Crystal structure of alluaudite-type NaMg3(HPO4)2(PO4)

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Crystal structure of alluaudite-type $NaMg_3(HPO_4)_2(PO_4)$

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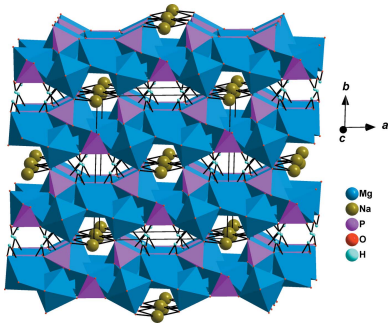
The title compound, sodium trimagnesium bis(hydrogen phosphate) phosphate, was obtained under hydrothermal conditions. In the crystal, two types of $[MgO_6]$ octahedra, one with point group symmetry 2, share edges to build chains extending parallel to $[10\bar{1}]$. These chains are linked together by two kinds of phosphate tetrahedra, HPO_4 and PO_4, the latter with point group symmetry 2. The three-dimensional framework delimits two different types of channels extending along [001]. One channel hosts the Na^+ cations (site symmetry 2) surrounded by eight O atoms, with Na—O bond lengths varying between 2.2974 (13) and 2.922 (2) Å. The OH group of the HPO_4 tetrahedron points into the other type of channel and exhibits a strong hydrogen bond to an O atom of the PO_4 tetrahedron on the opposite side.

1. Chemical context

By means of hydrothermal processes (Demazeau, 2008; Yoshimura & Byrappa, 2008), we have previously succeeded in the isolation of the mixed-valence manganese phosphates $MMn_2^{II}Mn^{III}(PO_4)_3$ (M = Ba, Pb, Sr) adopting the α-$CrPO_4$ structure type (Assani *et al.*, 2013; Alhakmi *et al.*, 2013*a*,*b*). In addition, within the pseudo-ternary systems Ag_2O–MO–P_2O_5, hydrothermal syntheses have allowed us to obtain other α-$CrPO_4$ isotype phosphates, *viz*. $Ag_2M_3(HPO_4)(PO_4)_2$ (M = Co, Ni) while $AgMg_3(HPO_4)_2(PO_4)$ is found to adopt the alluaudite structure type (Assani *et al.*, 2011*a*,*b*,*c*). Other hydrothermally grown phosphates with the alluaudite structure include $AgCo_3(HPO_4)_2(PO_4)$ (Guesmi & Driss, 2002), $AgNi_3(HPO_4)_2(PO_4)$ (Ben Smail & Jouini, 2002), $AMn_3(HPO_4)_2(PO_4)$ (A = Na, Ag) (Leroux *et al.*, 1995*a*,*b*) and $NaCo_3(HPO_4)_2(PO_4)$ (Lii & Shih, 1994). Phosphates belonging to either the α-$CrPO_4$ or alluaudite structure type or derivatives thereof are still in the focus of research owing to their promising applications as battery materials (Trad *et al.*, 2010; Essehli *et al.*, 2015*a*,*b*; Huang *et al.*, 2015).

The crystal structures of alluaudite-type phosphates exhibit channels in which the monovalent cations are localized. Indeed, this is strongly required for conductivity properties. The crystal structure of alluaudite can be formulated by the general formula $(A1)(A2)(M1)(M2)_2(PO_4)_3$, (Moore & Ito, 1979). The two A sites can be occupied by either mono- or divalent medium-sized cations while the two M cationic sites correspond to an octahedral environment generally occupied by transition metal cations. On the basis of literature research, it has been shown that the hydrothermal process allows, in general, stoechiometric phases to be obtained while solid-state



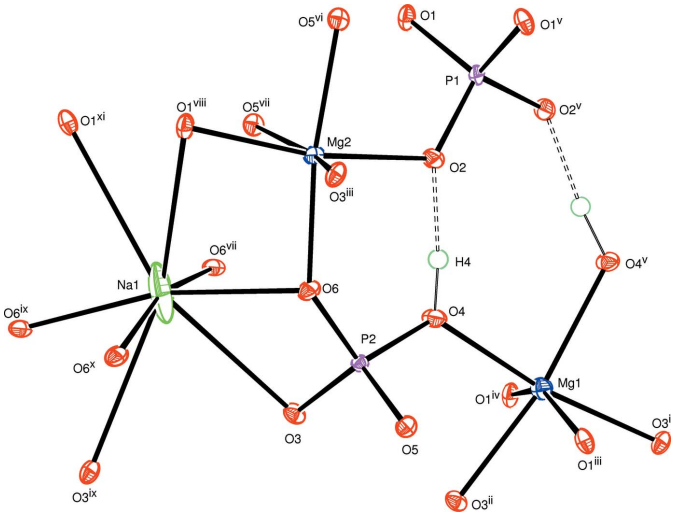


Figure 1
The principal building units in the structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are indicated by dashed lines [Symmetry codes: (i) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (iv) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z$; (v) $-x+1, -y+1, -z$; (vi) $-x+1, y, -z+\frac{1}{2}$; (vii) $x, -y+1, z+\frac{1}{2}$; (viii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ix) $-x+2, y, -z+\frac{3}{2}$; (x) $-x+2, -y+1, -z+1$; (xi) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (xii) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$; (xiii) $x, -y+1, z-\frac{1}{2}$.]

reactions give rather a statistical distribution of cations on either the *A* or *M* sites, leading to non-stoechiometric compounds (Bouraima *et al.*, 2015; Khmiyas *et al.*, 2015).

In line with our focus of interest, we hydrothermally synthesized the compound $NaMg_3(PO_4)(HPO_4)_2$ and report here its crystal structure.

2. Structural commentary

The principal building units of the allaudite structure of the title compound are represented in Fig. 1. The three atoms Mg1, Na1 and P1 are located on a twofold rotation axis (Wyckoff position 4*e*). Selected interatomic distances are compiled in Table 1. The three-dimensional framework of this structure consists of kinked chains of edge-sharing MgO_6 octahedra running parallel to $[10\bar{1}]$. The chains are held together by regular $P1O_4$ phosphate groups, forming sheets perpendicular to [010], as shown in Fig. 2. The stacked sheets delimit two types of channels along [001]. One of the channels is occupied by Na^+ cations surrounded by eight oxygen atoms (Table 1), whereas the second channel contains the hydrogen atoms of the $HP2O_4$ tetrahedra, as shown in Fig. 3. They form strong hydrogen bonds (Table 2, Figs. 1 and 3) with one of the oxygen atoms of PO_4 tetrahedra on opposite sides.

Table 1
Selected bond lengths (Å).

Mg1—O3^{i}	2.1224 (13)	Na1—O3	2.8840 (19)
Mg1—O1^{ii}	2.1312 (12)	Na1—O1^{vii}	2.922 (2)
Mg1—O4	2.1669 (14)	P1—O1^{viii}	1.5372 (12)
Mg2—O6	2.0234 (13)	P1—O1	1.5372 (12)
Mg2—O3^{ii}	2.0686 (13)	P1—O2^{viii}	1.5476 (13)
Mg2—O2	2.0696 (14)	P1—O2	1.5476 (13)
Mg2—O5^{iii}	2.0729 (13)	P2—O5	1.5234 (12)
Mg2—O5^{iv}	2.0955 (13)	P2—O6	1.5263 (12)
Mg2—O1^{v}	2.1153 (14)	P2—O3	1.5349 (13)
Na1—O6	2.2974 (13)	P2—O4	1.5806 (13)
Na1—O6^{vi}	2.4386 (13)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O2	0.93	1.57	2.4932 (17)	174

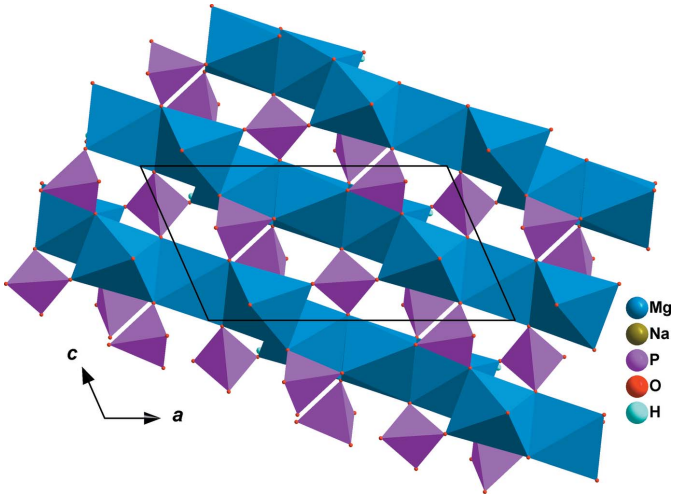


Figure 2
A sheet resulting from the linkage of kinked chains *via* vertices of PO_4 tetrahedra.

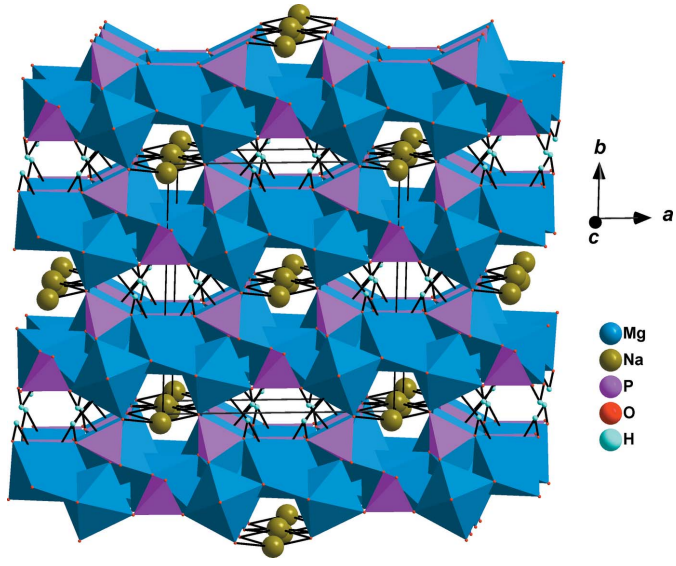


Figure 3
Polyhedral representation of the $NaMg_3(HPO_4)_2(PO_4)$ structure showing channels along [001]. The O—H···O hydrogen bonds are indicated by dashed lines.

Table 3
Experimental details.

Crystal data	
Chemical formula	$NaMg_3(HPO_4)_2(PO_4)$
M_r	382.85
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	296
a, *b*, *c* (Å)	11.8064 (6), 12.0625 (7), 6.4969 (4)
β (°)	113.805 (2)
V (Å^3)	846.54 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.06
Crystal size (mm)	0.36 × 0.24 × 0.18
Data collection	
Diffractometer	Bruker X8 APEX
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.504, 0.748
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9797, 1291, 1138
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.072, 1.09
No. of reflections	1291
No. of parameters	88
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.57, −0.54

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012). *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

3. Synthesis and crystallization

Colourless parallelepiped-shaped crystals of the title compound were grown under hydrothermal conditions, starting from a mixture of $Na_4P_2O_7{\cdot}10H_2O$, MgO and H_3PO_4 (85 wt%) in the molar ratio $Na_4P_2O_7{\cdot}10H_2O$:MgO:H_3PO_4 = 1:3:3. The hydrothermal reaction was conducted in a 23 ml Teflon-lined autoclave, filled to 50% with distilled water and under autogenous pressure at 483 K for four days.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The minimum and maximum electron densities are located 0.71 and 0.17 Å from O5 and H4, respectively. The O–bound H atom was initially located in a difference map and refined with an O—H distance restraint of 0.93 Å, and with U_{iso}(H) = 1.5U_{eq}(O).

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supporting information

Acta Cryst. (2015). E**71**, 813-815 [doi:10.1107/S205698901501155X]

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Sodium trimagnesium bis(hydrogen phosphate) phosphate

Crystal data

$NaMg_3(HPO_4)_2(PO_4)$
$M_r = 382.85$
Monoclinic, $C2/c$
$a = 11.8064$ (6) Å
$b = 12.0625$ (7) Å
$c = 6.4969$ (4) Å
$\beta = 113.805$ (2)°
$V = 846.54$ (8) Å^3
$Z = 4$
$F(000) = 760$
$D_x = 3.004$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1291 reflections
$\theta = 2.5$–30.5°
$\mu = 1.06$ mm^{-1}
$T = 296$ K
Block, colourless
0.36 × 0.24 × 0.18 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.504$, $T_{max} = 0.748$
9797 measured reflections
1291 independent reflections
1138 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 30.5°$, $\theta_{min} = 2.5°$
$h = -16\rightarrow16$
$k = -17\rightarrow17$
$l = -9\rightarrow8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.072$
$S = 1.09$
1291 reflections
88 parameters
0 restraints
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 1.4203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mg1	0.0000	0.27947 (7)	0.2500	0.00857 (18)
Mg2	0.29000 (6)	0.66219 (5)	0.37489 (10)	0.00643 (14)
Na1	0.5000	0.52321 (14)	0.7500	0.0308 (4)
P1	0.0000	0.68659 (5)	0.2500	0.00564 (14)
P2	0.28093 (4)	0.38887 (3)	0.38603 (7)	0.00494 (11)
O1	0.03662 (11)	0.75858 (10)	0.4624 (2)	0.0078 (2)
O2	0.10795 (12)	0.61003 (10)	0.2634 (2)	0.0084 (2)
O3	0.34567 (12)	0.32859 (10)	0.6116 (2)	0.0073 (2)
O4	0.14051 (11)	0.40754 (10)	0.3420 (2)	0.0085 (2)
H4	0.1241	0.4816	0.3033	0.013*
O5	0.28443 (11)	0.32046 (10)	0.1916 (2)	0.0068 (2)
O6	0.34273 (12)	0.50140 (10)	0.4000 (2)	0.0076 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0081 (4)	0.0088 (4)	0.0094 (4)	0.000	0.0041 (3)	0.000
Mg2	0.0073 (3)	0.0057 (3)	0.0067 (3)	0.0004 (2)	0.0031 (2)	0.0001 (2)
Na1	0.0118 (6)	0.0691 (11)	0.0091 (6)	0.000	0.0016 (5)	0.000
P1	0.0051 (3)	0.0063 (3)	0.0044 (3)	0.000	0.0007 (2)	0.000
P2	0.0060 (2)	0.00431 (19)	0.0043 (2)	−0.00006 (14)	0.00177 (16)	−0.00011 (14)
O1	0.0063 (6)	0.0110 (5)	0.0054 (5)	−0.0010 (4)	0.0014 (5)	−0.0022 (4)
O2	0.0060 (6)	0.0073 (5)	0.0114 (6)	0.0010 (4)	0.0031 (5)	−0.0007 (4)
O3	0.0086 (6)	0.0080 (5)	0.0049 (5)	0.0020 (4)	0.0024 (5)	0.0016 (4)
O4	0.0073 (6)	0.0058 (5)	0.0131 (6)	0.0009 (4)	0.0048 (5)	0.0004 (5)
O5	0.0077 (6)	0.0077 (5)	0.0052 (5)	0.0003 (4)	0.0028 (5)	−0.0009 (4)
O6	0.0083 (6)	0.0051 (5)	0.0093 (6)	−0.0014 (4)	0.0035 (5)	−0.0002 (4)

Geometric parameters (Å, º)

Mg1—O3^{i}	2.1224 (13)	Na1—O6^{x}	2.4386 (13)
Mg1—O3^{ii}	2.1224 (13)	Na1—O3	2.8840 (19)
Mg1—O1^{iii}	2.1312 (12)	Na1—O3^{ix}	2.8840 (19)
Mg1—O1^{iv}	2.1312 (12)	Na1—O1^{xi}	2.922 (2)
Mg1—O4^{v}	2.1669 (14)	Na1—O1^{viii}	2.922 (2)
Mg1—O4	2.1669 (14)	P1—O1^{v}	1.5372 (12)
Mg2—O6	2.0234 (13)	P1—O1	1.5372 (12)
Mg2—O3^{iii}	2.0686 (13)	P1—O2^{v}	1.5476 (13)
Mg2—O2	2.0696 (14)	P1—O2	1.5476 (13)

Mg2—O5^{vi}	2.0729 (13)	P2—O5	1.5234 (12)
Mg2—O5^{vii}	2.0955 (13)	P2—O6	1.5263 (12)
Mg2—O1^{viii}	2.1153 (14)	P2—O3	1.5349 (13)
Na1—O6	2.2974 (13)	P2—O4	1.5806 (13)
Na1—O6^{ix}	2.2974 (13)	O4—H4	0.9269
Na1—O6^{vii}	2.4386 (13)		

O3^{i}—Mg1—O3^{ii}	104.23 (8)	O6^{vii}—Na1—O6^{x}	166.01 (10)
O3^{i}—Mg1—O1^{iii}	86.53 (5)	O6—Na1—O3	56.06 (5)
O3^{ii}—Mg1—O1^{iii}	78.23 (5)	O6^{ix}—Na1—O3	111.84 (7)
O3^{i}—Mg1—O1^{iv}	78.23 (5)	O6^{vii}—Na1—O3	62.51 (5)
O3^{ii}—Mg1—O1^{iv}	86.53 (5)	O6^{x}—Na1—O3	105.27 (6)
O1^{iii}—Mg1—O1^{iv}	155.13 (8)	O6—Na1—O3^{ix}	111.84 (7)
O3^{i}—Mg1—O4^{v}	83.70 (5)	O6^{ix}—Na1—O3^{ix}	56.06 (5)
O3^{ii}—Mg1—O4^{v}	170.20 (5)	O6^{vii}—Na1—O3^{ix}	105.27 (6)
O1^{iii}—Mg1—O4^{v}	108.38 (5)	O6^{x}—Na1—O3^{ix}	62.51 (5)
O1^{iv}—Mg1—O4^{v}	89.53 (5)	O3—Na1—O3^{ix}	71.02 (6)
O3^{i}—Mg1—O4	170.20 (5)	O6—Na1—O1^{xi}	118.48 (6)
O3^{ii}—Mg1—O4	83.70 (5)	O6^{ix}—Na1—O1^{xi}	74.30 (5)
O1^{iii}—Mg1—O4	89.53 (5)	O6^{vii}—Na1—O1^{xi}	84.97 (5)
O1^{iv}—Mg1—O4	108.38 (5)	O6^{x}—Na1—O1^{xi}	107.88 (6)
O4^{v}—Mg1—O4	89.05 (7)	O3—Na1—O1^{xi}	146.62 (4)
O6—Mg2—O3^{iii}	85.88 (5)	O3^{ix}—Na1—O1^{xi}	129.17 (3)
O6—Mg2—O2	88.80 (5)	O6—Na1—O1^{viii}	74.30 (5)
O3^{iii}—Mg2—O2	111.03 (6)	O6^{ix}—Na1—O1^{viii}	118.48 (7)
O6—Mg2—O5^{vi}	172.05 (6)	O6^{vii}—Na1—O1^{viii}	107.88 (6)
O3^{iii}—Mg2—O5^{vi}	91.58 (5)	O6^{x}—Na1—O1^{viii}	84.97 (5)
O2—Mg2—O5^{vi}	85.07 (5)	O3—Na1—O1^{viii}	129.17 (3)
O6—Mg2—O5^{vii}	98.45 (5)	O3^{ix}—Na1—O1^{viii}	146.62 (4)
O3^{iii}—Mg2—O5^{vii}	162.38 (6)	O1^{xi}—Na1—O1^{viii}	51.46 (6)
O2—Mg2—O5^{vii}	86.23 (5)	O1^{v}—P1—O1	111.21 (10)
O5^{vi}—Mg2—O5^{vii}	86.22 (5)	O1^{v}—P1—O2^{v}	111.07 (7)
O6—Mg2—O1^{viii}	100.87 (6)	O1—P1—O2^{v}	108.34 (7)
O3^{iii}—Mg2—O1^{viii}	79.79 (5)	O1^{v}—P1—O2	108.34 (7)
O2—Mg2—O1^{viii}	166.18 (6)	O1—P1—O2	111.07 (7)
O5^{vi}—Mg2—O1^{viii}	86.06 (5)	O2^{v}—P1—O2	106.73 (10)
O5^{vii}—Mg2—O1^{viii}	82.62 (5)	O5—P2—O6	111.03 (7)
O6—Na1—O6^{ix}	166.85 (10)	O5—P2—O3	111.42 (7)
O6—Na1—O6^{vii}	86.56 (4)	O6—P2—O3	108.82 (7)
O6^{ix}—Na1—O6^{vii}	91.84 (4)	O5—P2—O4	107.74 (7)
O6—Na1—O6^{x}	91.84 (4)	O6—P2—O4	108.99 (7)
O6^{ix}—Na1—O6^{x}	86.56 (4)	O3—P2—O4	108.78 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O2	0.93	1.57	2.4932 (17)	174