Crystal structures of two alkaline earth (*M* = Ba and Sr) dimanganese(II) iron(III) tris(orthophosphates)

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Two new orthophosphates, BaMn$_2$Fe(PO$_4$)$_3$ [barium dimanganese(II) iron(III) tris(orthophosphate)] and SrMn$_2$Fe(PO$_4$)$_3$ [strontium dimanganese(II) iron(III) tris(orthophosphate)], were synthesized by solid-state reactions. They are isotypic and crystallize in the orthorhombic system with space group type *Pbcn*. Their crystal structures comprise infinite zigzag chains of edge-sharing FeO$_6$ octahedra (point group symmetry .2.) and Mn$_2$O$_{10}$ double octahedra running parallel to [001], linked by two types of PO$_4$ tetrahedra. The so-formed three-dimensional framework delineates channels running along [001], in which the alkaline earth cations (site symmetry .2.) are located within a neighbourhood of eight O atoms.

1. Chemical context

Considerable attention has been devoted to the preparation of new inorganic materials with open-framework structures (Rao *et al.*, 2001; Bouzidi *et al.*, 2015) due to their structural diversity covering a wide range of chemical compositions (Zhou *et al.*, 2002). In particular, transition-metal-based open-framework phosphates represent a highly attractive class of materials in industrial processes. In fact, their special framework structures lead to interesting properties that depend not only on the inclusion guest in the pores, but also on the chosen transition metal (Durio *et al.*, 2002; López *et al.*, 2004; Férey *et al.*, 2005). Typical examples are ion-exchangers (Jignasa *et al.*, 2006; Kullberg & Clearfield, 1981) and compounds with special magnetic (Chouaibi *et al.*, 2001; Ferdov *et al.*, 2008) and catalytic properties (Weng *et al.*, 2009).

In this context, our group focuses on the synthesis and characterization of new transition-metal phosphates crystallizing either in alluaudite- (Moore, 1971) or α-CrPO$_4$-type structures (Attfield *et al.*, 1988). In attempts to obtain new compounds belonging to the latter structure type, we have synthesized and structurally characterized several new phosphates, including those with oxidation states of both +II and +III for manganese. These compounds have the general formula MMn^{III}Mn$_2$^{II}(PO$_4$)$_3$ (M = Pb, Sr, Ba) (Alhakmi *et al.*, 2013*a*,*b*; Assani *et al.*, 2013) and adopt the α-CrPO$_4$ structure type. Recently, the phosphates Na$_2$Co$_2$Fe(PO$_4$)$_3$ (Bouraima *et al.*, 2015) and Na$_{1.67}$Zn$_{1.67}$Fe$_{1.33}$(PO$_4$)$_3$ (Khmiyas *et al.*, 2015) with an alluaudite-like structure were also reported. As a continuation in this regard, we have now extended our investigations to the quaternary system MO/MnO/Fe$_2$O$_3$/P$_2$O$_5$, where M is a divalent cation. The present work deals with the synthesis and the crystal structures of two new isotypic alkaline earth manganese iron phosphates, namely,


Sr
Fe
Mn
P
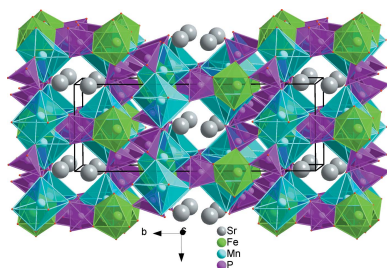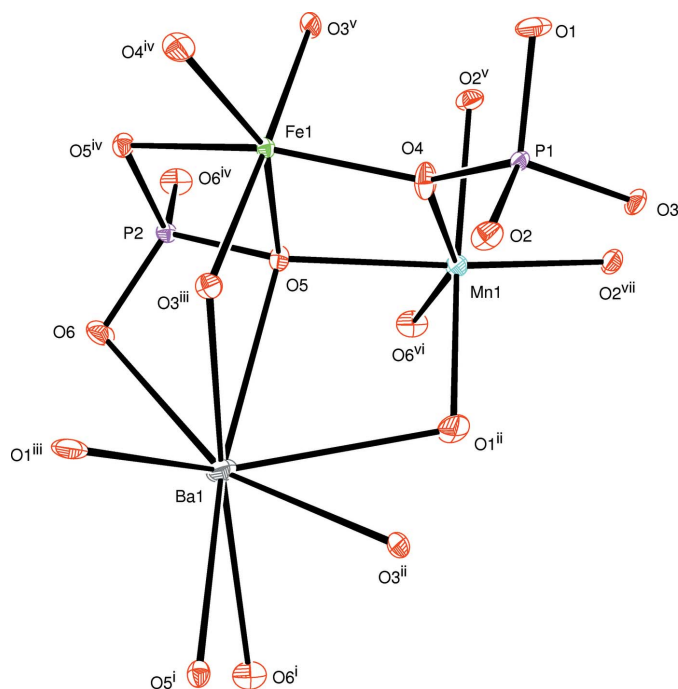
Figure 1
The principal building units in the structure of $BaMn_2Fe(PO_4)_3$. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) x, $-y + 1$, $z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}$, $-y + \frac{3}{2}$, $-z + 2$; (iii) x, y, $z + 1$; (iv) $-x + \frac{3}{2}$, $-y + \frac{3}{2}$, $-z + 1$; (v) $-x + 1$, y, $-z + \frac{3}{2}$; (vi) x, y, $z - 1$; (vii) $-x + 1$, y, $-z + \frac{1}{2}$; (viii) $x - \frac{1}{2}$, $-y + \frac{3}{2}$, $z - \frac{1}{2}$; (ix) $-x + 1$, $-y + 1$, $-z + 1$; (x) x, $-y + 1$, $z - \frac{1}{2}$; (xi) $-x + 2$, y, $-z + \frac{3}{2}$; (xii) $-x + 2$, $-y + 1$, $-z + 1$.]
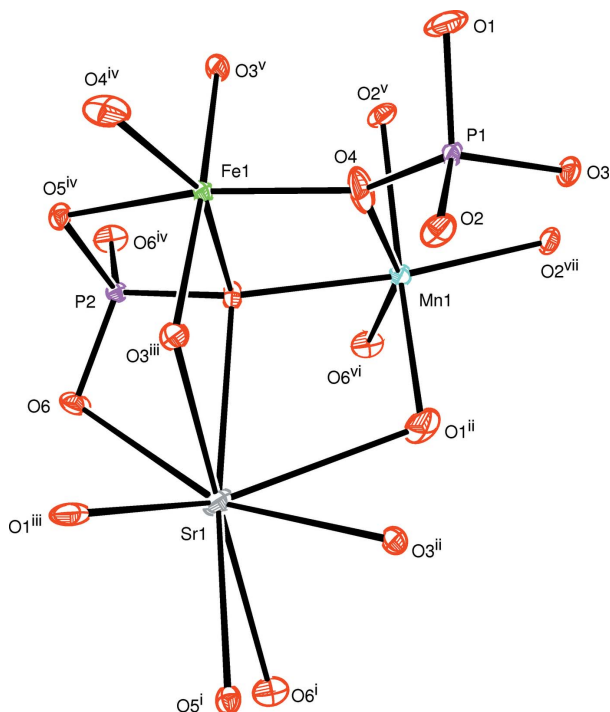
Figure 2
The principal building units in the structure of $SrMn_2Fe(PO_4)_3$. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) x, $-y + 1$, $z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}$, $-y + \frac{3}{2}$, $-z + 2$; (iii) x, y, $z + 1$; (iv) $-x + \frac{3}{2}$, $-y + \frac{3}{2}$, $-z + 1$; (v) $-x + 1$, y, $-z + \frac{3}{2}$; (vi) x, y, $z - 1$; (vii) $-x + 1$, y, $-z + \frac{1}{2}$; (viii) $x - \frac{1}{2}$, $-y + \frac{3}{2}$, $z - \frac{1}{2}$; (ix) $-x + 1$, $-y + 1$, $-z + 1$; (x) x, $-y + 1$, $z - \frac{1}{2}$; (xi) $-x + 2$, y, $-z + \frac{3}{2}$; (xii) $-x + 2$, $-y + 1$, $-z + 1$.]
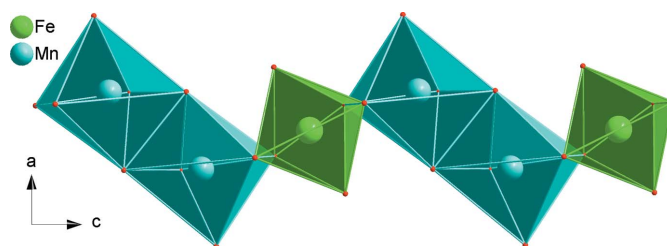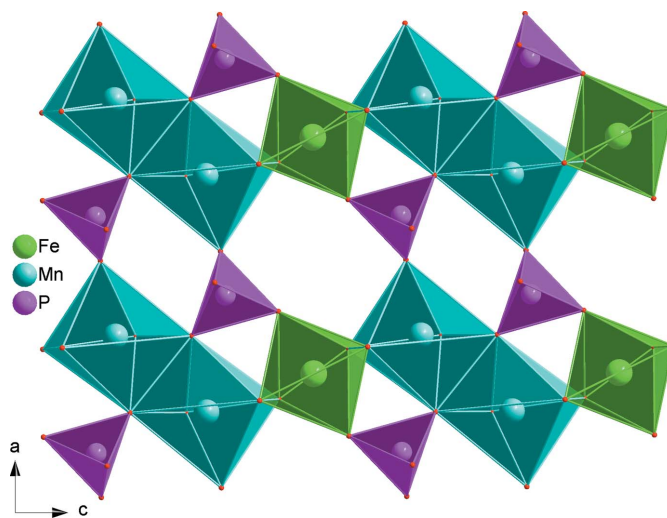

Figure 3
Edge-sharing $[FeO_6]$ octahedra and Mn_2O_{10} dimers forming an infinite zigzag chain running parallel to [001]. Data are from $BaMn_2Fe(PO_4)_3$.

$BaMn_2Fe(PO_4)_3$ and $SrMn_2Fe(PO_4)_3$. Their structures show a similarity with that of $AM_4(PO_4)_3$ phosphates where A is a monovalent cation and M a divalent cation (Daidouh *et al.*, 1999; Assaaoudi *et al.*, 2006).

2. Structural commentary

The principal building units in the crystal structures of both phosphates are distorted FeO_6 and MnO_6 octahedra, PO_4 tetrahedra and Ba^{2+} or Sr^{2+} cations as shown in Figs. 1 and 2. In each structure, two MnO_6 octahedra are linked together by a common edge to give a Mn_2O_{10} dimer to which FeO_6 octahedra (point group symmetry .2.) are alternately connected on both sides. In this way, infinite zigzag chains parallel to [001] are formed (Fig. 3). Adjacent chains are linked together by sharing corners with two types of PO_4 tetrahedra, forming a layer-like arrangement parallel to (010) as shown in Fig. 4. Such layers are stacked along [010] to form a three-dimensional framework (Fig. 5) with two types of channels running parallel to [001] in which the alkaline earth cations are located on a twofold rotation axis. They are coordinated by eight oxygen atoms (Figs. 1 and 6), with bond lengths ranging from 2.6803 (10) to 2.8722 (11) Å for the BaO_8 polyhedron and of 2.6020 (9) to 2.7358 (11) Å for the SrO_8 polyhedron.

Figure 4
A layer perpendicular to (010), resulting from the connection of metal oxide chains through PO_4 tetrahedra. Data are from $BaMn_2Fe(PO_4)_3$.

Table 1
Experimental details.

|	(I)	(II)
Crystal data		
Chemical formula	$BaMn_2Fe(PO_4)_3$	$SrMn_2Fe(PO_4)_3$
M_r	587.98	538.25
Crystal system, space group	Orthorhombic, *Pbcn*	Orthorhombic, *Pbcn*
Temperature (K)	296	296
a, b, c (Å)	6.5899 (2), 17.6467 (4), 8.5106 (2)	6.4304 (3), 17.8462 (7), 8.4906 (3)
V (Å^3)	989.70 (4)	974.37 (7)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	8.41	10.00
Crystal size (mm)	$0.32 \times 0.25 \times 0.22$	$0.30 \times 0.27 \times 0.23$
Data collection		
Diffractometer	Bruker X8 APEX	Bruker X8 APEX
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.596, 0.748	0.404, 0.748
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29422, 3088, 2731	23889, 2843, 2564
R_{int}	0.033	0.031
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.907	0.887
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.044, 1.05	0.021, 0.048, 1.08
No. of reflections	3088	2843
No. of parameters	89	89
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.29, −1.11	1.19, −0.81

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

Bond-valence-sum calculations (Brown & Altermatt, 1985) are in good agreement with the expected values for alkaline earth, manganese(II) and iron(III) cations and the phosphorus(V) atom. $BaMn_2Fe(PO_4)_3$ (values in valence units): Ba^{2+} 2.10; Mn^{2+} 2.00; Fe^{3+} 3.12; P^V 4.94. $SrMn_2Fe(PO_4)_3$: Sr^{2+} 1.80; Mn^{2+} 2.07; Fe^{3+} 3.18; P^V 5.00.

3. Database survey

A comparison between the structures of the title compounds and those of other phosphates such as the $AM_4(PO_4)_3$ compounds (A = monovalent cation and M = divalent cation) (Im *et al.*, 2014), reveals that all these compounds crystallize with orthorhombic symmetry and nearly the same unit-cell parameters despite the differences between their chemical formulae and space groups. In order to give an illustrative picture of the similarity between these two formula types, we can write the general formula of $AM_4(PO_4)_3$ compounds as follows: $M'^{2+}(A^+M^{2+})M_2^{2+}(PO_4)_3$ and that of the title compounds as $M'^{2+}Fe^{3+}Mn_2^{2+}(PO_4)_3$. The principal structures of the title compounds and that of the $AM_4(PO_4)_3$ compounds
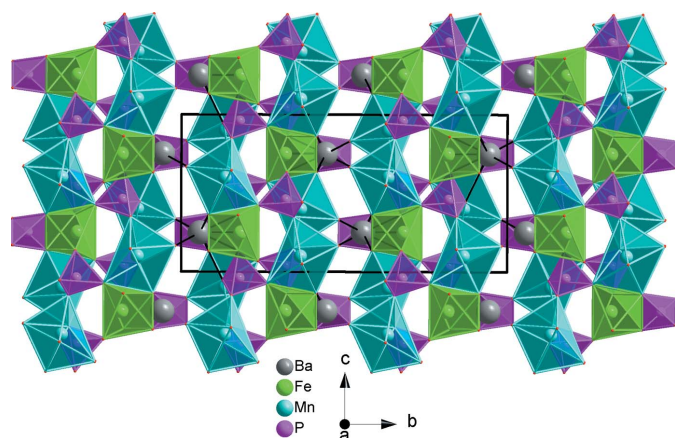
Figure 5
A view of stacked layers along [010]. Data are from $BaMn_2Fe(PO_4)_3$.
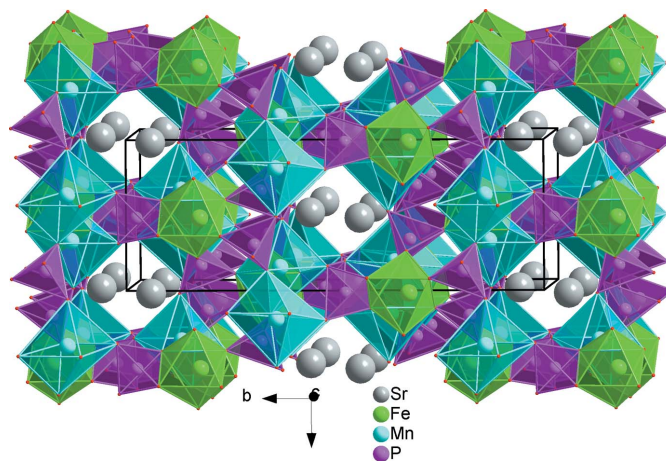
Figure 6
Polyhedral representation of the $BaMn_2Fe(PO_4)_3$ structure showing Ba^{2+} cations situated in channels running along [001].

are formed by stacking of the same infinite zigzag chains of edge-sharing octahedra. Furthermore, these structures are characterized by the presence of two types of channels in which the large cations are located.

4. Synthesis and crystallization

Single crystals of the title compounds were isolated as a result of solid-state reactions. Stoichiometric amounts of alkaline earth (M = Ba, Sr), manganese, iron and phosphate precursors in a molar ratio M:Mn:Fe:P = 1:2:1:3, were dissolved in 40 ml water that was placed into a 100 ml capacity pyrex glass beaker. The mixture was stirred at room temperature for 20 h and was evaporated under stirring at 363 K until dryness. The obtained black powder was ground in an agate mortar and pre-heated at 573 K in a platinum crucible for 24 h to eliminate gaseous materials. Subsequently, the resulting residue was reground and melted for 30 min at 1293 K, followed by slow cooling down to 1093 K at a rate 5K h^{-1} and a rapid cooling to room temperature by switching off the furnace. In the case of the BaO–MnO–Fe_2O_3–P_2O_5 system, the reaction product consisted of two types of crystals, *viz.* orange crystals of the title compound, $BaMn_2Fe(PO_4)_3$, and dark-violet crystals that were identified to be another new phase. In the case of the SrO–MnO–Fe_2O_3–P_2O_5 system, the reaction product contained dark-brown crystals corresponding to the title compound, $SrMn_2Fe(PO_4)_3$.

5. Refinement

Crystal data, data collection and structure refinement details for the two compounds are summarized in Table 1. For $BaMn_2Fe(PO_4)_3$, the maximum and minimum remaining electron densities are located 0.60 and 0.42 Å from atom Ba1. For $SrMn_2Fe(PO_4)_3$, they are 0.58 and 0.31 Å from Sr1.

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supporting information

Crystal structures of two alkaline earth (*M* = Ba and Sr) dimanganese(II) iron(III) tris(orthophosphates)

Ghaleb Alhakmi, Abderrazzak Assani, Mohamed Saadi and Lahcen El Ammari

Computing details

For both compounds, data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*). Molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006) for (I); *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) for (II). For both compounds, software used to prepare material for publication: *publCIF* (Westrip, 2010).

(I) Barium dimanganese(II) iron(III) tris(orthophosphate)

Crystal data

$BaMn_2Fe(PO_4)_3$	$D_x = 3.946$ Mg m^{-3}
$M_r = 587.98$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbcn*	Cell parameters from 3088 reflections
$a = 6.5899$ (2) Å	$\theta = 3.3$–40.1°
$b = 17.6467$ (4) Å	$\mu = 8.41$ mm^{-1}
$c = 8.5106$ (2) Å	$T = 296$ K
$V = 989.70$ (4) Å^3	Block, orange
$Z = 4$	$0.32 \times 0.25 \times 0.22$ mm
$F(000) = 1092$	

Data collection

Bruker X8 APEX diffractometer	29422 measured reflections
Radiation source: fine-focus sealed tube	3088 independent reflections
Graphite monochromator	2731 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.033$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$\theta_{max} = 40.1°$, $\theta_{min} = 3.3°$
	$h = -8 \rightarrow 11$
	$k = -31 \rightarrow 32$
$T_{min} = 0.596$, $T_{max} = 0.748$	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2 + 1.2088P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.018$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.044$	$\Delta\rho_{max} = 1.29$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -1.11$ e Å^{-3}
3088 reflections	Extinction correction: SHELXL2014 (Sheldrick, 2015*b*),
89 parameters	Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
0 restraints	Extinction coefficient: 0.00278 (15)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ba1	0.5000	0.44269 (2)	0.7500	0.01037 (3)
Fe1	1.0000	0.31799 (2)	0.7500	0.00461 (4)
Mn1	0.83899 (3)	0.36570 (2)	0.39874 (2)	0.00647 (4)
P1	0.83270 (5)	0.17935 (2)	0.53771 (3)	0.00490 (5)
P2	1.0000	0.47123 (2)	0.7500	0.00513 (7)
O1	1.01958 (15)	0.12822 (6)	0.55338 (13)	0.01186 (16)
O2	0.66250 (15)	0.15480 (5)	0.64868 (11)	0.00865 (14)
O3	0.76365 (15)	0.17592 (5)	0.36487 (10)	0.00794 (14)
O4	0.88706 (16)	0.26335 (5)	0.57277 (11)	0.01031 (15)
O5	0.89269 (15)	0.41422 (5)	0.63609 (10)	0.00656 (13)
O6	0.83805 (16)	0.51729 (5)	0.83211 (12)	0.00988 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.00562 (5)	0.01428 (5)	0.01119 (5)	0.000	−0.00082 (3)	0.000
Fe1	0.00537 (9)	0.00435 (8)	0.00411 (8)	0.000	0.00015 (7)	0.000
Mn1	0.00598 (7)	0.00785 (6)	0.00559 (7)	−0.00021 (5)	0.00041 (6)	0.00013 (5)
P1	0.00360 (11)	0.00666 (10)	0.00443 (10)	−0.00050 (9)	−0.00036 (9)	−0.00071 (8)
P2	0.00571 (17)	0.00355 (13)	0.00611 (15)	0.000	0.00000 (13)	0.000
O1	0.0058 (4)	0.0170 (4)	0.0128 (4)	0.0047 (3)	−0.0016 (3)	−0.0004 (3)
O2	0.0064 (3)	0.0126 (3)	0.0070 (3)	−0.0017 (3)	0.0007 (3)	0.0021 (3)
O3	0.0066 (4)	0.0127 (3)	0.0045 (3)	0.0002 (3)	−0.0018 (3)	−0.0017 (3)
O4	0.0136 (4)	0.0087 (3)	0.0086 (3)	−0.0047 (3)	−0.0002 (3)	−0.0028 (3)
O5	0.0084 (3)	0.0058 (3)	0.0055 (3)	−0.0007 (3)	−0.0009 (3)	−0.0003 (2)
O6	0.0091 (4)	0.0071 (3)	0.0134 (4)	0.0017 (3)	0.0011 (3)	−0.0031 (3)

Geometric parameters (Å, º)

Ba1—O6	2.6803 (10)	Mn1—O6[vi]	2.1413 (9)
Ba1—O6[i]	2.6803 (10)	Mn1—O1[ii]	2.1466 (10)
Ba1—O3[ii]	2.7861 (9)	Mn1—O2[vii]	2.1587 (9)
Ba1—O3[iii]	2.7861 (9)	Mn1—O2[v]	2.1997 (10)
Ba1—O5	2.8087 (10)	Mn1—O5	2.2223 (9)
Ba1—O5[i]	2.8087 (10)	Mn1—O4	2.3572 (10)
Ba1—O1[ii]	2.8722 (11)	P1—O2	1.5289 (10)
Ba1—O1[iii]	2.8722 (11)	P1—O1	1.5325 (10)
Fe1—O4	1.9387 (9)	P1—O3	1.5409 (9)
Fe1—O4[iv]	1.9387 (9)	P1—O4	1.5540 (9)

Fe1—O3^v	1.9965 (9)	P2—O6	1.5126 (10)
Fe1—O3^{iii}	1.9965 (9)	P2—O6^{iv}	1.5126 (10)
Fe1—O5^{iv}	2.0792 (9)	P2—O5	1.5659 (9)
Fe1—O5	2.0793 (9)	P2—O5^{iv}	1.5660 (9)
O6—Ba1—O6^i	121.17 (4)	O4^{iv}—Fe1—O5^{iv}	85.00 (4)
O6—Ba1—O3^{ii}	157.68 (3)	O3^v—Fe1—O5^{iv}	83.59 (4)
O6^i—Ba1—O3^{ii}	79.21 (3)	O3^{iii}—Fe1—O5^{iv}	91.36 (4)
O6—Ba1—O3^{iii}	79.21 (3)	O4—Fe1—O5	85.00 (4)
O6^i—Ba1—O3^{iii}	157.68 (3)	O4^{iv}—Fe1—O5	154.09 (4)
O3^{ii}—Ba1—O3^{iii}	82.60 (4)	O3^v—Fe1—O5	91.36 (4)
O6—Ba1—O5	53.99 (3)	O3^{iii}—Fe1—O5	83.59 (4)
O6^i—Ba1—O5	139.79 (3)	O5^{iv}—Fe1—O5	70.50 (5)
O3^{ii}—Ba1—O5	105.04 (3)	O6^{vi}—Mn1—O1^{ii}	89.96 (4)
O3^{iii}—Ba1—O5	58.11 (3)	O6^{vi}—Mn1—O2^{vii}	84.29 (4)
O6—Ba1—O5^i	139.79 (3)	O1^{ii}—Mn1—O2^{vii}	101.01 (4)
O6^i—Ba1—O5^i	53.99 (3)	O6^{vi}—Mn1—O2^v	96.48 (4)
O3^{ii}—Ba1—O5^i	58.11 (3)	O1^{ii}—Mn1—O2^v	173.39 (4)
O3^{iii}—Ba1—O5^i	105.04 (3)	O2^{vii}—Mn1—O2^v	78.23 (4)
O5—Ba1—O5^i	159.39 (3)	O6^{vi}—Mn1—O5	82.51 (4)
O6—Ba1—O1^{ii}	114.27 (3)	O1^{ii}—Mn1—O5	87.96 (4)
O6^i—Ba1—O1^{ii}	90.97 (3)	O2^{vii}—Mn1—O5	164.03 (4)
O3^{ii}—Ba1—O1^{ii}	51.86 (3)	O2^v—Mn1—O5	94.35 (4)
O3^{iii}—Ba1—O1^{ii}	87.88 (3)	O6^{vi}—Mn1—O4	154.91 (4)
O5—Ba1—O1^{ii}	64.56 (3)	O1^{ii}—Mn1—O4	92.91 (4)
O5^i—Ba1—O1^{ii}	105.89 (3)	O2^{vii}—Mn1—O4	119.45 (3)
O6—Ba1—O1^{iii}	90.97 (3)	O2^v—Mn1—O4	81.90 (4)
O6^i—Ba1—O1^{iii}	114.27 (3)	O5—Mn1—O4	72.70 (3)
O3^{ii}—Ba1—O1^{iii}	87.88 (3)	O2—P1—O1	111.65 (6)
O3^{iii}—Ba1—O1^{iii}	51.86 (3)	O2—P1—O3	111.22 (5)
O5—Ba1—O1^{iii}	105.89 (3)	O1—P1—O3	107.29 (6)
O5^i—Ba1—O1^{iii}	64.55 (3)	O2—P1—O4	108.71 (5)
O1^{ii}—Ba1—O1^{iii}	128.34 (4)	O1—P1—O4	111.08 (6)
O4—Fe1—O4^{iv}	120.35 (6)	O3—P1—O4	106.79 (5)
O4—Fe1—O3^v	88.85 (4)	O6—P2—O6^{iv}	115.00 (8)
O4^{iv}—Fe1—O3^v	94.22 (4)	O6—P2—O5	108.22 (5)
O4—Fe1—O3^{iii}	94.22 (4)	O6^{iv}—P2—O5	112.20 (5)
O4^{iv}—Fe1—O3^{iii}	88.85 (4)	O6—P2—O5^{iv}	112.20 (5)
O3^v—Fe1—O3^{iii}	173.83 (5)	O6^{iv}—P2—O5^{iv}	108.22 (5)
O4—Fe1—O5^{iv}	154.09 (4)	O5—P2—O5^{iv}	100.05 (7)

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

(II) Strontium dimanganese(II) iron(III) tris(orthophosphate)

Crystal data

SrMn$_2$Fe(PO$_4$)$_3$	Orthorhombic, $Pbcn$
M_r = 538.25	a = 6.4304 (3) Å

b = 17.8462 (7) Å
c = 8.4906 (3) Å
V = 974.37 (7) Å³
Z = 4
$F(000)$ = 1020
D_x = 3.669 Mg m⁻³
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2843 reflections
θ = 3.3–39.1°
μ = 10.00 mm⁻¹
T = 296 K
Block, dark brown
0.30 × 0.27 × 0.23 mm

Data collection

Bruker X8 APEX
   diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan
   (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.404, T_{max} = 0.748

23889 measured reflections
2843 independent reflections
2564 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 39.1°, θ_{min} = 3.3°
h = −11→10
k = −31→31
l = −8→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.048
S = 1.08
2843 reflections
89 parameters
0 restraints

$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 1.2279P]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.19 e Å⁻³
$\Delta\rho_{min}$ = −0.81 e Å⁻³
Extinction correction: SHELXL2014
   (Sheldrick, 2015*b*),
   Fc*=kFc[1+0.001xFc²λ³/sin(2θ)]⁻¹ᐟ⁴
Extinction coefficient: 0.0072 (3)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Sr1	0.5000	0.43233 (2)	0.7500	0.00986 (4)
Fe1	1.0000	0.31546 (2)	0.7500	0.00485 (4)
Mn1	0.83818 (3)	0.37163 (2)	0.39547 (2)	0.00679 (4)
P1	0.83555 (5)	0.17749 (2)	0.53581 (3)	0.00571 (5)
P2	1.0000	0.46759 (2)	0.7500	0.00485 (7)
O1	1.02378 (15)	0.12570 (6)	0.54770 (13)	0.01473 (18)
O2	0.66091 (14)	0.15203 (5)	0.64550 (11)	0.00922 (14)
O3	0.76936 (14)	0.17505 (5)	0.36165 (10)	0.00794 (14)
O4	0.89115 (17)	0.25971 (6)	0.57468 (12)	0.01448 (18)
O5	0.89256 (14)	0.41164 (5)	0.63388 (10)	0.00662 (13)
O6	0.82775 (15)	0.51251 (5)	0.82684 (12)	0.00991 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00601 (7)	0.01296 (7)	0.01060 (7)	0.000	−0.00134 (5)	0.000
Fe1	0.00567 (9)	0.00423 (8)	0.00466 (8)	0.000	0.00026 (7)	0.000
Mn1	0.00547 (7)	0.00927 (7)	0.00563 (7)	−0.00023 (5)	0.00064 (5)	−0.00056 (5)
P1	0.00382 (10)	0.00858 (11)	0.00473 (10)	−0.00077 (9)	−0.00010 (9)	−0.00167 (8)
P2	0.00502 (15)	0.00357 (13)	0.00597 (15)	0.000	−0.00017 (12)	0.000
O1	0.0066 (4)	0.0237 (5)	0.0139 (4)	0.0062 (3)	−0.0013 (3)	0.0010 (4)
O2	0.0061 (3)	0.0149 (4)	0.0067 (3)	−0.0015 (3)	0.0009 (3)	0.0025 (3)
O3	0.0067 (3)	0.0125 (3)	0.0046 (3)	0.0001 (3)	−0.0012 (3)	−0.0013 (3)
O4	0.0174 (4)	0.0133 (4)	0.0128 (4)	−0.0084 (3)	0.0029 (3)	−0.0074 (3)
O5	0.0085 (3)	0.0062 (3)	0.0052 (3)	−0.0009 (3)	−0.0016 (3)	−0.0006 (2)
O6	0.0085 (3)	0.0073 (3)	0.0140 (4)	0.0019 (3)	0.0015 (3)	−0.0032 (3)

Geometric parameters (Å, º)

Sr1—O3^i	2.6020 (9)	Mn1—O1^i	2.0790 (10)
Sr1—O3^{ii}	2.6020 (9)	Mn1—O2^v	2.1462 (9)
Sr1—O6^{iii}	2.6296 (9)	Mn1—O6^{vi}	2.1494 (9)
Sr1—O6	2.6296 (10)	Mn1—O2^{vii}	2.1641 (9)
Sr1—O5	2.7351 (9)	Mn1—O5	2.1748 (9)
Sr1—O5^{iii}	2.7351 (9)	Mn1—O4	2.5338 (12)
Sr1—O1^i	2.7358 (11)	P1—O1	1.5263 (10)
Sr1—O1^{ii}	2.7358 (11)	P1—O2	1.5281 (9)
Fe1—O4	1.9224 (10)	P1—O3	1.5394 (9)
Fe1—O4^{iv}	1.9224 (10)	P1—O4	1.5459 (10)
Fe1—O3^v	1.9818 (9)	P2—O6	1.5149 (9)
Fe1—O3^{ii}	1.9818 (9)	P2—O6^{iv}	1.5149 (9)
Fe1—O5	2.0966 (9)	P2—O5^{iv}	1.5641 (9)
Fe1—O5^{iv}	2.0966 (9)	P2—O5	1.5641 (9)
O3^i—Sr1—O3^{ii}	85.14 (4)	O4^{iv}—Fe1—O5	155.20 (4)
O3^i—Sr1—O6^{iii}	81.58 (3)	O3^v—Fe1—O5	89.60 (4)
O3^{ii}—Sr1—O6^{iii}	161.43 (3)	O3^{ii}—Fe1—O5	82.35 (4)
O3^i—Sr1—O6	161.43 (3)	O4—Fe1—O5^{iv}	155.20 (4)
O3^{ii}—Sr1—O6	81.58 (3)	O4^{iv}—Fe1—O5^{iv}	86.54 (4)
O6^{iii}—Sr1—O6	114.07 (4)	O3^v—Fe1—O5^{iv}	82.35 (4)
O3^i—Sr1—O5	107.18 (3)	O3^{ii}—Fe1—O5^{iv}	89.60 (4)
O3^{ii}—Sr1—O5	60.39 (3)	O5—Fe1—O5^{iv}	70.09 (5)
O6^{iii}—Sr1—O5	136.36 (3)	O1^i—Mn1—O2^v	169.25 (4)
O6—Sr1—O5	54.77 (3)	O1^i—Mn1—O6^{vi}	90.60 (4)
O3^i—Sr1—O5^{iii}	60.39 (3)	O2^v—Mn1—O6^{vi}	100.11 (4)
O3^{ii}—Sr1—O5^{iii}	107.18 (3)	O1^i—Mn1—O2^{vii}	103.58 (4)
O6^{iii}—Sr1—O5^{iii}	54.77 (3)	O2^v—Mn1—O2^{vii}	78.47 (4)
O6—Sr1—O5^{iii}	136.36 (3)	O6^{vi}—Mn1—O2^{vii}	85.52 (4)
O5—Sr1—O5^{iii}	164.49 (4)	O1^i—Mn1—O5	86.15 (4)
O3^i—Sr1—O1^i	54.30 (3)	O2^v—Mn1—O5	93.44 (4)

O3ii—Sr1—O1i	91.49 (3)	O6vi—Mn1—O5	86.65 (4)
O6iii—Sr1—O1i	91.23 (3)	O2vii—Mn1—O5	167.55 (4)
O6—Sr1—O1i	112.98 (3)	O1i—Mn1—O4	90.54 (4)
O5—Sr1—O1i	64.17 (3)	O2v—Mn1—O4	79.18 (4)
O5iii—Sr1—O1i	109.48 (3)	O6vi—Mn1—O4	157.72 (4)
O3i—Sr1—O1ii	91.49 (3)	O2vii—Mn1—O4	115.78 (3)
O3ii—Sr1—O1ii	54.30 (3)	O5—Mn1—O4	71.23 (3)
O6iii—Sr1—O1ii	112.98 (3)	O1—P1—O2	111.25 (6)
O6—Sr1—O1ii	91.23 (3)	O1—P1—O3	105.40 (6)
O5—Sr1—O1ii	109.48 (3)	O2—P1—O3	111.95 (5)
O5iii—Sr1—O1ii	64.17 (3)	O1—P1—O4	112.17 (6)
O1i—Sr1—O1ii	135.52 (5)	O2—P1—O4	108.80 (6)
O4—Fe1—O4iv	117.67 (7)	O3—P1—O4	107.21 (6)
O4—Fe1—O3v	89.54 (4)	O6—P2—O6iv	116.11 (7)
O4iv—Fe1—O3v	95.53 (4)	O6—P2—O5iv	112.91 (5)
O4—Fe1—O3ii	95.53 (4)	O6iv—P2—O5iv	106.63 (5)
O4iv—Fe1—O3ii	89.54 (4)	O6—P2—O5	106.64 (5)
O3v—Fe1—O3ii	170.19 (5)	O6iv—P2—O5	112.91 (5)
O4—Fe1—O5	86.54 (4)	O5iv—P2—O5	100.66 (7)

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