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Synthesis and crystal structure of a new magnesium phosphate $Na_3RbMg_7(PO_4)_6$

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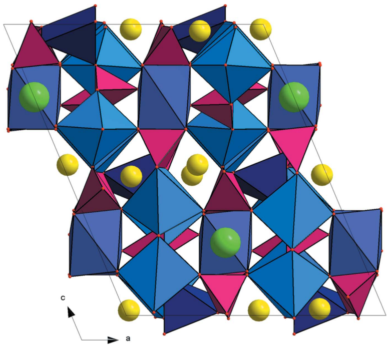
A new magnesium phosphate, $Na_3RbMg_7(PO_4)_6$ [trisodium rubidium heptamagnesium hexakis(orthophosphate)], has been synthesized as single crystals by the flux method and exhibits a new structure type. Its original structure is built up from MgO_x (x = 5 and 6) polyhedra linked directly to each other through common corners or edges and reinforced by corner-sharing with PO_4 tetrahedra. The resulting anionic three-dimensional framework leads to the formation of channels along the [010] direction, in which the Na^+ cations are located, while the Rb^+ cations are located in large interstitial cavities.



1. Chemical context

Magnesium phosphates are of increasing interest because of their potential applications as host materials for optically active rare earth ions (Seo, 2013; Kim *et al.*, 2013; Boukhris *et al.*, 2015). Moreover, these materials are very attractive in terms of basic research because they exhibit a rich structural chemistry due to their polymorphism (Ait Benhamou *et al.*, 2010; Orlova *et al.*, 2015).

Among the variety of magnesium monophosphates synthesized and characterized up to now, only four compounds belong to the system Na_3PO_4–$Mg_3(PO_4)_2$, namely $NaMgPO_4$, $NaMg_4(PO_4)_3$, $Na_2Mg_5(PO_4)_4$ and $Na_4Mg(PO_4)_2$ (Imura & Kawahara, 1997; Ben Amara *et al.*, 1983; Yamakawa *et al.*, 1994; Ghorbel *et al.*, 1974). $NaMgPO_4$ compound crystallizes in the orthorhombic system with space group $P2_12_12_1$. Its structure involves MgO_6 and MgO_5 polyhedra linked by the monophosphate groups that form a three-dimensional framework. $NaMg_4(PO_4)_3$ is also orthorhombic, space group *Pnma*. Its structure is built up from three kinds of MgO_5 units sharing edges and corners and linked to each other by the PO_4 tetrahedra, leading to a three-dimensional framework. $Na_2Mg_5(PO_4)_4$, synthesized under pressure, crystallizes in the triclinic system. Its structure results from a three-dimensional framework of MgO_6 and MgO_5 polyhedra connected either directly *via* common corners or by means of the phosphate groups. $Na_4Mg(PO_4)_2$ exhibits two polymorphs, which were only identified by their powder diffraction patterns.

Starting from these compounds, suitable replacements of magnesium and/or sodium by large cations induces their transformation into several structural types for different Mg/P atomic ratios. $NaMMg(PO_4)_2$ (M = Ca, Sr and Ba) compounds are related to the glaserite-type structure (Alkemper & Fuess, 1998; Boukhris *et al.*, 2012, 2013). They adopt an anionic two-dimensional network with different symmetries as a function of the size of the M^{2+} cation. For an atomic ratio M:P of 7:6,

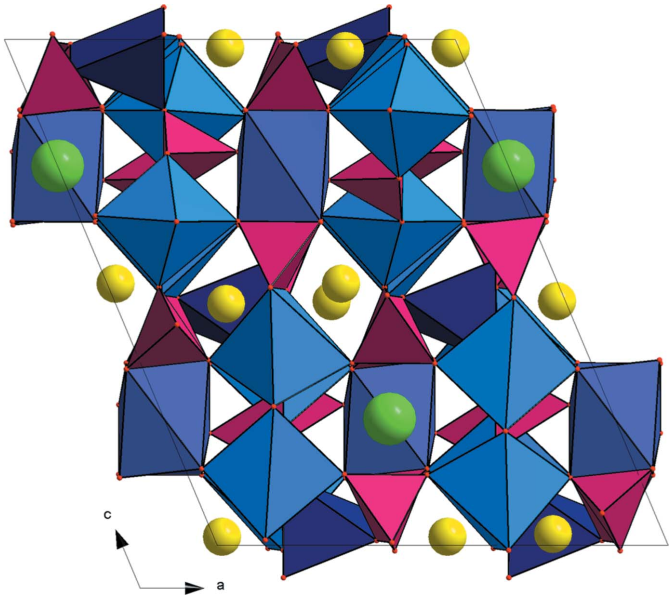


Figure 1
A view of the $Na_3RbMg_7(PO_4)_6$ structure along [010]. Colour key: MgO_x (x = 5 and 6; blue polyhedra), PO_4 (purple polyhedra), Rb (green spheres) and Na (yellow spheres).

magnesium phosphate compounds adopt a three-dimensional network related to the fillowite-type structure, as observed in $Na_4Ca_4Mg_{21}(PO_4)_{18}$, $Na_2CaMg_7(PO_4)_6$ and $Na_{2.5}Y_{0.5}Mg_7(PO_4)_6$ (Domanskii *et al.*, 1982; McCoy *et al.*, 1994; Jerbi *et al.*, 2010*a*). All of them crystallize with trigonal symmetry (space group $R\overline{3}$) and differ only by their cationic distributions. Three-dimensional anionic networks includes also original structures such as those observed in $Na_{18}Ca_{13}Mg_5(PO_4)_{18}$, $NaCa_9Mg(PO_4)_7$, $Na_7LnMg_{13}(PO_4)_{12}$ (Ln = La, Eu, Nd) (Yamakawa *et al.*, 1994; Morozov *et al.*, 1997; Jerbi *et al.*, 2010*b*, 2012).

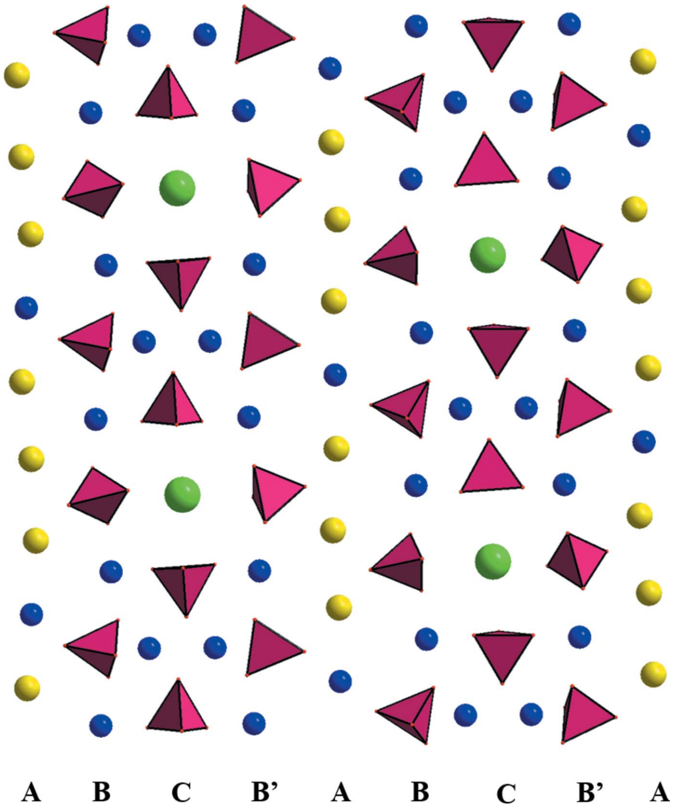


Figure 2
A view down the *b* axis, showing *ABCB*' rows made of PO_4 tetrahedra and Mg, Na and Rb atoms.

As a contribution to the investigation of the above-mentioned systems, we report here the structural characterization of a new magnesium phosphate $Na_3RbMg_7(PO_4)_6$, which is, to our knowledge, the first magnesium phosphate revealing an original structure for an atomic ratio Mg/P equal to 7/6.

2. Structural commentary

To the best of our knowledge, $Na_3RbMg_7(PO_4)_6$ exhibits a new structure type. A projection along the [010] direction of its structure (Fig. 1) clearly evidences the three-dimensional character of its anionic framework, which is built up from five different polyhedra MgO_x (x = 5, 6) and three kinds of PO_4 tetrahedra connected together by sharing edges and corners. The Na^+ cations are located within channels running along the [010] direction while the Rb^+ cations are found in the large interstitial cavities.

A projection of the structure on the (012) plane (Fig. 2) shows that it can also be described on the basis of three kinds of rows (*A*, *B* and *C*) running parallel to the [100] direction. The first row (*A;* Fig. 3), consists of units with edge-sharing between one $Na1O_8$ and two $Na2O_6$ polyhedra. Such units alternate with $Mg1O_5$ polyhedra, leading to the sequence

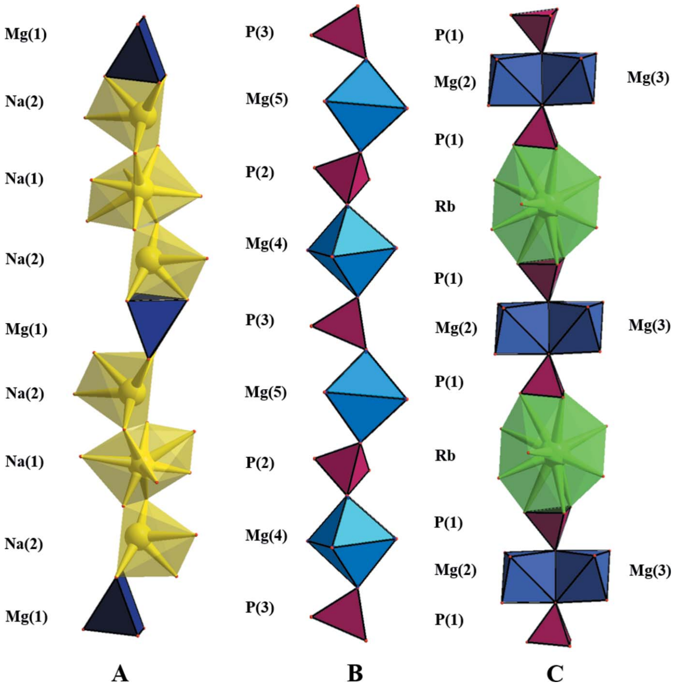


Figure 3
A view of parallel rows of *ABC* polyhedra.

–Mg1–Na2–Na1–Na2–. The second row (*B*) consists of corner-sharing P2O$_4$, P3O$_4$, Mg4O$_6$ and Mg5O$_5$ polyhedra, forming the sequence –P3–Mg4–P2–Mg5–. Rows *B* and *B*′ are symmetrical with respect to the inversion centre located on the *A* row. The last row (*C*) includes units with corner-sharing between P1O$_4$ tetrahedra and Mg$_2$O$_{10}$ dimers, which consist of edge-sharing Mg*i*O$_6$ (*i* = 2, 3) octahedra. These units alternate with RbO$_{12}$ polyhedra to form a –P1–[Mg2,Mg3]–P1–Rb– sequence. These rows, connected to each other through common corners or edges, occur with a sequence of *ABCB*′.

There are five distinct Mg sites. The Mg1 atom is displaced slightly from the inversion center, statistically occupying two symmetry-related positions. As a consequence, the Mg1O$_6$ polyhedron exhibits two distances that are long [2.241 (5) Å] compared to the other Mg1—O distances, which vary from 1.969 (10) to 2.030 (10) Å. Thus, this environment can be considered as [4 + 1]. The average value of 2.005 (10) Å calculated from the four short distances is slightly higher but consistent with that of 1.930 (2) Å reported for the tetra-coordinated Mg^{2+} cation in KMgPO$_4$ (Wallez *et al.*,1998). Sites Mg2 and Mg3 are located on twofold rotation axes and have slightly distorted octahedral environments with Mg—O distances varying from 2.052 (3) to 2.202 (2) Å for Mg2 and from 2.042 (2) to 2.169 (2) Å for Mg3. The corresponding average values of 2.123 and 2.103 Å, respectively, are in a good agreement with that of 2.14 Å observed for hexa-coordinated Mg^{2+} ions in Mg$_3$(PO$_4$)$_2$ (Jaulmes *et al.*, 1997). Site Mg4 is [5 + 1]-coordinated, with five short distances varying from 1.981 (3) to 2.050 (3) Å and a sixth longer distance of 2.5734 (3) Å. A similar environment has already been observed in Mg$_3$(PO$_4$)$_2$ (Jaulmes *et al.*, 1997). Site Mg5 is five-coordinated with Mg—O distances ranging from 2.020 (3) to 2.148 (3) Å. The corresponding mean distance of 2.07 Å is close to that of 2.08 Å observed for Mg^{2+} with the same coordination in NaMg$_4$(PO$_4$)$_3$ (Ben Amara *et al.*, 1983). The P—O distances within the PO$_4$ tetrahedra are in the range of 1.518 (2)–1.552 (2) Å with an overall mean value of 1.539 Å, very close to that of 1.537 Å predicted by Baur (1974) for monophosphate groups.

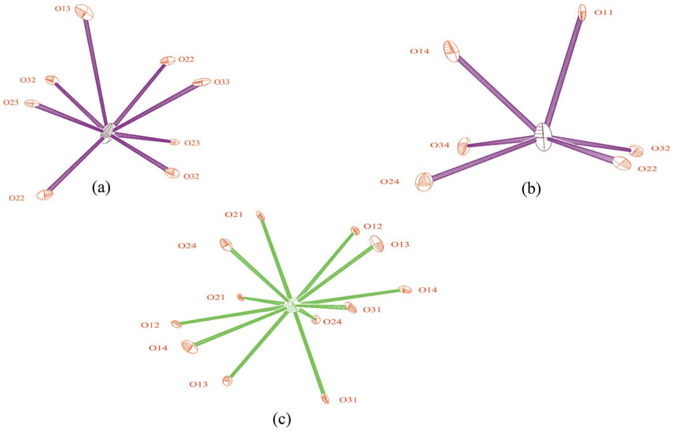


Figure 4
The environment of the (*a*) Na1$^+$, (*b*) Na2$^+$ and (*c*) Rb$^+$ cations, showing displacement ellipsoids drawn at the 50% probability level.

Table 1
Experimental details.

Crystal data	
Chemical formula	Na$_3$RbMg$_7$(PO$_4$)$_6$
M_r	894.43
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	12.734 (3), 10.685 (3), 15.498 (5)
β (°)	112.83 (2)
V (Å^3)	1943.5 (10)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	3.47
Crystal size (mm)	0.16 × 0.10 × 0.07
Data collection	
Diffractometer	Enraf–Nonius Turbo CAD-4
Absorption correction	Part of the refinement model (Δ*F*) (Parkin *et al.*, 1995)
T_{min}, T_{max}	0.377, 0.485
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2333, 2333, 1968
R_{int}	0.020
(sin θ/λ)$_{max}$ (Å^{-1})	0.660
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.036, 0.100, 1.07
No. of reflections	2333
No. of parameters	196
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.87, −1.49

Computer programs: *CAD-4 EXPRESS* (Enraf–Nonius, 1994), *XCAD4* (Harms & Wocadlo, 1995), *SIR92* (Altomare *et al.*, 1993), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg *et al.*, 1999) and *WinGX* (Farrugia, 2012).

The environments of the alkali cations are shown in Fig. 4. Those of the two crystallographic distinct Na sites were determined assuming a maximum sodium–oxygen distance L_{max} of 3.13 Å, as suggested by Donnay & Allmann (1970). As in the case of the Mg1 atom, the sodium atom Na1 is also moved slightly away from the inversion center and statistically occupying two symmetry-related positions. This moving probably occurs to accommodate the environment of the Na1 site, which then consists of eight oxygen atoms with Na—O distances varying from 2.303 (7) to 2.963 (6) Å. Na2 is bound to only six oxygen atoms, with Na2—O distances in the range 2.246 (3)–2.962 (3) Å. The Rb$^+$ ion is located on a twofold rotation axis and occupies a single site whose environment was determined assuming all Rb—O distances to be shorter than the shortest distance between Rb$^+$ and its nearest cation. This environment then consists of twelve oxygen atoms with Rb—O distances ranging from 2.923 (3) to 3.517 (2) Å.

3. Synthesis and crystallization

Single crystals of Na$_3$RbMg$_7$(PO$_4$)$_6$ were grown in a flux of sodium molybdate, Na$_2$MoO$_4$, with a P:Mo atomic ratio of 2:1. Appropriate amounts of the starting reactants (NH$_4$)H$_2$PO$_4$, Na$_2$CO$_3$, Rb$_2$CO$_3$, (MgCO$_3$)$_4$Mg(OH)$_2$·5H$_2$O and Na$_2$MoO$_4$·2H$_2$O were dissolved in nitric acid and the obtained solution was evaporated to dryness. The residue was homogenized by grinding in an agate mortar, and subsequently heated in a platinum crucible for 24 h at 673 K and then for 12 h at 873 K. After being reground, the sample was melted for 2 h at 1273 K and then cooled slowly down to room temperature at a rate of 10 K h^{-1}. The solidified melt was washed with boiling water to dissolve the flux. Colourless, irregularly shaped crystals were extracted from the final product.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The refinement was performed on the basis of electric neutrality and similar works. The atomic positions are determined by comparison with the refinements reported by Jerbi *et al.* (2010*a*) and McCoy *et al.* (1994).

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Synthesis and crystal structure of a new magnesium phosphate $Na_3RbMg_7(PO_4)_6$

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Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg *et al.*, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Trisodium rubidium heptamagnesium hexakis(orthophosphate)

Crystal data

$Mg_7Na_3O_{24}P_6Rb$	$F(000) = 1744$
$M_r = 894.43$	$D_x = 3.057$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 12.734$ (3) Å	Cell parameters from 25 reflections
$b = 10.685$ (3) Å	$\theta = 7.5–10.8°$
$c = 15.498$ (5) Å	$\mu = 3.47$ mm^{-1}
$\beta = 112.83$ (2)°	$T = 293$ K
$V = 1943.5$ (10) Å^3	Prism, colourless
$Z = 4$	0.16 × 0.10 × 0.07 mm

Data collection

Enraf–Nonius Turbo CAD-4 diffractometer	1968 reflections with $I > 2\sigma(I)$
non–profiled $\omega/2\tau$ scans	$R_{int} = 0.020$
Absorption correction: part of the refinement model (ΔF) (Parkin *et al.*, 1995)	$\theta_{max} = 28.0°$, $\theta_{min} = 2.6°$
$T_{min} = 0.377$, $T_{max} = 0.485$	$h = -16 \rightarrow 15$
2333 measured reflections	$k = 0 \rightarrow 14$
2333 independent reflections	$l = 0 \rightarrow 20$
	2 standard reflections every 60 min
	intensity decay: −2%

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 7.6361P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.036$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.100$	$\Delta\rho_{max} = 0.87$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -1.49$ e Å^{-3}
2333 reflections	
196 parameters	

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*	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
Rb	0.5000	0.74607 (5)	0.7500	0.02406 (16)	
Na1	0.2552 (5)	0.7550 (6)	0.0226 (3)	0.0279 (12)	0.5
Na2	−0.01858 (14)	0.76242 (14)	0.98277 (13)	0.0226 (4)	
Mg1	0.2487 (8)	0.2471 (9)	0.0142 (4)	0.0098 (10)	0.5
Mg2	0.0000	0.58859 (15)	0.7500	0.0071 (3)	
Mg3	0.5000	0.62142 (14)	0.2500	0.0059 (3)	
Mg4	0.18422 (9)	0.54259 (10)	0.12717 (7)	0.0065 (2)	
Mg5	0.19042 (9)	0.99696 (11)	0.14183 (7)	0.0081 (2)	
P1	0.28980 (7)	0.76938 (7)	0.27439 (6)	0.00668 (18)	
O11	0.41297 (19)	0.7658 (2)	0.27801 (17)	0.0097 (5)	
O12	0.25429 (18)	0.9074 (2)	0.27435 (15)	0.0084 (4)	
O13	0.2043 (2)	0.7106 (3)	0.18543 (18)	0.0164 (5)	
O14	0.2884 (2)	0.6963 (2)	0.36018 (17)	0.0146 (5)	
P2	0.41165 (6)	0.50005 (7)	0.08098 (5)	0.00531 (18)	
O21	0.53692 (18)	0.5150 (2)	0.15135 (15)	0.0084 (4)	
O22	0.38853 (19)	0.5698 (2)	0.98959 (16)	0.0113 (5)	
O23	0.34627 (19)	0.5654 (2)	0.13363 (15)	0.0085 (4)	
O24	0.38345 (19)	0.3619 (2)	0.06370 (17)	0.0119 (5)	
P3	0.09357 (6)	0.50198 (7)	0.92791 (5)	0.00484 (18)	
O31	−0.03126 (18)	0.4851 (2)	0.86059 (16)	0.0100 (5)	
O32	0.10990 (18)	0.6126 (2)	0.99444 (15)	0.0103 (5)	
O33	0.15211 (18)	0.5301 (2)	0.85956 (16)	0.0109 (5)	
O34	0.1418 (2)	0.3884 (2)	0.99025 (18)	0.0136 (5)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb	0.0278 (3)	0.0250 (3)	0.0200 (3)	0.000	0.0099 (2)	0.000
Na1	0.0132 (16)	0.0218 (17)	0.050 (4)	−0.0034 (12)	0.014 (3)	0.009 (3)
Na2	0.0180 (8)	0.0166 (7)	0.0412 (10)	−0.0006 (6)	0.0202 (7)	−0.0027 (6)
Mg1	0.0043 (9)	0.0081 (11)	0.015 (3)	0.0002 (8)	0.001 (2)	−0.001 (3)
Mg2	0.0052 (7)	0.0109 (7)	0.0054 (7)	0.000	0.0021 (5)	0.000
Mg3	0.0044 (7)	0.0099 (7)	0.0050 (6)	0.000	0.0037 (5)	0.000
Mg4	0.0035 (5)	0.0114 (5)	0.0052 (5)	−0.0010 (4)	0.0024 (4)	0.0014 (4)
Mg5	0.0036 (5)	0.0166 (6)	0.0055 (5)	0.0009 (4)	0.0033 (4)	−0.0002 (4)
P1	0.0030 (3)	0.0093 (4)	0.0098 (4)	−0.0003 (3)	0.0046 (3)	−0.0010 (3)
O11	0.0045 (10)	0.0115 (11)	0.0158 (11)	0.0007 (8)	0.0070 (9)	0.0000 (9)
O12	0.0059 (10)	0.0106 (11)	0.0097 (11)	0.0019 (8)	0.0042 (9)	−0.0004 (8)
O13	0.0076 (11)	0.0216 (13)	0.0179 (12)	−0.0027 (10)	0.0026 (9)	−0.0117 (11)

O14	0.0149 (12)	0.0142 (12)	0.0203 (13)	0.0005 (10)	0.0129 (10)	0.0051 (10)
P2	0.0029 (4)	0.0105 (4)	0.0038 (4)	−0.0006 (3)	0.0028 (3)	−0.0011 (3)
O21	0.0027 (10)	0.0169 (11)	0.0056 (10)	−0.0002 (8)	0.0017 (8)	−0.0028 (8)
O22	0.0098 (11)	0.0191 (12)	0.0060 (10)	−0.0007 (9)	0.0043 (9)	0.0011 (9)
O23	0.0065 (10)	0.0139 (11)	0.0072 (10)	0.0000 (8)	0.0049 (8)	−0.0026 (9)
O24	0.0081 (11)	0.0112 (11)	0.0165 (12)	−0.0023 (9)	0.0049 (9)	−0.0042 (9)
P3	0.0025 (4)	0.0090 (4)	0.0040 (4)	0.0005 (3)	0.0024 (3)	0.0008 (3)
O31	0.0027 (10)	0.0181 (12)	0.0089 (11)	−0.0016 (9)	0.0018 (8)	−0.0003 (9)
O32	0.0091 (11)	0.0144 (11)	0.0082 (11)	0.0003 (9)	0.0041 (9)	−0.0034 (9)
O33	0.0044 (10)	0.0232 (12)	0.0066 (10)	0.0001 (9)	0.0037 (8)	0.0014 (9)
O34	0.0093 (11)	0.0141 (11)	0.0197 (12)	0.0061 (9)	0.0080 (9)	0.0088 (10)

Geometric parameters (Å, º)

Rb—O24^{i}	2.923 (3)	Mg2—O33^{xvi}	2.115 (2)
Rb—O24^{ii}	2.923 (3)	Mg2—O33	2.115 (2)
Rb—O13^{iii}	3.163 (3)	Mg2—O31	2.202 (2)
Rb—O13^{iv}	3.163 (3)	Mg2—O31^{xvi}	2.202 (2)
Rb—O31^{v}	3.186 (2)	Mg3—O11	2.042 (2)
Rb—O31^{vi}	3.186 (2)	Mg3—O11^{xvii}	2.042 (2)
Rb—O21^{i}	3.301 (2)	Mg3—O21	2.100 (2)
Rb—O21^{ii}	3.301 (2)	Mg3—O21^{xvii}	2.100 (2)
Rb—O14^{iii}	3.452 (3)	Mg3—O23^{xvii}	2.169 (2)
Rb—O14^{iv}	3.452 (3)	Mg3—O23	2.169 (2)
Rb—O12^{iv}	3.517 (2)	Mg4—O13	1.981 (3)
Rb—O12^{iii}	3.517 (2)	Mg4—O12^{xv}	2.026 (3)
Na1—O32^{vii}	2.303 (7)	Mg4—O23	2.041 (2)
Na1—O32^{iv}	2.318 (7)	Mg4—O32^{vii}	2.043 (3)
Na1—O22^{iv}	2.573 (7)	Mg4—O31^{xviii}	2.050 (2)
Na1—O23	2.620 (7)	Mg4—O34^{vii}	2.573 (3)
Na1—O22^{vii}	2.782 (7)	Mg5—O22^{iv}	2.020 (3)
Na1—O13	2.878 (5)	Mg5—O21^{xix}	2.026 (2)
Na1—O33^{iv}	2.886 (6)	Mg5—O33^{iv}	2.034 (2)
Na1—O23^{viii}	2.963 (6)	Mg5—O12	2.121 (3)
Na2—O32	2.246 (3)	Mg5—O14^{xx}	2.148 (3)
Na2—O24^{ix}	2.340 (3)	P1—O13	1.521 (3)
Na2—O22^{x}	2.365 (3)	P1—O12	1.542 (2)
Na2—O34^{xi}	2.396 (3)	P1—O11	1.548 (2)
Na2—O14^{xii}	2.495 (3)	P1—O14	1.548 (2)
Na2—O11^{xii}	2.962 (3)	P2—O24	1.518 (2)
Mg1—O34^{vii}	1.969 (10)	P2—O22^{vii}	1.524 (2)
Mg1—O24	2.004 (10)	P2—O23	1.541 (2)
Mg1—O24^{xiii}	2.017 (10)	P2—O21	1.552 (2)
Mg1—O34^{xiv}	2.030 (10)	P3—O34	1.524 (2)
Mg1—O14^{xv}	2.241 (4)	P3—O32	1.528 (2)
Mg2—O11^{iv}	2.052 (3)	P3—O31	1.537 (2)
Mg2—O11^{xii}	2.052 (3)	P3—O33	1.543 (2)

O24^{i}—Rb—O24^{ii}	133.51 (9)	O24^{ix}—Na2—O22^{x}	92.29 (10)
O24^{i}—Rb—O13^{iii}	84.83 (7)	O32—Na2—O34^{xi}	90.71 (10)
O24^{ii}—Rb—O13^{iii}	101.86 (7)	O24^{ix}—Na2—O34^{xi}	71.97 (10)
O24^{i}—Rb—O13^{iv}	101.86 (7)	O22^{x}—Na2—O34^{xi}	159.77 (12)
O24^{ii}—Rb—O13^{iv}	84.83 (7)	O32—Na2—O14^{xii}	131.25 (11)
O13^{iii}—Rb—O13^{iv}	163.19 (10)	O24^{ix}—Na2—O14^{xii}	75.82 (9)
O24^{i}—Rb—O31^{v}	136.57 (6)	O22^{x}—Na2—O14^{xii}	114.69 (10)
O24^{ii}—Rb—O31^{v}	84.63 (6)	O34^{xi}—Na2—O14^{xii}	74.54 (9)
O13^{iii}—Rb—O31^{v}	110.05 (7)	O32—Na2—O11^{xii}	85.19 (9)
O13^{iv}—Rb—O31^{v}	54.74 (6)	O24^{ix}—Na2—O11^{xii}	128.61 (10)
O24^{i}—Rb—O31^{vi}	84.63 (6)	O22^{x}—Na2—O11^{xii}	99.52 (9)
O24^{ii}—Rb—O31^{vi}	136.57 (6)	O34^{xi}—Na2—O11^{xii}	100.27 (10)
O13^{iii}—Rb—O31^{vi}	54.74 (6)	O14^{xii}—Na2—O11^{xii}	53.75 (8)
O13^{iv}—Rb—O31^{vi}	110.05 (7)	O34^{vii}—Mg1—O24	91.7 (4)
O31^{v}—Rb—O31^{vi}	73.42 (9)	O34^{vii}—Mg1—O24^{xiii}	88.6 (4)
O24^{i}—Rb—O21^{i}	47.00 (6)	O24—Mg1—O24^{xiii}	166.9 (2)
O24^{ii}—Rb—O21^{i}	90.86 (6)	O34^{vii}—Mg1—O34^{xiv}	167.0 (2)
O13^{iii}—Rb—O21^{i}	72.22 (6)	O24—Mg1—O34^{xiv}	87.2 (4)
O13^{iv}—Rb—O21^{i}	123.54 (6)	O24^{xiii}—Mg1—O34^{xiv}	89.6 (4)
O31^{v}—Rb—O21^{i}	175.28 (6)	O34^{vii}—Mg1—O14^{xv}	89.2 (3)
O31^{vi}—Rb—O21^{i}	110.99 (6)	O24—Mg1—O14^{xv}	104.7 (3)
O24^{i}—Rb—O21^{ii}	90.86 (6)	O24^{xiii}—Mg1—O14^{xv}	88.4 (3)
O24^{ii}—Rb—O21^{ii}	47.00 (6)	O34^{xiv}—Mg1—O14^{xv}	103.6 (3)
O13^{iii}—Rb—O21^{ii}	123.54 (6)	O11^{iv}—Mg2—O11^{xii}	81.37 (14)
O13^{iv}—Rb—O21^{ii}	72.22 (7)	O11^{iv}—Mg2—O33^{xvi}	117.11 (10)
O31^{v}—Rb—O21^{ii}	110.99 (6)	O11^{xii}—Mg2—O33^{xvi}	89.56 (10)
O31^{vi}—Rb—O21^{ii}	175.28 (6)	O11^{iv}—Mg2—O33	89.56 (10)
O21^{i}—Rb—O21^{ii}	64.66 (8)	O11^{xii}—Mg2—O33	117.11 (10)
O24^{i}—Rb—O14^{iii}	126.45 (6)	O33^{xvi}—Mg2—O33	145.64 (16)
O24^{ii}—Rb—O14^{iii}	63.05 (6)	O11^{iv}—Mg2—O31	145.19 (10)
O13^{iii}—Rb—O14^{iii}	44.16 (6)	O11^{xii}—Mg2—O31	86.60 (9)
O13^{iv}—Rb—O14^{iii}	131.70 (6)	O33^{xvi}—Mg2—O31	95.21 (10)
O31^{v}—Rb—O14^{iii}	85.51 (6)	O33—Mg2—O31	67.21 (9)
O31^{vi}—Rb—O14^{iii}	78.00 (6)	O11^{iv}—Mg2—O31^{xvi}	86.60 (9)
O21^{i}—Rb—O14^{iii}	93.70 (6)	O11^{xii}—Mg2—O31^{xvi}	145.19 (10)
O21^{ii}—Rb—O14^{iii}	103.71 (6)	O33^{xvi}—Mg2—O31^{xvi}	67.21 (9)
O24^{i}—Rb—O14^{iv}	63.05 (6)	O33—Mg2—O31^{xvi}	95.20 (9)
O24^{ii}—Rb—O14^{iv}	126.45 (6)	O31—Mg2—O31^{xvi}	119.70 (14)
O13^{iii}—Rb—O14^{iv}	131.70 (6)	O11—Mg3—O11^{xvii}	81.88 (14)
O13^{iv}—Rb—O14^{iv}	44.16 (6)	O11—Mg3—O21	149.00 (10)
O31^{v}—Rb—O14^{iv}	78.00 (6)	O11^{xvii}—Mg3—O21	87.76 (9)
O31^{vi}—Rb—O14^{iv}	85.51 (6)	O11—Mg3—O21^{xvii}	87.76 (9)
O21^{i}—Rb—O14^{iv}	103.71 (6)	O11^{xvii}—Mg3—O21^{xvii}	149.00 (10)
O21^{ii}—Rb—O14^{iv}	93.70 (6)	O21—Mg3—O21^{xvii}	114.43 (14)
O14^{iii}—Rb—O14^{iv}	159.44 (9)	O11—Mg3—O23^{xvii}	114.89 (10)
O24^{i}—Rb—O12^{iv}	67.45 (6)	O11^{xvii}—Mg3—O23^{xvii}	89.77 (9)
O24^{ii}—Rb—O12^{iv}	90.89 (6)	O21—Mg3—O23^{xvii}	94.09 (9)
O13^{iii}—Rb—O12^{iv}	150.50 (6)	O21^{xvii}—Mg3—O23^{xvii}	68.28 (9)

O13^{iv}—Rb—O12^{iv}	42.77 (6)	O11—Mg3—O23	89.77 (9)
O31^{v}—Rb—O12^{iv}	97.43 (6)	O11^{xvii}—Mg3—O23	114.89 (10)
O31^{vi}—Rb—O12^{iv}	128.18 (6)	O21—Mg3—O23	68.28 (9)
O21^{i}—Rb—O12^{iv}	81.20 (5)	O21^{xvii}—Mg3—O23	94.09 (9)
O21^{ii}—Rb—O12^{iv}	50.59 (5)	O23^{xvii}—Mg3—O23	147.97 (14)
O14^{iii}—Rb—O12^{iv}	153.49 (6)	O13—Mg4—O12^{xv}	111.06 (11)
O14^{iv}—Rb—O12^{iv}	43.24 (6)	O13—Mg4—O23	85.41 (10)
O24^{i}—Rb—O12^{iii}	90.89 (6)	O12^{xv}—Mg4—O23	87.74 (10)
O24^{ii}—Rb—O12^{iii}	67.45 (6)	O13—Mg4—O32^{vii}	93.13 (12)
O13^{iii}—Rb—O12^{iii}	42.77 (6)	O12^{xv}—Mg4—O32^{vii}	155.80 (11)
O13^{iv}—Rb—O12^{iii}	150.50 (6)	O23—Mg4—O32^{vii}	94.02 (10)
O31^{v}—Rb—O12^{iii}	128.18 (6)	O13—Mg4—O31^{xviii}	92.75 (11)
O31^{vi}—Rb—O12^{iii}	97.43 (6)	O12^{xv}—Mg4—O31^{xviii}	86.03 (10)
O21^{i}—Rb—O12^{iii}	50.59 (5)	O23—Mg4—O31^{xviii}	172.38 (11)
O21^{ii}—Rb—O12^{iii}	81.20 (5)	O32^{vii}—Mg4—O31^{xviii}	93.46 (10)
O14^{iii}—Rb—O12^{iii}	43.24 (6)	O13—Mg4—O34^{vii}	154.80 (11)
O14^{iv}—Rb—O12^{iii}	153.49 (6)	O12^{xv}—Mg4—O34^{vii}	93.48 (10)
O12^{iv}—Rb—O12^{iii}	124.43 (8)	O23—Mg4—O34^{vii}	90.10 (9)
O32^{vii}—Na1—O32^{iv}	163.38 (18)	O32^{vii}—Mg4—O34^{vii}	62.42 (9)
O32^{vii}—Na1—O22^{iv}	88.3 (2)	O31^{xviii}—Mg4—O34^{vii}	94.64 (9)
O32^{iv}—Na1—O22^{iv}	94.9 (3)	O22^{iv}—Mg5—O21^{xix}	89.44 (10)
O32^{vii}—Na1—O23	74.4 (2)	O22^{iv}—Mg5—O33^{iv}	92.64 (10)
O32^{iv}—Na1—O23	112.8 (3)	O21^{xix}—Mg5—O33^{iv}	175.75 (11)
O22^{iv}—Na1—O23	137.03 (19)	O22^{iv}—Mg5—O12	132.14 (11)
O32^{vii}—Na1—O22^{vii}	89.9 (2)	O21^{xix}—Mg5—O12	89.48 (10)
O32^{iv}—Na1—O22^{vii}	83.2 (2)	O33^{iv}—Mg5—O12	86.38 (10)
O22^{iv}—Na1—O22^{vii}	166.37 (17)	O22^{iv}—Mg5—O14^{xx}	110.57 (11)
O23—Na1—O22^{vii}	54.84 (15)	O21^{xix}—Mg5—O14^{xx}	92.12 (10)
Na1^{viii}—Na1—O13	150.6 (12)	O33^{iv}—Mg5—O14^{xx}	90.63 (10)
O32^{vii}—Na1—O13	67.64 (15)	O12—Mg5—O14^{xx}	117.28 (10)
O32^{iv}—Na1—O13	129.0 (2)	O13—P1—O12	106.71 (14)
O22^{iv}—Na1—O13	77.79 (16)	O13—P1—O11	112.40 (14)
O23—Na1—O13	59.29 (12)	O12—P1—O11	108.47 (12)
O22^{vii}—Na1—O13	113.9 (2)	O13—P1—O14	109.11 (15)
O32^{vii}—Na1—O33^{iv}	138.3 (2)	O12—P1—O14	112.44 (13)
O32^{iv}—Na1—O33^{iv}	56.44 (15)	O11—P1—O14	107.79 (13)
O22^{iv}—Na1—O33^{iv}	64.67 (16)	O24—P2—O22^{vii}	111.34 (14)
O23—Na1—O33^{iv}	103.37 (17)	O24—P2—O23	113.25 (13)
O22^{vii}—Na1—O33^{iv}	123.6 (2)	O22^{vii}—P2—O23	108.74 (13)
O13—Na1—O33^{iv}	75.63 (12)	O24—P2—O21	109.41 (13)
O32^{vii}—Na1—O23^{viii}	102.1 (2)	O22^{vii}—P2—O21	112.20 (13)
O32^{iv}—Na1—O23^{viii}	67.63 (16)	O23—P2—O21	101.56 (12)
O22^{iv}—Na1—O23^{viii}	52.91 (14)	O34—P3—O32	105.79 (14)
O23—Na1—O23^{viii}	168.2 (2)	O34—P3—O31	113.15 (14)
O22^{vii}—Na1—O23^{viii}	114.48 (15)	O32—P3—O31	112.52 (13)
O13—Na1—O23^{viii}	130.4 (2)	O34—P3—O33	114.02 (13)
O33^{iv}—Na1—O23^{viii}	86.8 (2)	O32—P3—O33	109.69 (14)

O32—Na2—O24^{ix}	143.52 (12)	O31—P3—O33	101.82 (13)
O32—Na2—O22^{x}	95.11 (10)		

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1/2, −*y*+3/2, *z*+1/2; (iv) −*x*+1/2, −*y*+3/2, −*z*+1; (v) *x*+1/2, *y*+1/2, *z*; (vi) −*x*+1/2, *y*+1/2, −*z*+3/2; (vii) *x*, *y*, *z*−1; (viii) −*x*+1/2, −*y*+3/2, −*z*; (ix) *x*−1/2, *y*+1/2, *z*+1; (x) −*x*+1/2, −*y*+3/2, −*z*+2; (xi) −*x*, −*y*+1, −*z*+2; (xii) *x*−1/2, −*y*+3/2, *z*+1/2; (xiii) −*x*+1/2, −*y*+1/2, −*z*; (xiv) −*x*+1/2, −*y*+1/2, −*z*+1; (xv) −*x*+1/2, *y*−1/2, −*z*+1/2; (xvi) −*x*, *y*, −*z*+3/2; (xvii) −*x*+1, *y*, −*z*+1/2; (xviii) −*x*, −*y*+1, −*z*+1; (xix) *x*−1/2, *y*+1/2, *z*; (xx) −*x*+1/2, *y*+1/2, −*z*+1/2.