octahedra through common corners to form crossing zigzag chains that run parallel to the [011] and [01 $\bar{1}$ ] directions (Fig. 1). These chains are linked by the PO<sub>4</sub> tetrahedra, giving rise to a three-dimensional framework.

The environments of the different coordination polyhedra are shown in Fig. 2. Each CuO<sub>5</sub> polyhedron is linked to four PO<sub>4</sub> tetrahedra, by sharing three corners with three tetrahedra and one edge with the fourth, the two O atoms forming the shared edge being also shared by two FeO<sub>6</sub> octahedra (Fig. 2a). Each FeO<sub>6</sub> octahedron is corner-linked to six PO<sub>4</sub> tetrahedra, two of its corners being also shared with two CuO<sub>5</sub> polyhedra (Fig. 2b). Each PO<sub>4</sub> tetrahedron shares one edge with one CuO<sub>5</sub> polyhedron and four corners, one with a CuO<sub>5</sub> polyhedron and three with three FeO<sub>6</sub> octahedra (Fig. 2c). Each PO<sub>4</sub> tetrahedron shares three corners with three FeO<sub>6</sub> octahedra, the remaining corner being doubly shared with two CuO<sub>5</sub> polyhedra (Fig. 2d). The anionic framework induced by this mode of connectivity forms quasi-elliptic tunnels along the [101] direction (Fig. 3).

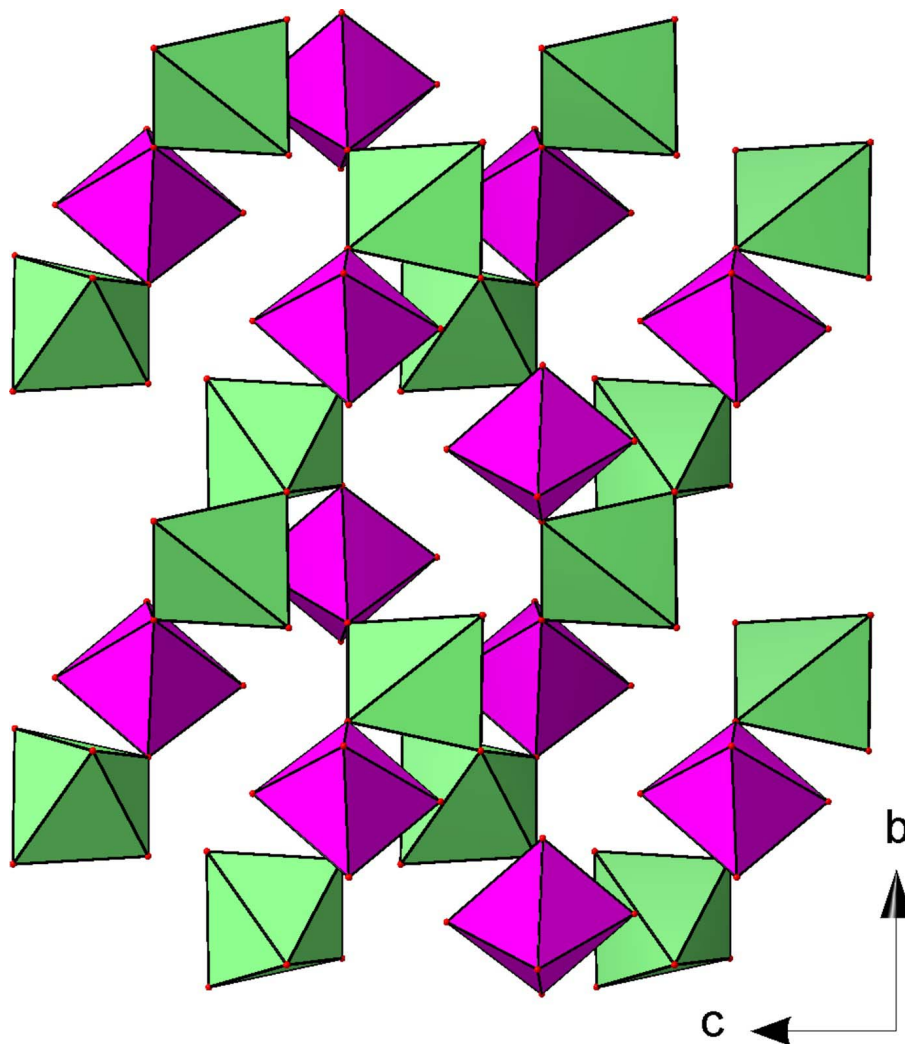
From an examination of the cation–oxygen distances, the CuO<sub>5</sub> polyhedron is highly deformed, with one longer Cu—O distance of 2.174 (3) Å compared to the four others [from 1.916 (3) to 2.030 (3) Å]. Such deformation has already been observed in KCuFe(PO<sub>4</sub>)<sub>2</sub> and it can be attributed to the Jahn–Teller effect accentuated for the Cu<sup>2+</sup> ions with d<sup>9</sup> configuration. The FeO<sub>6</sub> octahedron is also highly distorted, with Fe—O distances varying between 1.937 (4) and 2.187 (3) Å. Corresponding mean <Fe—O> distance of 2.018 Å is close to 2.03 Å predicted by Shannon for octahedral Fe<sup>3+</sup> ions (Shannon, 1976). The P—O distances within the PO<sub>4</sub> tetrahedra are in the range 1.518 (3) and 1.576 (3) Å, with an overall distances of 1.540 (3) Å consistent with 1.537 Å calculated by Baur for the monophosphate groups (Baur, 1974). The Rb<sup>+</sup> ions occupy a single distinct site. Their environment was determined assuming all cation–oxygen distances shorter than the shortest distance between Rb<sup>+</sup> and its nearest cation. This environment (Fig. 4) is then constituted by nine O atoms, with Rb—O distances ranging from 2.887 (3) to 3.123 (3) Å.

## S2. Experimental

Single crystals of  $\text{RbCuFe}(\text{PO}_4)_2$  were grown in a flux of rubidium dimolybdate,  $\text{Rb}_2\text{Mo}_2\text{O}_7$ , in an atomic ratio P:Mo = 4:1. Appropriate amounts of  $\text{Rb}_2\text{CO}_3$  (Fluka, 99%),  $\text{Cu}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (Acros, 99%),  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  (Fisher, 98.6%),  $(\text{NH}_4)_2\text{HPO}_4$  (Merck, 99%) and  $\text{MoO}_3$  (Acros, 99%) were dissolved in aqueous nitric acid and the obtained solution was evaporated to dryness. The obtained residue was homogenized by grinding and then gradually heated up to 873 K in a platinum crucible. After being reground, the mixture was melted for 1 h at 1173 K and subsequently cooled at a rate of 10  $\text{K h}^{-1}$  down to 673 K, after which the furnace was turned off. The crystals extracted from the flux by washing with warm water, are essentially composed by dark-green plate crystals of  $\text{RbCuFe}(\text{PO}_4)_2$ .

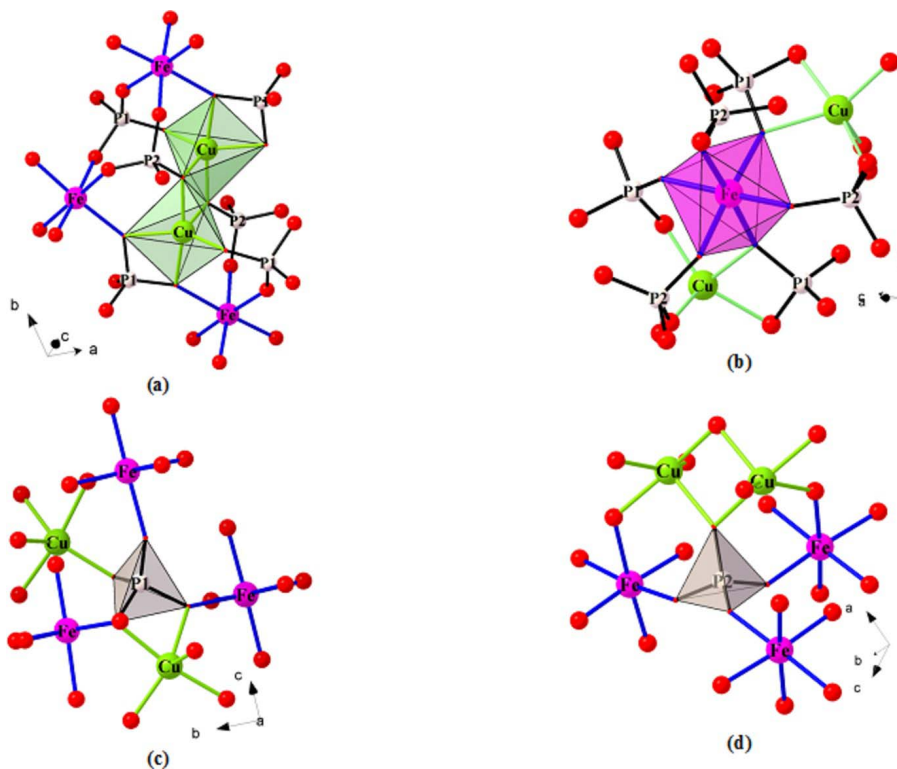
## S3. Refinement

Due to the poor quality of the crystal, anisotropic structure refinement led to non-positive definite thermal parameters for the Fe, P1, P2, O11, O13, O21 and O23 atoms. Then, all the atoms were refined isotropically. The obtained largest positive and negative difference electron densities are closest to the Rb atoms.

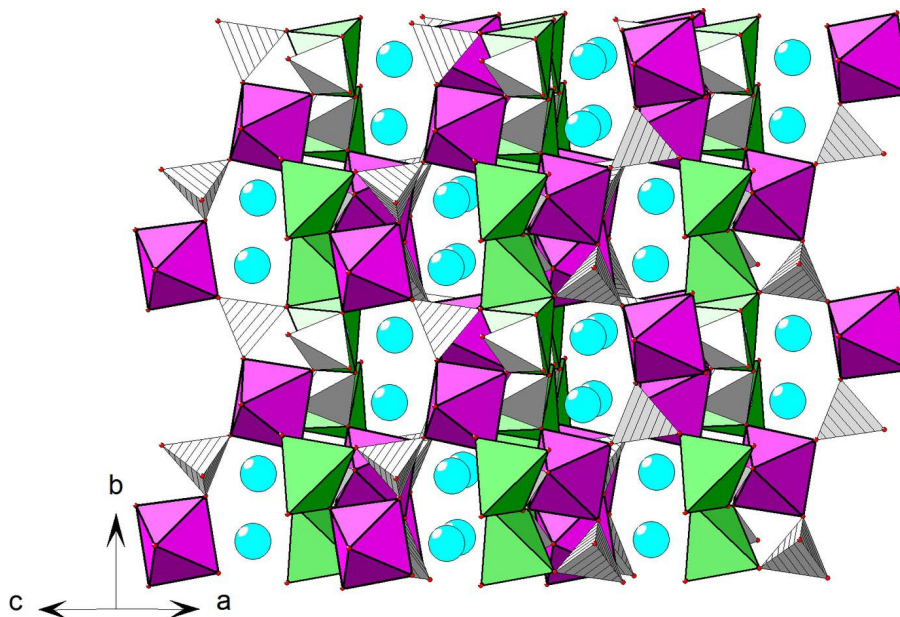


**Figure 1**

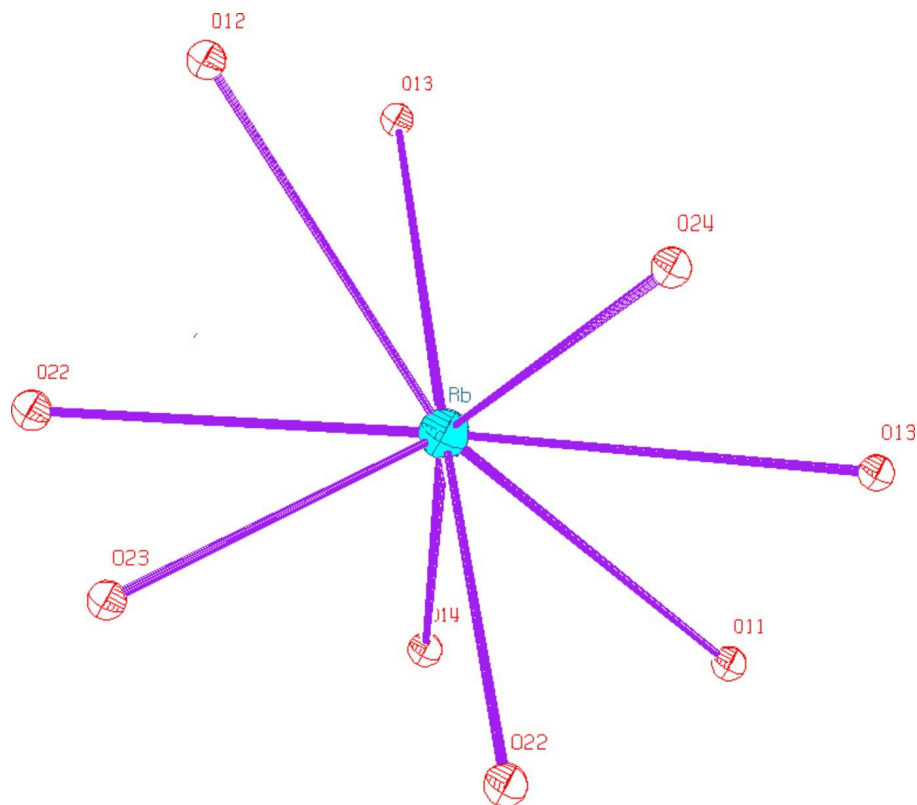
The crossing chains of the alternating  $\text{Cu}_2\text{O}_8$  units and  $\text{FeO}_6$  octahedra. The  $\text{FeO}_6$  octahedra and the  $\text{CuO}_5$  trigonal bipyramids are represented by purple and green polyhedra, respectively.

**Figure 2**

The environments of the  $\text{CuO}_5$  (a),  $\text{FeO}_6$  (b),  $\text{P1O}_4$  (c) and  $\text{P2O}_4$  (d) polyhedra.

**Figure 3**

A projection along the  $[101]$  direction of the structure showing the large tunnels occupied by the  $\text{Rb}^+$  cations.  $\text{FeO}_6$ ,  $\text{CuO}_5$ ,  $\text{P1O}_4$  and  $\text{P2O}_4$  are represented by purple, green, solid grey and hatched grey polyhedra, respectively. The  $\text{Rb}$  atoms are illustrated by cyan circles.

**Figure 4**

The environment of the Rb cations showing the thermal ellipsoids drawn at the 50% probability level.

### Rubidium copper iron bis(phosphate)

#### Crystal data

RbCuFe(PO<sub>4</sub>)<sub>2</sub>  
 $M_r = 394.80$   
 Monoclinic,  $P2_1/n$   
 Hall symbol: -P 2yn  
 $a = 8.054 (1) \text{ \AA}$   
 $b = 9.906 (3) \text{ \AA}$   
 $c = 9.140 (1) \text{ \AA}$   
 $\beta = 115.47 (1)^\circ$   
 $V = 658.3 (2) \text{ \AA}^3$   
 $Z = 4$

$F(000) = 744$   
 $D_x = 3.983 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 25 reflections  
 $\theta = 2.8\text{--}26.9^\circ$   
 $\mu = 13.28 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$   
 Plate, green  
 $0.25 \times 0.21 \times 0.14 \text{ mm}$

#### Data collection

Enraf–Nonius CAD4  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega/2\theta$  scans  
 Absorption correction: part of the refinement  
 model ( $\Delta F$ )  
 (SHELXL97; Sheldrick 2008)  
 $T_{\min} = 0.060$ ,  $T_{\max} = 0.119$   
 1939 measured reflections

1437 independent reflections  
 1236 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.046$   
 $\theta_{\max} = 26.9^\circ$ ,  $\theta_{\min} = 2.8^\circ$   
 $h = -1 \rightarrow 10$   
 $k = -1 \rightarrow 12$   
 $l = -11 \rightarrow 10$   
 2 standard reflections every 120 min  
 intensity decay: 1%

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.126$   
 $S = 1.08$   
 1437 reflections  
 54 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 $w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 8.1747P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 3.25 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -2.25 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXL97* (Sheldrick,  
 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.056 (3)

Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Rb	0.08146 (10)	-0.36746 (7)	0.92434 (9)	0.0187 (3)*
Cu	0.36913 (11)	-0.11858 (8)	0.94182 (10)	0.0103 (3)*
Fe	0.98385 (13)	0.12391 (9)	0.75520 (11)	0.0084 (3)*
P1	1.2630 (2)	0.08995 (18)	0.1423 (2)	0.0082 (4)*
O11	0.4087 (7)	0.0231 (5)	0.0958 (6)	0.0116 (10)*
O12	0.2147 (7)	-0.0101 (5)	0.2460 (6)	0.0116 (10)*
O13	0.8515 (7)	0.2895 (5)	0.7505 (6)	0.0123 (10)*
O14	0.0942 (7)	0.1317 (5)	0.9900 (6)	0.0115 (10)*
P2	0.1321 (2)	-0.15855 (18)	0.6387 (2)	0.0087 (4)*
O21	0.4575 (7)	-0.2610 (5)	0.1010 (6)	0.0138 (10)*
O22	0.1462 (7)	-0.1108 (5)	0.4869 (6)	0.0119 (10)*
O23	0.3040 (7)	-0.2436 (5)	0.7543 (6)	0.0118 (10)*
O24	0.1483 (7)	-0.0378 (5)	0.7545 (6)	0.0112 (10)*

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Rb—O13 <sup>i</sup>	2.888 (5)	Fe—O14 <sup>vii</sup>	1.940 (5)
Rb—O21 <sup>ii</sup>	2.947 (5)	Fe—O13	1.946 (5)
Rb—O12 <sup>iii</sup>	2.952 (5)	Fe—O12 <sup>vi</sup>	1.952 (5)
Rb—O21 <sup>iii</sup>	2.969 (5)	Fe—O22 <sup>vi</sup>	2.005 (5)
Rb—O14 <sup>iv</sup>	3.003 (5)	Fe—O24 <sup>vii</sup>	2.081 (5)
Rb—O12 <sup>v</sup>	3.085 (5)	Fe—O23 <sup>viii</sup>	2.185 (5)
Rb—O23	3.087 (5)	P1—O13 <sup>ix</sup>	1.519 (5)
Rb—O11 <sup>iii</sup>	3.120 (5)	P1—O14 <sup>x</sup>	1.526 (5)
Rb—O22 <sup>v</sup>	3.122 (5)	P1—O12 <sup>vii</sup>	1.533 (5)

Cu—O11 <sup>ii</sup>	1.915 (5)	P1—O11 <sup>vii</sup>	1.557 (5)
Cu—O21 <sup>ii</sup>	1.930 (5)	P2—O22	1.515 (5)
Cu—O23	1.993 (5)	P2—O21 <sup>iii</sup>	1.521 (5)
Cu—O24	2.028 (5)	P2—O24	1.565 (5)
Cu—O11 <sup>vi</sup>	2.178 (5)	P2—O23	1.576 (5)
O13 <sup>i</sup> —Rb—O21 <sup>ii</sup>	69.35 (14)	O11 <sup>ii</sup> —Cu—O23	170.6 (2)
O13 <sup>i</sup> —Rb—O12 <sup>iii</sup>	112.20 (14)	O21 <sup>ii</sup> —Cu—O23	94.0 (2)
O21 <sup>ii</sup> —Rb—O12 <sup>iii</sup>	176.53 (14)	O11 <sup>ii</sup> —Cu—O24	98.0 (2)
O13 <sup>i</sup> —Rb—O21 <sup>iii</sup>	138.05 (14)	O21 <sup>ii</sup> —Cu—O24	146.1 (2)
O21 <sup>ii</sup> —Rb—O21 <sup>iii</sup>	102.61 (12)	O23—Cu—O24	73.0 (2)
O12 <sup>iii</sup> —Rb—O21 <sup>iii</sup>	78.36 (14)	O11 <sup>ii</sup> —Cu—O11 <sup>vi</sup>	84.8 (2)
O13 <sup>i</sup> —Rb—O14 <sup>iv</sup>	54.85 (14)	O21 <sup>ii</sup> —Cu—O11 <sup>vi</sup>	112.0 (2)
O21 <sup>ii</sup> —Rb—O14 <sup>iv</sup>	93.87 (14)	O23—Cu—O11 <sup>vi</sup>	93.67 (19)
O12 <sup>iii</sup> —Rb—O14 <sup>iv</sup>	89.52 (14)	O24—Cu—O11 <sup>vi</sup>	100.20 (19)
O21 <sup>iii</sup> —Rb—O14 <sup>iv</sup>	86.08 (14)	O14 <sup>vii</sup> —Fe—O13	88.7 (2)
O13 <sup>i</sup> —Rb—O12 <sup>v</sup>	48.09 (13)	O14 <sup>vii</sup> —Fe—O12 <sup>vi</sup>	90.8 (2)
O21 <sup>ii</sup> —Rb—O12 <sup>v</sup>	68.83 (13)	O13—Fe—O12 <sup>vi</sup>	92.7 (2)
O12 <sup>iii</sup> —Rb—O12 <sup>v</sup>	109.70 (11)	O14 <sup>vii</sup> —Fe—O22 <sup>vi</sup>	176.0 (2)
O21 <sup>iii</sup> —Rb—O12 <sup>v</sup>	168.12 (14)	O13—Fe—O22 <sup>vi</sup>	90.5 (2)
O14 <sup>iv</sup> —Rb—O12 <sup>v</sup>	102.37 (13)	O12 <sup>vi</sup> —Fe—O22 <sup>vi</sup>	85.3 (2)
O13 <sup>i</sup> —Rb—O23	121.31 (14)	O14 <sup>vii</sup> —Fe—O24 <sup>vii</sup>	92.6 (2)
O21 <sup>ii</sup> —Rb—O23	56.71 (14)	O13—Fe—O24 <sup>vii</sup>	172.8 (2)
O12 <sup>iii</sup> —Rb—O23	123.04 (13)	O12 <sup>vi</sup> —Fe—O24 <sup>vii</sup>	94.4 (2)
O21 <sup>iii</sup> —Rb—O23	49.30 (14)	O22 <sup>vi</sup> —Fe—O24 <sup>vii</sup>	88.73 (19)
O14 <sup>iv</sup> —Rb—O23	105.24 (13)	O14 <sup>vii</sup> —Fe—O23 <sup>viii</sup>	91.5 (2)
O12 <sup>v</sup> —Rb—O23	119.56 (13)	O13—Fe—O23 <sup>viii</sup>	85.59 (19)
O13 <sup>i</sup> —Rb—O11 <sup>iii</sup>	158.60 (14)	O12 <sup>vi</sup> —Fe—O23 <sup>viii</sup>	177.11 (19)
O21 <sup>ii</sup> —Rb—O11 <sup>iii</sup>	129.19 (14)	O22 <sup>vi</sup> —Fe—O23 <sup>viii</sup>	92.38 (19)
O12 <sup>iii</sup> —Rb—O11 <sup>iii</sup>	48.65 (13)	O24 <sup>vii</sup> —Fe—O23 <sup>viii</sup>	87.29 (19)
O21 <sup>iii</sup> —Rb—O11 <sup>iii</sup>	55.53 (14)	O13 <sup>ix</sup> —P1—O14 <sup>x</sup>	111.4 (3)
O14 <sup>iv</sup> —Rb—O11 <sup>iii</sup>	124.74 (13)	O13 <sup>ix</sup> —P1—O12 <sup>vii</sup>	106.2 (3)
O12 <sup>v</sup> —Rb—O11 <sup>iii</sup>	122.91 (13)	O14 <sup>x</sup> —P1—O12 <sup>vii</sup>	112.1 (3)
O23—Rb—O11 <sup>iii</sup>	80.05 (13)	O13 <sup>ix</sup> —P1—O11 <sup>vii</sup>	108.3 (3)
O13 <sup>i</sup> —Rb—O22 <sup>v</sup>	98.03 (14)	O14 <sup>x</sup> —P1—O11 <sup>vii</sup>	110.3 (3)
O21 <sup>ii</sup> —Rb—O22 <sup>v</sup>	72.07 (14)	O12 <sup>vii</sup> —P1—O11 <sup>vii</sup>	108.4 (3)
O12 <sup>iii</sup> —Rb—O22 <sup>v</sup>	104.52 (14)	O22—P2—O21 <sup>iii</sup>	112.5 (3)
O21 <sup>iii</sup> —Rb—O22 <sup>v</sup>	119.17 (14)	O22—P2—O24	111.3 (3)
O14 <sup>iv</sup> —Rb—O22 <sup>v</sup>	152.82 (13)	O21 <sup>iii</sup> —P2—O24	110.7 (3)
O12 <sup>v</sup> —Rb—O22 <sup>v</sup>	51.19 (13)	O22—P2—O23	113.0 (3)
O23—Rb—O22 <sup>v</sup>	86.70 (13)	O21 <sup>iii</sup> —P2—O23	109.4 (3)
O11 <sup>iii</sup> —Rb—O22 <sup>v</sup>	80.87 (13)	O24—P2—O23	99.3 (3)
O11 <sup>ii</sup> —Cu—O21 <sup>ii</sup>	95.2 (2)		

Symmetry codes: (i)  $-x+1, -y, -z+2$ ; (ii)  $x, y, z+1$ ; (iii)  $x-1/2, -y-1/2, z+1/2$ ; (iv)  $-x, -y, -z+2$ ; (v)  $-x+1/2, y-1/2, -z+3/2$ ; (vi)  $-x+1, -y, -z+1$ ; (vii)  $x+1, y, z$ ; (viii)  $-x+3/2, y+1/2, -z+3/2$ ; (ix)  $x+1/2, -y+1/2, z-1/2$ ; (x)  $x+1, y, z-1$ .