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$K_2[Fe^{II}_3(P_2O_7)_2(H_2O)_2]$

Juan Yang, Xin Zhang, Biao Liu, Wei Sun and Ya-Xi Huang*

Department of Materials Science and Engineering, College of Materials, Xiamen University, Xiamen 361005, Fujian Province, People's Republic of China
Correspondence e-mail: yaxihuang@xmu.edu.cn

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Key indicators: single-crystal X-ray study; *T* = 173 K; mean σ(P–O) = 0.003 Å; *R* factor = 0.032; *wR* factor = 0.074; data-to-parameter ratio = 13.0.

The title compound, dipotassium diaquabis(diphosphato)triferrate(II), $K_2[Fe^{II}_3(P_2O_7)_2(H_2O)_2]$, was synthesized under solvothermal conditions. The crystal structure is isotypic with its Co analogue. In the structure, there are two crystallographically distinct Fe positions; one lies on an inversion center, the other on a general position. The first Fe^{2+} cation adopts a regular octahedral coordination with six O atoms, whereas the other is coordinated by five O atoms and a water molecule. The $[FeO_6]$ octahedron shares its *trans*-edges with an adjacent $[FeO_5(H_2O)]$ octahedron; in turn, the $[FeO_5(H_2O)]$ octahedron shares skew-edges with a neighbouring $[FeO_6]$ octahedron and an $[FeO_5(H_2O)]$ octahedron, resulting in a zigzag octahedral chain running along [001]. The zigzag chains are linked to each other by the P_2O_7 diphosphate groups, leading to a corrugated iron diphosphate layer, $[Fe_3(P_2O_7)_2(H_2O)_2]^{2-}$, parallel to (100). The interlayer space is occupied by K^+ cations, which adopt an eight-coordination to seven O atoms and one water molecule from a neighbouring iron diphosphate layer. Thus, the K^+ ions not only compensate the negative charge of the layer but also link the layers into a network structure.

Related literature

For background to iron compounds, see: Mi *et al.* (2004); Huang *et al.* (2012). For related structures, see: Chippindale *et al.* (2003) for $(NH_4)_2[Mn_3(P_2O_7)_2(H_2O)_2]$; Lightfoot *et al.* (1990) for $K_2[Co_3(P_2O_7)_2(H_2O)_2]$; Liu *et al.* (2012) for $(NH_4)_2[Fe^{II}_3(P_2O_7(H_2O)_2)_2]$; Liu *et al.* (2004) for $Na(NH_4)[Ni_3(P_2O_7)_2(H_2O)_2]$; Wei *et al.* (2010) for $(NH_4)_2[Ni_3(P_2O_7)_2(H_2O)_2]$. For bond-valence calculations, see: Brown (2002).

Experimental

Crystal data

$K_2[Fe_3(P_2O_7)_2(H_2O)_2]$
M_r = 629.66
Monoclinic, $P2_1/c$
a = 9.1517 (16) Å
b = 8.1737 (15) Å
c = 9.3147 (17) Å
β = 98.860 (3)°
V = 688.5 (2) Å^3
Z = 2
Mo *K*α radiation
μ = 4.28 mm^{-1}
T = 173 K
0.09 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SMART*; Bruker, 2001)
T_{min} = 0.687, T_{max} = 0.710
4006 measured reflections
1596 independent reflections
1460 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.074
S = 1.07
1596 reflections
123 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H1···O3^{i}	0.82 (5)	1.90 (5)	2.716 (4)	171 (5)
O8—H2···O7^{ii}	0.76 (4)	1.95 (4)	2.696 (4)	164 (4)

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005) and *ATOMS* (Dowty, 2004); software used to prepare material for publication: *SHELXL97* and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2202).

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supporting information

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$K_2[Fe^{II}_3(P_2O_7)_2(H_2O)_2]$

Juan Yang, Xin Zhang, Biao Liu, Wei Sun and Ya-Xi Huang

S1. Comment

A class of layered transition metal diphosphates with the general formula of $A_2M_3(P_2O_7)_2(H_2O)_2$ (A = K or NH_4, M = transition metal (II)) has recently attracted much attention. Since the first publication of $K_2Co_3(P_2O_7)_2(H_2O)_2$ (Lightfoot *et al.*, 1990) in 1990, a few examples of ammonium substituted compounds, $(NH_4)_2M_3(P_2O_7)_2(H_2O)_2$ (M = Mn^{2+}, Ni^{2+}) (Chippindale *et al.*, 2003; Wei *et al.*, 2010), have been synthesized by using either solvothermal or ionothermal method. Their magnetic and ion exchange behaviors have also been discussed. Besides, a compound with mixed cations, $Na(NH_4)[Ni_3(P_2O_7)_2(H_2O)_2]$, has also been reported (Liu *et al.*, 2004). Although compounds incorporating with Mn^{2+}, Co^{2+}, and Ni^{2+} have been known, as a very close relationship to these elements, Fe^{2+} was not yet found in this class of compounds until very recently an ammonium iron diphosphate, $(NH_4)_2[Fe_3^{II}(P_2O_7)_2(H_2O)_2]$, was reported by our group which was synthesized by using iron powder as iron source and applying the weak reductive agent pyridine as solvent (Liu *et al.*, 2012). During our systematically investigation on iron compounds (Mi *et al.*, 2004; Huang *et al.*, 2012), we obtained a new member in this class of compounds with the formula of $K_2[Fe^{II}_3(P_2O_7)_2(H_2O)_2]$.

In the crystal structure of the title compound, there are two crystallographically distinct iron sites, one potassium, and two independent phosphorus (shown in Figure 1). Fe(2) lies on an inversion center (2*a*, -1) while Fe(1) on a general position (4*e*, 1). Fe(2) adopts a regular octahedral coordination with six oxygen atoms, whereas Fe(1) coordinates to five oxygen atoms and a water molecule in the form of $Fe(1)O_5(OH_2)$. Each $Fe(2)O_6$ octahedron shares trans-edges with adjacent $Fe(1)O_5(OH_2)$ octahedra, and in turn, $Fe(1)O_5(OH_2)$ octahedron shares skew-edges with the neighboring $Fe(2)O_6$ and $Fe(1)O_5(OH_2)$ octahedra, which finally leads to the formation of FeO_6-based zigzag chains parallel to [010] (see Figure 2a). Two independent phosphorus atoms adopt a four-fold coordination with one long P–O bond and three general P–O bonds which are often found in diphosphates. Every two PO_4 tetrahedra share the common O-vertex (O2) to constitute a P_2O_7 group which acts as a bidentate ligand to link FeO_6-based chains along [001], resulting in a undulating iron diphosphate layer, $[Fe_3(P_2O_7)_2(H_2O)_2]^{2-}$, parallel to the (100) (see Figure 2b). The layers stack along the *a*-axis direction in AAA fashion with the potassium atoms locating at the interlayer space (see Figure 2c). The potassium ion is 8-coordinated with seven oxygens and a water molecule from the neighbouring layers with one long bond and seven relatively short bonds (see Figure 2d). Bond-valence sum calculations (Brown, 2002) suggests both two iron atoms are in the 2+ valence state (Cald.: 2.008 v.u. for Fe(1) and 2.112 v.u. for Fe(2) and the potassium should be +1 oxidation (Cald.: 1.054 v.u. for K1). Comparing the crystal structure of NH_4- and K-compounds, both of them possess the same conformation of iron diphosphate layer, however, the interlayer distance of K-compound is relatively smaller than that of NH_4-compound identified by the *a*-value (9.1517 (16) Å for KFe-compound and 9.4131 (17) Å for NH_4Fe-compound) which is consistent with the ion radius of K^+ and NH_4^+.

S2. Experimental

The title compound has been synthesized under solvothermal condition. In a typical synthesis, 1 mmol Fe powder and 2.5 mmol KH_2PO_4 were added into the mixed solvent of 2 mL pyridine and 2 mL 1,2-propanediol. Then, 2 mL H_3PO_4 (85%) was dropped into the above solution to adjust pH value to 6-7. After stirred for 5 minutes, the mixture was transferred into a 15 mL Teflon-lined stainless steel autoclave which was heated at 436 K for 7 days and then was cooled down to room temperature. The final product, colourless block-like crystals, was washed with distilled water and filtrated by vacuum. The powder X-ray diffraction of the sample showed that it is isotypic to our recently reported compound $[NH_4]_2[Fe^{II}_3(H_2O)_2(P_2O_7)_2]$.

S3. Refinement

The hydrogen atoms bonded to water (O8) were located from the difference Fourier maps and refined without applying any constraints on the distance of O–H and the displacement parameter of H atoms.

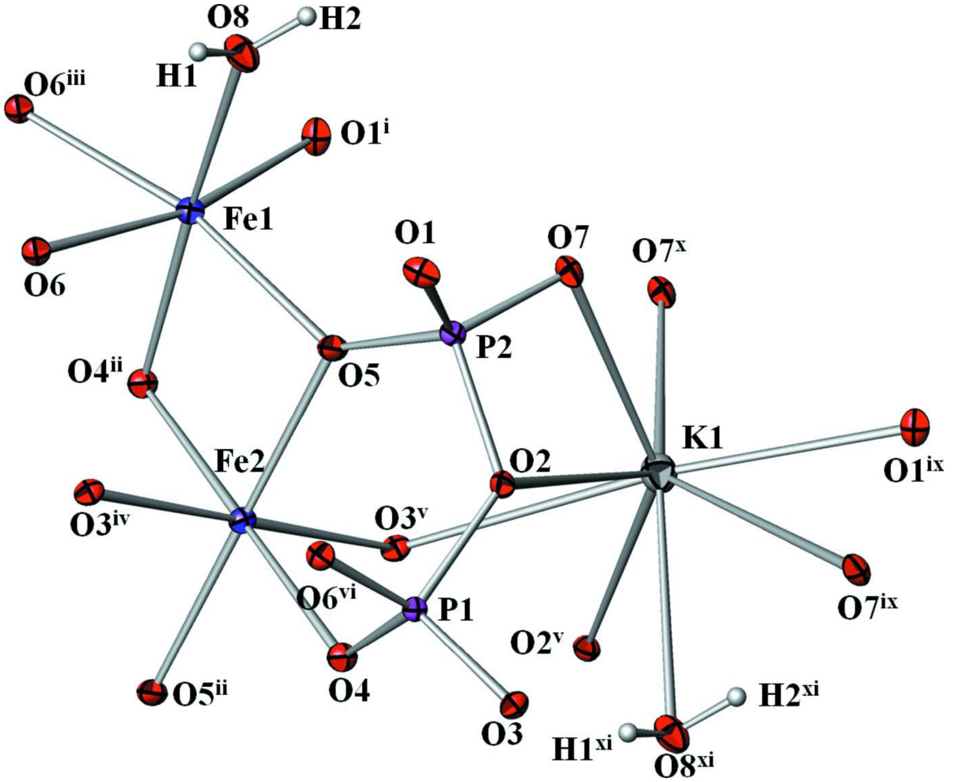

Figure 1

Structural unit of $K_2[Fe^{II}_3(P_2O_7)_2(H_2O)_2]$, showing the coordination environments of Fe, K, and P atoms. Thermal ellipsoids were drawn at the 50% probability level. Symmetry codes: (i) *x*, –*y*+3/2, *z*+1/2; (ii) –*x*+2, –*y*+1, –*z*+1; (iii) –*x*+2,–*y*+2, –*z*+1; (iv) –*x*+2, *y*+1/2, –*z*+1/2; (v) *x*, –*y*+1/2, *z*+1/2; (vi) –*x*+2, *y*–1/2, –*z*+1/2; (vii) *x*, –*y*+1/2, *z*–1/2; (viii) –*x*+1, *y*+1/2, –*z*+1/2; (ix) *x*+1, *y*–1/2, –*z*+1/2; (x) –*x*+1, –*y*+1, –*z*+1; (xi) *x*, *y*–1, *z*; (xii) *x*, –*y*+3/2, *z*–1/2; (xiii) *x*, *y*+1, *z*.

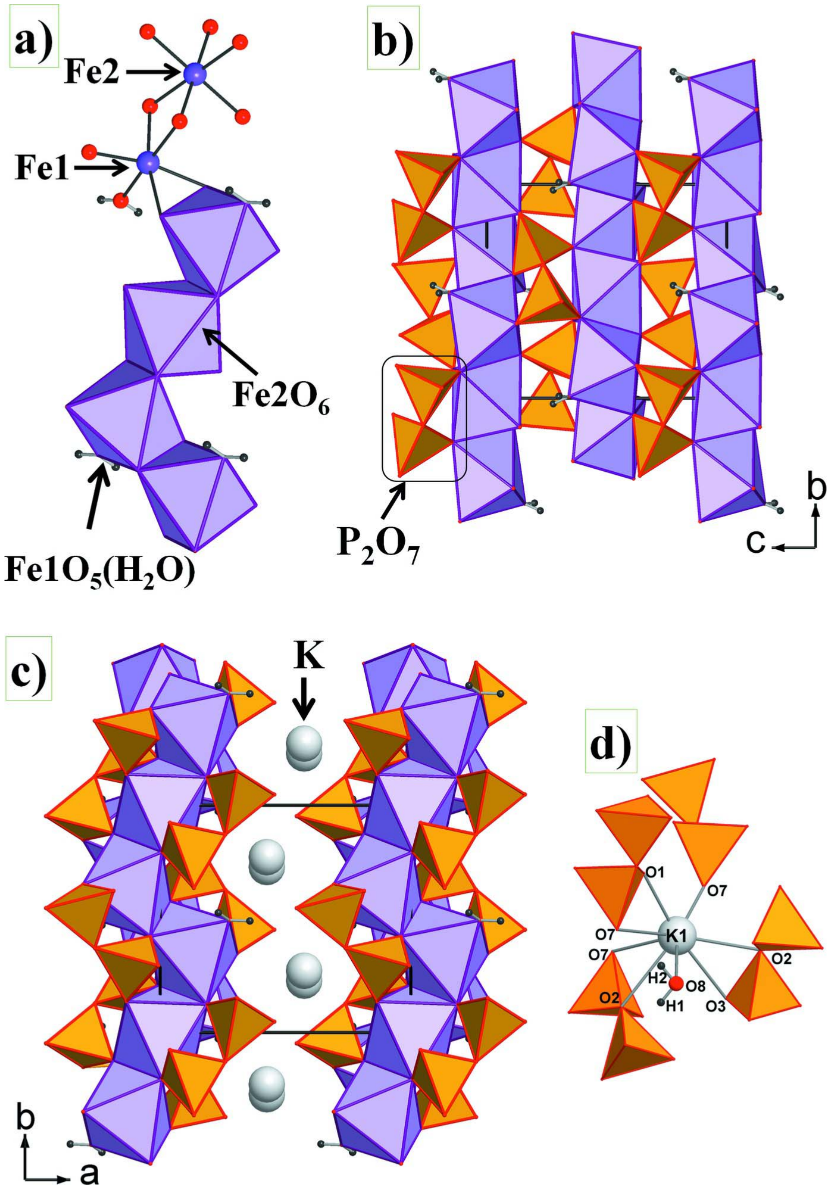

Figure 2

Polyhedral presentation of the crystal structure of $K_2[Fe^{II}_3(P_2O_7)_2(H_2O)_2]$, (a) zigzag edge-sharing iron octahedral chain is built from FeO_6 and $FeO_5(H_2O)$ octahedra by sharing their trans- or skew-edges running along [010]; (b) P_2O_7 groups act as a bidentate ligand to link FeO_6-based chains along [001] to form a corrugated iron diphosphate layer $[Fe_3(P_2O_7)_2(H_2O)_2]^{2-}$; (c) the iron diphosphate layers stack along [100] in AAA fashion with the potassium atoms locating at the interlayer space; (d) the K atom is 8-coordinated to seven oxygen atoms and a H_2O molecule coming from adjacent iron diphosphate layers to form an irregular polyhedron. Purple octahedron: FeO_6, orange tetrahedron: PO_4, light grey sphere: K atom, dark grey sphere: H atom.

Dipotassium diaquabis(diphosphato)triferrate(II)

Crystal data

$K_2[Fe_3(P_2O_7)_2(H_2O)_2]$	$F(000) = 616$
$M_r = 629.66$	$D_x = 3.037$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4006 reflections
$a = 9.1517$ (16) Å	$\theta = 2.3$–$28.3°$
$b = 8.1737$ (15) Å	$\mu = 4.28$ mm^{-1}
$c = 9.3147$ (17) Å	$T = 173$ K
$\beta = 98.860$ (3)°	Block, colourless
$V = 688.5$ (2) Å^3	0.09 × 0.09 × 0.08 mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	4006 measured reflections
Radiation source: fine-focus sealed tube	1596 independent reflections
Graphite monochromator	1460 reflections with $I > 2\sigma(I)$
1265 images,φ=0, 90, 180 degree, and $\Delta\omega$=0.3 degree, χ= 54.74 degree scans	$R_{\rm int} = 0.027$
Absorption correction: multi-scan (*SMART*; Bruker, 2001)	$\theta_{\rm max} = 28.3°$, $\theta_{\rm min} = 2.3°$
$T_{\rm min} = 0.687$, $T_{\rm max} = 0.710$	$h = -11 \rightarrow 12$
	$k = -10 \rightarrow 10$
	$l = -12 \rightarrow 8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.032$	All H-atom parameters refined
$wR(F^2) = 0.074$	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 1.280P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\rm max} < 0.001$
1596 reflections	$\Delta\rho_{\rm max} = 0.57$ e Å^{-3}
123 parameters	$\Delta\rho_{\rm min} = -0.66$ e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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 (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Fe1	0.86324 (5)	0.85888 (6)	0.50352 (5)	0.00807 (13)
Fe2	1.0000	0.5000	0.5000	0.00754 (16)
P1	0.89966 (9)	0.30110 (10)	0.20949 (9)	0.00652 (18)

P2	0.69498 (9)	0.56235 (10)	0.26759 (9)	0.00744 (18)
K1	0.57440 (8)	0.27162 (10)	0.48169 (9)	0.01682 (19)
O1	0.6935 (3)	0.6515 (3)	0.1248 (3)	0.0111 (5)
O2	0.7397 (2)	0.3719 (3)	0.2360 (2)	0.0090 (5)
O3	0.8654 (2)	0.1362 (3)	0.1376 (2)	0.0084 (5)
O4	0.9925 (2)	0.2944 (3)	0.3595 (2)	0.0094 (5)
O5	0.8140 (2)	0.6235 (3)	0.3887 (3)	0.0103 (5)
O6	1.0389 (2)	0.9230 (3)	0.3891 (2)	0.0089 (5)
O7	0.5448 (2)	0.5477 (3)	0.3129 (3)	0.0120 (5)
O8	0.7250 (3)	0.9942 (3)	0.3420 (3)	0.0146 (5)
H1	0.770 (5)	1.027 (6)	0.278 (5)	0.023 (13)*
H2	0.645 (5)	0.991 (5)	0.302 (5)	0.013 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0087 (2)	0.0085 (2)	0.0070 (2)	0.00054 (17)	0.00131 (17)	0.00043 (17)
Fe2	0.0088 (3)	0.0075 (3)	0.0061 (3)	0.0003 (2)	0.0004 (2)	0.0000 (2)
P1	0.0070 (4)	0.0068 (4)	0.0058 (4)	0.0001 (3)	0.0008 (3)	−0.0002 (3)
P2	0.0072 (4)	0.0081 (4)	0.0069 (4)	0.0007 (3)	0.0007 (3)	−0.0007 (3)
K1	0.0152 (4)	0.0183 (4)	0.0164 (4)	−0.0009 (3)	0.0007 (3)	0.0013 (3)
O1	0.0113 (11)	0.0142 (12)	0.0083 (11)	0.0030 (9)	0.0029 (9)	0.0019 (9)
O2	0.0072 (11)	0.0086 (11)	0.0113 (12)	−0.0005 (8)	0.0015 (9)	−0.0025 (9)
O3	0.0105 (11)	0.0075 (11)	0.0071 (11)	−0.0004 (8)	0.0014 (9)	−0.0016 (9)
O4	0.0103 (11)	0.0096 (11)	0.0079 (11)	0.0005 (9)	0.0002 (9)	−0.0006 (9)
O5	0.0096 (11)	0.0089 (11)	0.0114 (12)	0.0017 (9)	−0.0014 (9)	−0.0020 (9)
O6	0.0091 (11)	0.0094 (12)	0.0082 (11)	−0.0001 (9)	0.0021 (9)	−0.0014 (9)
O7	0.0072 (11)	0.0134 (12)	0.0158 (13)	−0.0004 (9)	0.0028 (9)	−0.0008 (10)
O8	0.0097 (13)	0.0200 (14)	0.0140 (14)	0.0006 (10)	0.0009 (11)	0.0061 (10)

Geometric parameters (Å, º)

Fe1—O1^{i}	2.058 (2)	P1—O2	1.628 (2)
Fe1—O4^{ii}	2.103 (2)	P2—O7	1.503 (2)
Fe1—O8	2.121 (3)	P2—O1	1.515 (2)
Fe1—O6	2.127 (2)	P2—O5	1.527 (2)
Fe1—O6^{iii}	2.169 (2)	P2—O2	1.648 (2)
Fe1—O5	2.214 (2)	K1—O1^{vii}	2.685 (2)
Fe2—O5^{ii}	2.109 (2)	K1—O7	2.740 (3)
Fe2—O5	2.109 (2)	K1—O7^{viii}	2.771 (3)
Fe2—O4^{ii}	2.124 (2)	K1—O2^{iv}	2.859 (2)
Fe2—O4	2.124 (2)	K1—O3^{iv}	2.929 (2)
Fe2—O3^{iv}	2.210 (2)	K1—O2	3.043 (2)
Fe2—O3^{v}	2.210 (2)	K1—O8^{ix}	3.047 (3)
P1—O3	1.516 (2)	K1—O7^{vii}	3.339 (3)
P1—O6^{vi}	1.520 (2)	O8—H1	0.82 (5)
P1—O4	1.521 (2)	O8—H2	0.76 (4)

O1^{i}—Fe1—O4^{ii}	95.66 (9)	O1^{vii}—K1—O7	94.87 (7)
O1^{i}—Fe1—O8	89.59 (10)	O1^{vii}—K1—O7^{viii}	90.91 (7)
O4^{ii}—Fe1—O8	172.30 (10)	O7—K1—O7^{viii}	86.72 (8)
O1^{i}—Fe1—O6	167.91 (9)	O1^{vii}—K1—O2^{iv}	119.53 (7)
O4^{ii}—Fe1—O6	89.92 (9)	O7—K1—O2^{iv}	143.75 (7)
O8—Fe1—O6	86.00 (10)	O7^{viii}—K1—O2^{iv}	81.99 (7)
O1^{i}—Fe1—O6^{iii}	94.22 (9)	O1^{vii}—K1—O3^{iv}	170.43 (7)
O4^{ii}—Fe1—O6^{iii}	91.94 (9)	O7—K1—O3^{iv}	94.29 (7)
O8—Fe1—O6^{iii}	93.29 (10)	O7^{viii}—K1—O3^{iv}	86.85 (7)
O6—Fe1—O6^{iii}	74.83 (10)	O2^{iv}—K1—O3^{iv}	50.94 (6)
O1^{i}—Fe1—O5	96.59 (9)	O1^{vii}—K1—O2	110.62 (7)
O4^{ii}—Fe1—O5	80.63 (9)	O7—K1—O2	50.46 (7)
O8—Fe1—O5	93.20 (10)	O7^{viii}—K1—O2	132.06 (7)
O6—Fe1—O5	94.90 (9)	O2^{iv}—K1—O2	118.20 (8)
O6^{iii}—Fe1—O5	167.42 (9)	O3^{iv}—K1—O2	77.53 (6)
O5^{ii}—Fe2—O5	180.0	O1^{vii}—K1—O8^{ix}	91.01 (8)
O5^{ii}—Fe2—O4^{ii}	97.39 (9)	O7—K1—O8^{ix}	112.28 (8)
O5—Fe2—O4^{ii}	82.61 (9)	O7^{viii}—K1—O8^{ix}	160.66 (8)
O5^{ii}—Fe2—O4	82.61 (9)	O2^{iv}—K1—O8^{ix}	80.33 (7)
O5—Fe2—O4	97.39 (9)	O3^{iv}—K1—O8^{ix}	88.08 (7)
O4^{ii}—Fe2—O4	180.0	O2—K1—O8^{ix}	64.50 (7)
O5^{ii}—Fe2—O3^{iv}	87.34 (9)	O1^{vii}—K1—O7^{vii}	48.08 (6)
O5—Fe2—O3^{iv}	92.66 (9)	O7—K1—O7^{vii}	89.37 (3)
O4^{ii}—Fe2—O3^{iv}	90.54 (9)	O7^{viii}—K1—O7^{vii}	138.28 (9)
O4—Fe2—O3^{iv}	89.46 (9)	O2^{iv}—K1—O7^{vii}	121.35 (7)
O5^{ii}—Fe2—O3^{v}	92.66 (9)	O3^{iv}—K1—O7^{vii}	134.87 (7)
O5—Fe2—O3^{v}	87.34 (9)	O2—K1—O7^{vii}	70.56 (6)
O4^{ii}—Fe2—O3^{v}	89.46 (9)	O8^{ix}—K1—O7^{vii}	49.70 (7)
O4—Fe2—O3^{v}	90.54 (9)	P2—O1—Fe1^{x}	123.83 (14)
O3^{iv}—Fe2—O3^{v}	180.0	P1—O2—P2	128.09 (15)
O3—P1—O6^{vi}	112.74 (13)	P1—O3—Fe2^{vi}	127.45 (13)
O3—P1—O4	114.99 (13)	P1—O4—Fe1^{ii}	142.06 (15)
O6^{vi}—P1—O4	111.86 (13)	P1—O4—Fe2	119.89 (13)
O3—P1—O2	104.68 (12)	Fe1^{ii}—O4—Fe2	98.04 (9)
O6^{vi}—P1—O2	106.47 (13)	P2—O5—Fe2	129.55 (14)
O4—P1—O2	105.14 (13)	P2—O5—Fe1	135.27 (14)
O7—P2—O1	113.58 (13)	Fe2—O5—Fe1	95.14 (9)
O7—P2—O5	113.47 (14)	P1^{v}—O6—Fe1	121.29 (13)
O1—P2—O5	113.57 (14)	P1^{v}—O6—Fe1^{iii}	130.73 (13)
O7—P2—O2	103.75 (13)	Fe1—O6—Fe1^{iii}	105.17 (10)
O1—P2—O2	105.48 (13)	H1—O8—H2	102 (4)
O5—P2—O2	105.80 (13)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H1···O3^{xi}	0.82 (5)	1.90 (5)	2.716 (4)	171 (5)
O8—H2···O7^{xii}	0.76 (4)	1.95 (4)	2.696 (4)	164 (4)

Symmetry codes: (xi) *x*, *y*+1, *z*; (xii) −*x*+1, *y*+1/2, −*z*+1/2.