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Distrontium trimanganese(II) bis(hydrogenphosphate) bis(orthophosphate)

Jamal Khmiyas,* Abderrazzak Assani, Mohamed Saadi and Lahcen El Ammari

Laboratoire de Chimie du Solide Appliquée, Faculté des Sciences, Université Mohammed V-Agdal, Avenue Ibn Battouta, BP 1014, Rabat, Morocco
Correspondence e-mail: j_khmiyas@yahoo.fr

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ(P–O) = 0.001 Å; R factor = 0.019; wR factor = 0.045; data-to-parameter ratio = 27.3.

The title compound, $Sr_2Mn_3(HPO_4)_2(PO_4)_2$, was synthesized under hydrothermal conditions. In the structure, one of two Mn atoms is located on an inversion centre, whereas all others atoms are located in general positions. The framework structure is built up from two types of MnO_6 octahedra (one almost undistorted, one considerably distorted), one PO_3OH and one PO_4 tetrahedron. The centrosymmetric MnO_6 octahedron is linked to two other MnO_6 octahedra by edge-sharing, forming infinite zigzag chains parallel to [010]. The PO_3OH and PO_4 tetrahedra connect these chains through common vertices or edges, resulting in the formation of sheets parallel to (100). The Sr^{2+} cation is located in the interlayer space and is bonded to nine O atoms in form of a distorted polyhedron and enhances the cohesion of the layers. Additional stabilization is achieved by a strong interlayer O—H···O hydrogen bond between the PO_3OH and PO_4 units. The structure of the title phosphate is isotypic to that of $Pb_2Mn_3(HPO_4)_2(PO_4)_2$.

Related literature

For isotypic $Pb_2Mn_3(HPO_4)_2(PO_4)_2$, see: Assani *et al.* (2012*b*). For related structures, see: Assani *et al.* (2012*a*); Effenberger (1999). For the thermal stability of similar compounds, see: Morozov *et al.* (2003). For applications of phosphates, see: Cheetham *et al.* (1999); Viter & Nagornyi (2009); Forster *et al.* (2003); Clearfield (1988); Joschi *et al.* (2008); Trad *et al.* (2010).

Experimental

Crystal data

$Sr_2Mn_3(HPO_4)_2(PO_4)_2$
M_r = 721.96
Monoclinic, $P2_1/c$
a = 7.8535 (1) Å
b = 8.7793 (2) Å
c = 9.6165 (2) Å
β = 101.434 (1)°
V = 649.88 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.58 mm^{-1}
T = 296 K
0.33 × 0.24 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.046, T_{max} = 0.215
12425 measured reflections
3138 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.045
S = 1.06
3138 reflections
115 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8···O4	0.82	1.66	2.4828 (14)	177

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2758).

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Distrontium trimanganese(II) bis(hydrogenphosphate) bis(orthophosphate)

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S1. Comment

Widespread studies were devoted to metal-based phosphates, either with open-framework structures, or in terms of porous materials. Within those materials, the anionic framework, generally constructed from PO_4 tetrahedra connected to metal (M) cations in different coordination environments MO_n (with n = 4, 5 and 6), can generate pores and channels offering a suitable environment to accommodate various other cations. Besides their high chemical activity and their thermal stability (Morozov *et al.*, 2003), such metal-based phosphates have some interesting properties leading to applications such as in catalysis (Cheetham *et al.*, 1999; Viter & Nagornyi, 2009), ion-exchangers (Clearfield, 1988; Joschi *et al.*, 2008), gas sorption (Forster *et al.*, 2003), or batteries (Trad *et al.*, 2010).

Our interest is particularly focused on hydrothermally synthesized orthophosphates within the ternary systems MO–$M'O$–P_2O_5 with M and M' = divalent cations. We have recently characterized some new lead cobalt or manganese phosphates, *viz*. $Co_2Pb(HPO_4)(PO_4)OH{\cdot}H_2O$ (Assani *et al.*, 2012*a*) and $Pb_2Mn_3(HPO_4)_2(PO_4)_2$ (Assani *et al.*, 2012*b*). In line with the focus of our research, the present paper describes the hydrothermal synthesis and the structural characterization of a new strontium manganese phosphate, $Sr_2Mn_3(HPO_4)_2(PO_4)_2$, that is isotypic with its lead analogue, $Pb_2Mn_3(HPO_4)_2(PO_4)_2$. These two phosphates are characterized by an Mn:P ratio = 3:4, which is rarely observed, with the exception of some copper-based orthophosphates, $Pb_3Cu_3(PO_4)_4$ and $Sr_3Cu_3(PO_4)_4$ (Effenberger, 1999), also with Cu:P = 3:4.

In the structure of the title compound, one of the two manganese sites (Mn1) is located on a centre of inversion, while all remaining atoms are in general positions. A part of the structure, as given in Fig. 1, shows the different types of polyhedra around the metal positions and the P atoms. The centrosymmetric $Mn1O_6$ octahedron is linked to two distorted $Mn2O_6$ octahedra by a common edge, thus forming infinite zigzag chains with composition $[Mn_3O_{14}]_\infty$ running parallel to [010] (Fig. 2). Adjacent chains are linked to each other through PO_4 and PO_3OH tetrahedra, *via* common corners or edges, leading to the formation of layers parallel to (100). The cohesion of the crystal structure is ensured on one hand by the presence of the Sr^{2+} cations in the interlayer space and on the other hand by strong O—H···O hydrogen bonds between sheets (Fig. 2 and Table 2).

In the structure of the title compound, the Sr^{2+} cation is surrounded by nine O atoms instead of eight as in the case of $Pb_2Mn_3(HPO_4)_2(PO_4)_2$. All other bond lengths and angles are similar in the two structures, with the exception of the Mn2—O bond lengths. In the title structure, four medium-long bonds in the range 2.1189 (10) to 2.1875 (9) Å and two longer bonds of 2.4079 (12) and 2.4609 (11) Å are observed, whereas in the lead analogue five medium-long bonds in the range 2.094 (4) to 2.235 (4) Å and one considerably long bond of 2.610 (4) Å is observed.

S2. Experimental

Transparent crystals of $Sr_2Mn_3(HPO_4)_2(PO_4)_2$ were isolated from hydrothermal treatment of the reaction mixture of strontium, manganese, sodium and phosphate precursors in a proportion corresponding to the molar ratio Sr: Mn: Na: P:

= 4: 4.5: 1: 6. The hydrothermal reaction was conducted in a 23 ml Teflon-lined autoclave filled to 50% with distilled water and under autogenously pressure at 473 K for five days. After being filtered off, washed with deionized water and air-dried, the reaction product consisted of colourless crystals with a platy form.

S3. Refinement

The O-bound H atom was initially located in a difference map and refined with O—H distance restraint of 0.82 (1) Å. In the last cycle it was refined in the riding model approximation with $U_{\rm iso}$(H) set to 1.5Ueq(O). The highest peak and the deepest hole in the final Fourier map are at 0.64 Å and 0.55 Å, from Mn2.

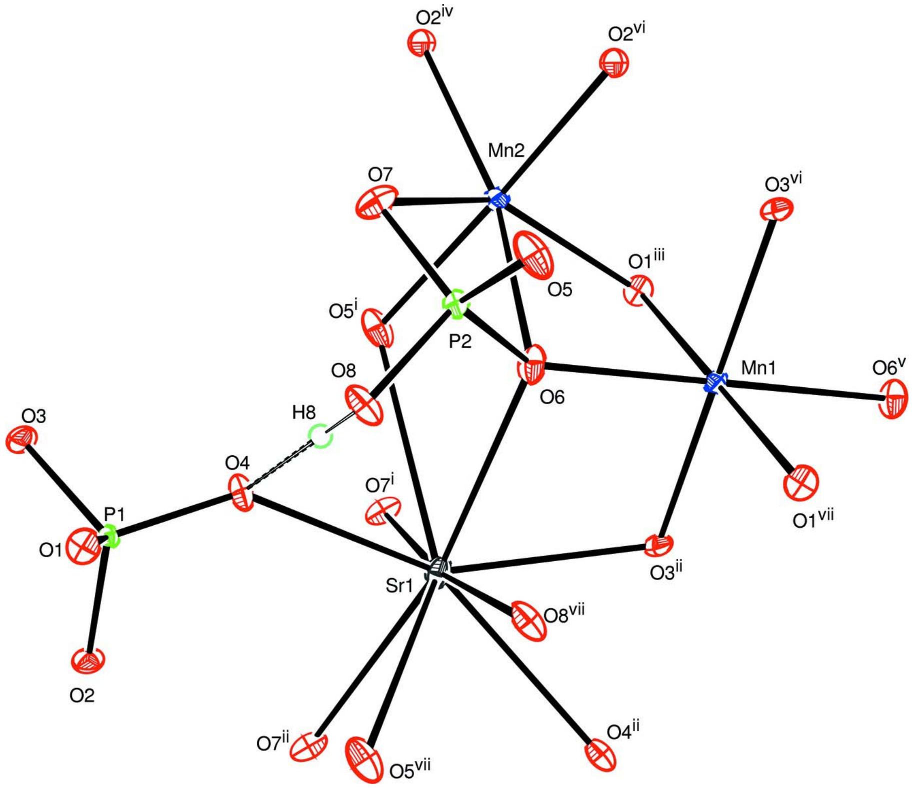

Figure 1

A partial plot of the crystal structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) -*x* + 1, *y* - 1/2, -*z* + 1/2; (ii) -*x* + 1, -*y* + 1, -*z* + 1; (iii) *x*, -*y* + 3/2, *z* - 1/2; (iv) -*x* + 2, -*y* + 1, -*z* + 1; (v) *x* + 1, -*y* + 3/2, *z* + 1/2; (vi) *x* + 1, *y*, *z*; (vii) -*x* + 1, *y* + 1/2, -*z* + 1/2; (viii) *x*, -*y* + 3/2, *z* + 1/2.

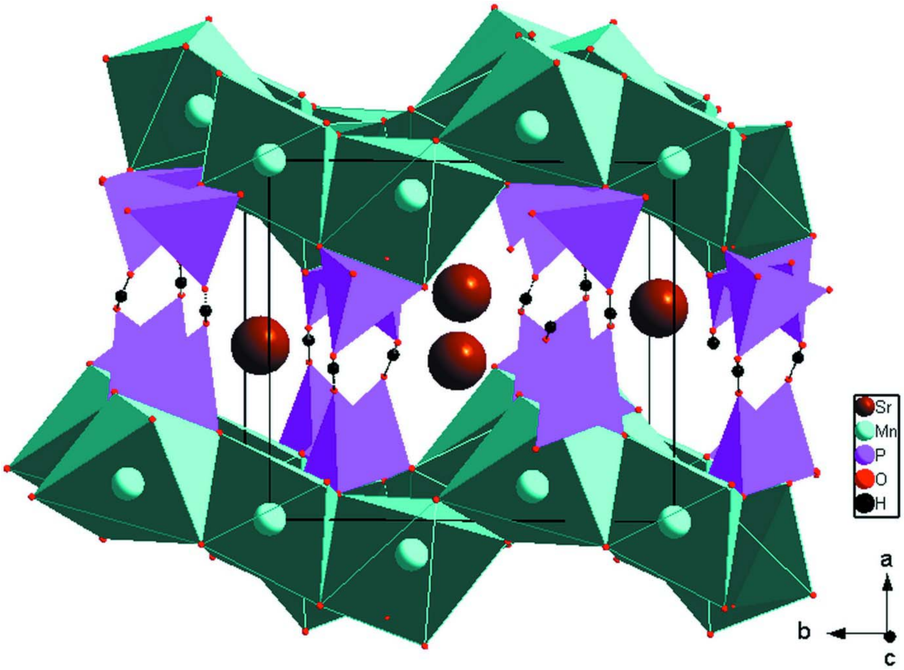

Figure 2

Polyhedral representation of $Sr_2Mn_3(HPO_4)_2(PO_4)_2$, showing Sr^{2+} cations between layers and O—H···O hydrogen bonds (dashed lines) between the sheets.

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Crystal data

$Sr_2Mn_3(HPO_4)_2(PO_4)_2$
$M_r = 721.96$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.8535$ (1) Å
$b = 8.7793$ (2) Å
$c = 9.6165$ (2) Å
$\beta = 101.434$ (1)°
$V = 649.88$ (2) Å^3
$Z = 2$

$F(000) = 682$
$D_x = 3.689$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3138 reflections
$\theta = 2.7$–$36.3°$
$\mu = 11.58$ mm^{-1}
$T = 296$ K
Sheet, colourless
0.33 × 0.24 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker (2009)
$T_{min} = 0.046$, $T_{max} = 0.215$

12425 measured reflections
3138 independent reflections
2874 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 36.3°$, $\theta_{min} = 2.7°$
$h = -13 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.045$
$S = 1.06$
3138 reflections
115 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 0.239P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.58$ e Å^{-3}
$\Delta\rho_{\min} = -0.54$ e Å^{-3}

Special details

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

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Sr1	0.573794 (17)	0.478038 (15)	0.234323 (14)	0.00999 (3)
Mn1	1.0000	0.5000	0.5000	0.00677 (5)
Mn2	0.89650 (3)	0.85638 (2)	0.40357 (2)	0.00891 (4)
P1	0.14462 (4)	0.70256 (4)	0.22974 (3)	0.00542 (6)
P2	0.65079 (4)	0.71451 (4)	0.56233 (3)	0.00649 (6)
O1	0.06059 (13)	0.67784 (12)	0.35944 (10)	0.00966 (17)
O2	0.06622 (13)	0.59473 (11)	0.10796 (10)	0.01019 (17)
O3	0.11920 (13)	0.86980 (11)	0.18530 (11)	0.01016 (17)
O4	0.34252 (13)	0.67330 (12)	0.27411 (10)	0.01050 (17)
O5	0.70244 (14)	0.69325 (14)	0.72158 (10)	0.0141 (2)
O6	0.75819 (13)	0.62546 (12)	0.47491 (11)	0.01179 (18)
O7	0.65059 (15)	0.88211 (12)	0.51673 (11)	0.01383 (19)
O8	0.45824 (13)	0.65486 (13)	0.53325 (11)	0.01209 (19)
H8	0.4169	0.6607	0.4482	0.018*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00960 (6)	0.01026 (6)	0.01085 (5)	0.00204 (4)	0.00384 (4)	0.00216 (4)
Mn1	0.00742 (11)	0.00597 (11)	0.00692 (11)	0.00076 (8)	0.00144 (8)	−0.00002 (8)
Mn2	0.00962 (9)	0.00758 (9)	0.00837 (8)	0.00006 (6)	−0.00103 (6)	−0.00030 (6)
P1	0.00572 (12)	0.00557 (12)	0.00475 (12)	−0.00013 (10)	0.00052 (9)	0.00000 (9)
P2	0.00632 (13)	0.00796 (13)	0.00540 (12)	0.00034 (10)	0.00167 (10)	−0.00007 (10)
O1	0.0108 (4)	0.0108 (4)	0.0085 (4)	0.0003 (3)	0.0047 (3)	0.0012 (3)
O2	0.0137 (4)	0.0079 (4)	0.0073 (4)	−0.0001 (3)	−0.0019 (3)	−0.0020 (3)

O3	0.0126 (4)	0.0057 (4)	0.0109 (4)	0.0000 (3)	−0.0007 (3)	0.0021 (3)
O4	0.0064 (4)	0.0154 (5)	0.0093 (4)	0.0019 (3)	0.0007 (3)	0.0004 (3)
O5	0.0105 (4)	0.0256 (6)	0.0055 (4)	−0.0009 (4)	0.0002 (3)	0.0008 (4)
O6	0.0109 (4)	0.0151 (5)	0.0104 (4)	0.0054 (4)	0.0047 (3)	−0.0002 (3)
O7	0.0202 (5)	0.0076 (4)	0.0148 (4)	−0.0001 (4)	0.0061 (4)	0.0003 (3)
O8	0.0074 (4)	0.0203 (5)	0.0083 (4)	−0.0033 (4)	0.0008 (3)	0.0009 (3)

Geometric parameters (Å, º)

Sr1—O3^{i}	2.5641 (10)	Mn2—O1^{vi}	2.1248 (10)
Sr1—O4	2.5806 (10)	Mn2—O5^{iii}	2.1256 (10)
Sr1—O8^{ii}	2.5775 (11)	Mn2—O2^{v}	2.1875 (9)
Sr1—O7^{iii}	2.5981 (11)	Mn2—O7	2.4079 (12)
Sr1—O5^{ii}	2.7409 (11)	Mn2—O6	2.4609 (11)
Sr1—O4^{i}	2.7599 (11)	P1—O3	1.5312 (10)
Sr1—O6	2.7923 (10)	P1—O2	1.5365 (10)
Sr1—O7^{i}	2.8207 (11)	P1—O1	1.5377 (10)
Sr1—O5^{iii}	3.0680 (12)	P1—O4	1.5494 (10)
Mn1—O6	2.1670 (10)	P2—O5	1.5160 (10)
Mn1—O6^{iv}	2.1670 (10)	P2—O6	1.5201 (11)
Mn1—O3^{v}	2.1672 (9)	P2—O7	1.5352 (11)
Mn1—O3^{i}	2.1672 (9)	P2—O8	1.5721 (11)
Mn1—O1^{ii}	2.1786 (10)	P2—Sr1^{viii}	3.2838 (4)
Mn1—O1^{vi}	2.1786 (10)	O8—H8	0.8200
Mn2—O2^{vii}	2.1189 (10)		

O3^{i}—Sr1—O4	148.09 (3)	O6^{iv}—Mn1—O3^{i}	92.85 (4)
O3^{i}—Sr1—O8^{ii}	79.54 (3)	O3^{v}—Mn1—O3^{i}	180.0
O4—Sr1—O8^{ii}	88.83 (3)	O6—Mn1—O1^{ii}	97.99 (4)
O3^{i}—Sr1—O7^{iii}	93.63 (3)	O6^{iv}—Mn1—O1^{ii}	82.01 (4)
O4—Sr1—O7^{iii}	95.05 (3)	O3^{v}—Mn1—O1^{ii}	88.84 (4)
O8^{ii}—Sr1—O7^{iii}	172.09 (3)	O3^{i}—Mn1—O1^{ii}	91.16 (4)
O3^{i}—Sr1—O5^{ii}	118.41 (3)	O6—Mn1—O1^{vi}	82.01 (4)
O4—Sr1—O5^{ii}	74.91 (4)	O6^{iv}—Mn1—O1^{vi}	97.99 (4)
O8^{ii}—Sr1—O5^{ii}	53.21 (3)	O3^{v}—Mn1—O1^{vi}	91.16 (4)
O7^{iii}—Sr1—O5^{ii}	134.52 (3)	O3^{i}—Mn1—O1^{vi}	88.84 (4)
O3^{i}—Sr1—O4^{i}	55.56 (3)	O1^{ii}—Mn1—O1^{vi}	180.0
O4—Sr1—O4^{i}	145.79 (2)	O2^{vii}—Mn2—O1^{vi}	128.50 (4)
O8^{ii}—Sr1—O4^{i}	69.60 (3)	O2^{vii}—Mn2—O5^{iii}	104.08 (4)
O7^{iii}—Sr1—O4^{i}	109.86 (3)	O1^{vi}—Mn2—O5^{iii}	92.78 (4)
O5^{ii}—Sr1—O4^{i}	70.92 (3)	O2^{vii}—Mn2—O2^{v}	77.72 (4)
O3^{i}—Sr1—O6	67.65 (3)	O1^{vi}—Mn2—O2^{v}	92.21 (4)
O4—Sr1—O6	80.44 (3)	O5^{iii}—Mn2—O2^{v}	171.78 (4)
O8^{ii}—Sr1—O6	67.36 (3)	O2^{vii}—Mn2—O7	93.58 (4)
O7^{iii}—Sr1—O6	106.45 (3)	O1^{vi}—Mn2—O7	137.06 (4)
O5^{ii}—Sr1—O6	114.99 (3)	O5^{iii}—Mn2—O7	83.28 (4)
O4^{i}—Sr1—O6	112.72 (3)	O2^{v}—Mn2—O7	88.62 (4)
O3^{i}—Sr1—O7^{i}	122.54 (3)	O2^{vii}—Mn2—O6	154.34 (4)

O4—Sr1—O7$^{\mathrm{i}}$	89.23 (3)
O8$^{\mathrm{ii}}$—Sr1—O7$^{\mathrm{i}}$	117.08 (3)
O7$^{\mathrm{iii}}$—Sr1—O7$^{\mathrm{i}}$	69.95 (4)
O5$^{\mathrm{ii}}$—Sr1—O7$^{\mathrm{i}}$	65.75 (3)
O4$^{\mathrm{i}}$—Sr1—O7$^{\mathrm{i}}$	78.31 (3)
O6—Sr1—O7$^{\mathrm{i}}$	168.81 (3)
O3$^{\mathrm{i}}$—Sr1—O5$^{\mathrm{iii}}$	93.62 (3)
O4—Sr1—O5$^{\mathrm{iii}}$	68.17 (3)
O8$^{\mathrm{ii}}$—Sr1—O5$^{\mathrm{iii}}$	123.36 (3)
O7$^{\mathrm{iii}}$—Sr1—O5$^{\mathrm{iii}}$	52.59 (3)
O5$^{\mathrm{ii}}$—Sr1—O5$^{\mathrm{iii}}$	143.06 (3)
O4$^{\mathrm{i}}$—Sr1—O5$^{\mathrm{iii}}$	145.93 (3)
O6—Sr1—O5$^{\mathrm{iii}}$	58.42 (3)
O7$^{\mathrm{i}}$—Sr1—O5$^{\mathrm{iii}}$	113.67 (3)
O6—Mn1—O6$^{\mathrm{iv}}$	180.0
O6—Mn1—O3$^{\mathrm{v}}$	92.85 (4)
O6$^{\mathrm{iv}}$—Mn1—O3$^{\mathrm{v}}$	87.15 (4)
O6—Mn1—O3$^{\mathrm{i}}$	87.15 (4)
O1$^{\mathrm{vi}}$—Mn2—O6	76.51 (4)
O5$^{\mathrm{iii}}$—Mn2—O6	77.09 (4)
O2$^{\mathrm{v}}$—Mn2—O6	97.77 (4)
O7—Mn2—O6	60.88 (4)
O3—P1—O2	111.57 (5)
O3—P1—O1	107.97 (6)
O2—P1—O1	111.08 (6)
O3—P1—O4	107.70 (6)
O2—P1—O4	109.65 (6)
O1—P1—O4	108.76 (6)
O5—P2—O6	115.38 (6)
O5—P2—O7	113.04 (6)
O6—P2—O7	107.71 (6)
O5—P2—O8	101.19 (6)
O6—P2—O8	110.48 (6)
O7—P2—O8	108.78 (6)
O5—P2—Mn2	120.08 (4)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*+1, −*y*+3/2, *z*+1/2; (vi) *x*+1, *y*, *z*; (vii) −*x*+1, *y*+1/2, −*z*+1/2; (viii) *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—H8···O4	0.82	1.66	2.4828 (14)	177