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# Heptamagnesium bis(phosphate) tetrakis(hydrogen phosphate) with strong hydrogen bonds: $Mg_7(PO_4)_2(HPO_4)_4$

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Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(P–O) = 0.002 Å; $R$ factor = 0.026; $wR$ factor = 0.072; data-to-parameter ratio = 11.4.

The title compound, $Mg_7(PO_4)_2(HPO_4)_4$, was synthesized by the hydrothermal method. The structure is based on a framework of edge- and corner-sharing $MgO_6$ and $MgO_4(OH)_2$ octahedra, an $MgO_5$ polyhedron, $PO_4$ and $PO_3(OH)$ tetrahedra. All atoms are in general positions except for one Mg atom, which is located on a crystallographic inversion centre. The OH groups, bridging Mg–(OH)–P, are involved in strong hydrogen bonds. Compounds with the general formula $M_7(PO_4)_2(HPO_4)_4$ ($M$ = Mg, Mn, Fe and Co) are all isostructural with their homologue arsenate $Mg_7(AsO_4)_2(HAsO_4)_4$.

## Related literature

For background to metal phosphates, see: Viter & Nagornyi (2009); Clearfield (1988); Trad *et al.* (2010). For the hydrothermal method, see: Assani *et al.* (2010, 2011*a*,*b*). For isostructural compounds, see: Zhou *et al.* (2002); Riou *et al.* (1987); Rojo *et al.* (2002); Lightfoot & Cheetham (1988); Kolitsch & Bartu (2004).

## Experimental

### *Crystal data*

$Mg_7(PO_4)_2(HPO_4)_4$
$M_r$ = 744.02
Triclinic, $P\overline{1}$
$a$ = 6.4204 (5) Å
$b$ = 7.8489 (4) Å
$c$ = 9.4315 (5) Å
$\alpha$ = 104.442 (3)°
$\beta$ = 108.505 (5)°
$\gamma$ = 101.189 (8)°
$V$ = 416.70 (4) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.06 mm$^{-1}$
$T$ = 296 K
0.16 × 0.10 × 0.07 mm

### *Data collection*

Bruker X8 APEX Diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.881, $T_{max}$ = 0.929
9421 measured reflections
1923 independent reflections
1715 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.072
$S$ = 1.07
1923 reflections
169 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4···O7$^{i}$ | 0.86 | 1.61 | 2.460 (2) | 172 |
| O12—H12···O10$^{ii}$ | 0.86 | 1.80 | 2.656 (2) | 171 |

Symmetry codes: (i) $x, y-1, z$; (ii) $-x-1, -y+1, -z-1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5638).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, i52 [ **doi:10.1107/S1600536811036361** ]

# Heptamagnesium bis(phosphate) tetrakis(hydrogen phosphate) with strong hydrogen bonds: $Mg_7(PO_4)_2(HPO_4)_4$

**A. Assani, M. Saadi, M. Zriouil and L. El Ammari**

## Comment

Widespread studies are devoted to the metal phosphate owing to their impressive structural diversity and to their prospective applications in catalysis (Viter & Nagornyi, 2009), ion-exchangers (Clearfield, 1988)) and in batteries performance (Trad *et al.*, (2010)). Mainly, our most attention has been paid to the hydrothermal synthesis of new metal based phosphate. Accordingly, we have recently succeed to obtain new phosphates, such as $Ni_2Sr(PO_4)_2\ 2H_2O$ (Assani *et al.* (2010)), $AgMg_3(PO_4)(HPO_4)_2$ (Assani *et al.* (2011*b*)) and $Ag_2Ni_3(HPO_4)(PO_4)_2$ (Assani *et al.* (2011*a*)).

Besides, the investigation of the MO—$P_2O_5$ systems (*M*=divalent cations) has allowed to isolate a new member of the metal phosphates, with a general formula $M_7(PO_4)_2(HPO_4)_4$. The present paper aims to develop the hydrothermal synthesis and the structural characterization of the $Mg_7(PO_4)_2(HPO_4)_4$ which is isostructural with $Fe_7(PO_4)_2(HPO_4)_4$ (Zhou *et al.* (2002)), $Mn_7(PO_4)_2(HPO_4)_4$ (Riou *et al.* (1987) and (Rojo *et al.* (2002)), $Co_7(PO_4)_2(HPO_4)_4$ (Lightfoot & Cheetham, (1988)) and with their homologue arsenate $Mg_7(AsO_4)_2(HAsO_4)_4$ (Kolitsch & Bartu, (2004)).

The crystal structure of $Mg_7(PO_4)_2(HPO_4)_4$ is built up from $MgO_6$, $MgO_4(OH)_2$ octahedra, $MgO_5$ polyhedron, $PO_4$ and $PO_3(OH)$ tetrahedra, sharing corners and edges to form a three-dimensional framework as shown in Fig.1 and Fig.2. In the asymmetric unit, all atoms are in general positions except for atom Mg2, which is located at a crystallographic inversion centre (0, 0, 0). Each OH group is bonded to an Mg and an P atom. Atom Mg2 is located at the centre of an $Mg2O_6$ octahedron with significant bond-length distortion as shown in Table 1. In contrast, $Mg1O_6$ and $Mg3O_4(OH)_2$ represent less distorted octahedra, and atom Mg4 is surrounded by five O ligands, forming a distorted $Mg4O_5$ trigonal bipyramid. In this structure, each $Mg1O_6$ and $Mg3O_6$ octahedron shares an edge with its symmetrical to form a dimer. Both dimers, $Mg1O_{10}$ and $Mg3O_{10}$ are bound by $Mg4O_5$ by sharing two edges to form a zigzag chaine. The $Mg2O_6$ octahedron and $PO_4$ tetrahedra are linked to neighboring polyhedra by vertices. The three crystallographically independent P atoms show tetrahedral coordination. The $PO_4$ groups are relatively regular, although the two protonated groups, centred by P1 and P3, show a stronger angular and bond-length distortion in comparison with the unprotonated $P2O_4$ tetrahedron as shown in Table 1. Moreover the OH groups, bridging Mg–(OH)–P, are involved in strong hydrogen bonds (Table 2).

## Experimental

The crystals of the title compound is isolated from the hydrothermal treatment of the reaction mixture of magnesium oxide (MgO) and 85%wt phosphoric acid ($H_3PO_4$) in the nominal proportion corresponding to the molar ratio Mg: P = 7:6. The hydrothermal reaction was conducted in a 23 ml Teflon-lined autoclave, filled to 50% with distilled water and under autogenously pressure at 468 K for two days. After being filtered off, washed with deionized water and air dried, the reaction product consists of a white powder and colourless parallelepipedic crystals corresponding to the title compound.

### Refinement

The H atoms were initially located in a difference map and refined with O—H distance restraints of 0.86 (1). In a the last cycle they were refined in the riding model approximation with $U_{iso}$(H) set to 1.2$U_{eq}$(O).

### Figures

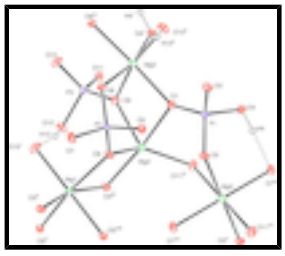

Fig. 1. Partial plot of $Mg_7(PO_4)_2(HPO_4)_4$ crystal structure. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) -*x* - 1, -*y* + 1, -*z* - 1; (ii) -*x*, -*y* + 1, -*z*; (iii) *x* - 1, *y*, *z*; (iv) *x*, *y* - 1, *z*; (v) -*x*, -*y*, -*z*; (vi) -*x* - 1, -*y*, -*z* - 1; (vii) *x* + 1, *y*, *z* + 1; (viii) -*x*, -*y*, -*z* - 1; (ix) -*x*, -*y* + 1, -*z* - 1; (*x*) *x* + 1, *y*, *z*; (xi) *x*, *y* + 1, *z*; (xii) *x* - 1, *y*, *z* - 1.

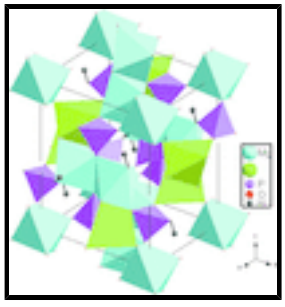

Fig. 2. A three-dimensional polyhedral view of the crystal structure of the $Mg_7(PO_4)_2(HPO_4)_4$ showing polyhedra linkage.

### Heptamagnesium bis(phosphate) tetrakis(hydrogen phosphate)

*Crystal data*

| | |
|---|---|
| $Mg_7(PO_4)_2(HPO_4)_4$ | $Z = 1$ |
| $M_r = 744.02$ | $F(000) = 370$ |
| Triclinic, $P\overline{1}$ | $D_x = 2.965$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 6.4204$ (5) Å | Cell parameters from 1923 reflections |
| $b = 7.8489$ (4) Å | $\theta = 2.4$–$27.6°$ |
| $c = 9.4315$ (5) Å | $\mu = 1.06$ mm$^{-1}$ |
| $\alpha = 104.442$ (3)° | $T = 296$ K |
| $\beta = 108.505$ (5)° | Parallelepipedic, colourless |
| $\gamma = 101.189$ (8)° | 0.16 × 0.10 × 0.07 mm |
| $V = 416.70$ (4) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker X8 APEX Diffractometer | 1923 independent reflections |
| Radiation source: fine-focus sealed tube | 1715 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.036$ |
| φ and ω scans | $\theta_{max} = 27.6°$, $\theta_{min} = 2.4°$ |
| Absorption correction: multi-scan | $h = -8 \rightarrow 8$ |

(*SADABS*; Bruker, 2005)

$T_{min}$ = 0.881, $T_{max}$ = 0.929

9421 measured reflections

$k$ = −10→10

$l$ = −11→12

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.026

$wR(F^2)$ = 0.072

$S$ = 1.07

1923 reflections

169 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

$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 0.6237P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$

$\Delta\rho_{min}$ = −0.42 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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mg1 | −0.38348 (12) | 0.54390 (10) | −0.10950 (8) | 0.00639 (17) |
| Mg2 | 0.0000 | 0.0000 | 0.0000 | 0.0094 (2) |
| Mg3 | −0.05324 (13) | 0.28758 (10) | −0.51536 (9) | 0.00821 (17) |
| Mg4 | −0.27778 (13) | 0.19081 (11) | −0.28530 (9) | 0.00902 (17) |
| P1 | 0.22691 (9) | 0.14512 (8) | −0.22413 (6) | 0.00561 (13) |
| P2 | 0.08899 (9) | 0.58025 (7) | −0.17255 (6) | 0.00465 (13) |
| P3 | −0.59090 (9) | 0.23141 (8) | −0.62865 (7) | 0.00658 (14) |
| O1 | 0.0189 (3) | 0.1762 (2) | −0.33779 (18) | 0.0081 (3) |
| O2 | 0.2208 (3) | 0.1877 (2) | −0.05694 (18) | 0.0074 (3) |
| O3 | 0.4517 (3) | 0.2446 (2) | −0.22968 (18) | 0.0077 (3) |
| O4 | 0.2013 (3) | −0.0667 (2) | −0.27972 (18) | 0.0091 (3) |
| H4 | 0.1828 | −0.1148 | −0.2104 | 0.011* |
| O5 | 0.3069 (3) | 0.5385 (2) | −0.08555 (18) | 0.0068 (3) |
| O6 | 0.0589 (3) | 0.5452 (2) | −0.34643 (18) | 0.0073 (3) |
| O7 | 0.1098 (3) | 0.7857 (2) | −0.09645 (19) | 0.0094 (3) |
| O8 | −0.1240 (3) | 0.4602 (2) | −0.16487 (18) | 0.0070 (3) |

| | | | | |
|---|---|---|---|---|
| O9 | −0.3803 (3) | 0.2112 (2) | −0.50853 (19) | 0.0104 (3) |
| O10 | −0.5267 (3) | 0.3827 (2) | −0.69363 (19) | 0.0106 (3) |
| O11 | −0.7360 (3) | 0.0488 (2) | −0.76029 (19) | 0.0097 (3) |
| O12 | −0.7344 (3) | 0.2950 (2) | −0.52719 (19) | 0.0111 (3) |
| H12 | −0.6495 | 0.3935 | −0.4485 | 0.013* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mg1 | 0.0064 (4) | 0.0077 (4) | 0.0058 (4) | 0.0022 (3) | 0.0028 (3) | 0.0028 (3) |
| Mg2 | 0.0120 (5) | 0.0086 (5) | 0.0095 (5) | 0.0035 (4) | 0.0061 (4) | 0.0034 (4) |
| Mg3 | 0.0091 (4) | 0.0083 (4) | 0.0076 (4) | 0.0021 (3) | 0.0037 (3) | 0.0029 (3) |
| Mg4 | 0.0093 (4) | 0.0082 (4) | 0.0104 (4) | 0.0027 (3) | 0.0047 (3) | 0.0031 (3) |
| P1 | 0.0055 (3) | 0.0055 (3) | 0.0056 (3) | 0.0011 (2) | 0.0024 (2) | 0.0016 (2) |
| P2 | 0.0045 (3) | 0.0052 (3) | 0.0047 (3) | 0.0017 (2) | 0.0019 (2) | 0.0020 (2) |
| P3 | 0.0058 (3) | 0.0073 (3) | 0.0067 (3) | 0.0019 (2) | 0.0023 (2) | 0.0025 (2) |
| O1 | 0.0056 (7) | 0.0103 (8) | 0.0084 (8) | 0.0024 (6) | 0.0019 (6) | 0.0041 (6) |
| O2 | 0.0086 (7) | 0.0070 (7) | 0.0056 (7) | 0.0010 (6) | 0.0031 (6) | 0.0008 (6) |
| O3 | 0.0056 (7) | 0.0078 (7) | 0.0088 (7) | −0.0002 (6) | 0.0037 (6) | 0.0019 (6) |
| O4 | 0.0133 (8) | 0.0067 (7) | 0.0085 (8) | 0.0025 (6) | 0.0057 (6) | 0.0030 (6) |
| O5 | 0.0053 (7) | 0.0094 (7) | 0.0068 (7) | 0.0034 (6) | 0.0024 (6) | 0.0034 (6) |
| O6 | 0.0097 (7) | 0.0081 (7) | 0.0053 (7) | 0.0036 (6) | 0.0035 (6) | 0.0030 (6) |
| O7 | 0.0119 (8) | 0.0060 (7) | 0.0109 (8) | 0.0038 (6) | 0.0050 (6) | 0.0021 (6) |
| O8 | 0.0049 (7) | 0.0071 (7) | 0.0091 (7) | 0.0010 (6) | 0.0037 (6) | 0.0020 (6) |
| O9 | 0.0085 (8) | 0.0157 (8) | 0.0086 (8) | 0.0059 (6) | 0.0030 (6) | 0.0052 (6) |
| O10 | 0.0117 (8) | 0.0093 (8) | 0.0087 (8) | −0.0002 (6) | 0.0018 (6) | 0.0048 (6) |
| O11 | 0.0098 (7) | 0.0073 (7) | 0.0102 (8) | 0.0014 (6) | 0.0025 (6) | 0.0025 (6) |
| O12 | 0.0084 (8) | 0.0137 (8) | 0.0099 (8) | 0.0037 (6) | 0.0042 (6) | 0.0010 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Mg1—O10$^{i}$ | 2.0235 (17) | P1—O2 | 1.5431 (16) |
| Mg1—O5$^{ii}$ | 2.0462 (17) | P1—O4 | 1.5718 (16) |
| Mg1—O5$^{iii}$ | 2.0643 (17) | P2—O5 | 1.5237 (16) |
| Mg1—O8 | 2.0698 (17) | P2—O6 | 1.5350 (16) |
| Mg1—O2$^{ii}$ | 2.1093 (17) | P2—O8 | 1.5362 (16) |
| Mg1—O3$^{iii}$ | 2.2065 (17) | P2—O7 | 1.5533 (16) |
| Mg2—O7$^{iv}$ | 2.0630 (16) | P3—O10 | 1.5131 (16) |
| Mg2—O7$^{ii}$ | 2.0630 (16) | P3—O11 | 1.5245 (17) |
| Mg2—O2 | 2.1296 (15) | P3—O9 | 1.5287 (16) |
| Mg2—O2$^{v}$ | 2.1296 (15) | P3—O12 | 1.5853 (17) |
| Mg2—O11$^{vi}$ | 2.2395 (16) | O2—Mg1$^{ii}$ | 2.1093 (17) |
| Mg2—O11$^{vii}$ | 2.2395 (16) | O3—Mg4$^{x}$ | 2.0549 (17) |
| Mg3—O4$^{viii}$ | 2.0415 (17) | O3—Mg1$^{x}$ | 2.2065 (17) |
| Mg3—O1 | 2.0443 (17) | O4—Mg3$^{viii}$ | 2.0415 (17) |
| Mg3—O6 | 2.0606 (17) | O4—H4 | 0.8601 |

| | | | |
|---|---|---|---|
| Mg3—O6$^{ix}$ | 2.0649 (17) | O5—Mg1$^{ii}$ | 2.0462 (17) |
| Mg3—O12$^{x}$ | 2.0759 (17) | O5—Mg1$^{x}$ | 2.0643 (17) |
| Mg3—O9 | 2.0954 (17) | O6—Mg3$^{ix}$ | 2.0649 (17) |
| Mg4—O8 | 2.0041 (17) | O7—Mg2$^{xi}$ | 2.0630 (16) |
| Mg4—O11$^{vi}$ | 2.0426 (18) | O10—Mg1$^{i}$ | 2.0235 (17) |
| Mg4—O9 | 2.0544 (17) | O11—Mg4$^{vi}$ | 2.0426 (18) |
| Mg4—O3$^{iii}$ | 2.0549 (17) | O11—Mg2$^{xii}$ | 2.2395 (16) |
| Mg4—O1 | 2.1312 (17) | O12—Mg3$^{iii}$ | 2.0759 (17) |
| P1—O3 | 1.5252 (16) | O12—H12 | 0.8600 |
| P1—O1 | 1.5297 (16) | | |
| O10$^{i}$—Mg1—O5$^{ii}$ | 177.45 (7) | O1—Mg3—O12$^{x}$ | 90.91 (7) |
| O10$^{i}$—Mg1—O5$^{iii}$ | 93.60 (7) | O6—Mg3—O12$^{x}$ | 95.01 (7) |
| O5$^{ii}$—Mg1—O5$^{iii}$ | 84.54 (7) | O6$^{ix}$—Mg3—O12$^{x}$ | 82.93 (7) |
| O10$^{i}$—Mg1—O8 | 89.62 (7) | O4$^{viii}$—Mg3—O9 | 82.41 (7) |
| O5$^{ii}$—Mg1—O8 | 91.62 (7) | O1—Mg3—O9 | 80.21 (7) |
| O5$^{iii}$—Mg1—O8 | 161.77 (7) | O6—Mg3—O9 | 96.14 (7) |
| O10$^{i}$—Mg1—O2$^{ii}$ | 97.16 (7) | O6$^{ix}$—Mg3—O9 | 108.15 (7) |
| O5$^{ii}$—Mg1—O2$^{ii}$ | 84.67 (7) | O12$^{x}$—Mg3—O9 | 165.63 (8) |
| O5$^{iii}$—Mg1—O2$^{ii}$ | 92.32 (7) | O8—Mg4—O11$^{vi}$ | 135.86 (7) |
| O8—Mg1—O2$^{ii}$ | 105.09 (7) | O8—Mg4—O9 | 97.00 (7) |
| O10$^{i}$—Mg1—O3$^{iii}$ | 96.93 (7) | O11$^{vi}$—Mg4—O9 | 124.27 (7) |
| O5$^{ii}$—Mg1—O3$^{iii}$ | 81.15 (6) | O8—Mg4—O3$^{iii}$ | 83.43 (7) |
| O5$^{iii}$—Mg1—O3$^{iii}$ | 83.53 (6) | O11$^{vi}$—Mg4—O3$^{iii}$ | 102.94 (7) |
| O8—Mg1—O3$^{iii}$ | 78.27 (6) | O9—Mg4—O3$^{iii}$ | 98.66 (7) |
| O2$^{ii}$—Mg1—O3$^{iii}$ | 165.53 (7) | O8—Mg4—O1 | 88.96 (7) |
| O7$^{iv}$—Mg2—O7$^{ii}$ | 180.00 (7) | O11$^{vi}$—Mg4—O1 | 84.69 (7) |
| O7$^{iv}$—Mg2—O2 | 91.18 (6) | O9—Mg4—O1 | 79.14 (7) |
| O7$^{ii}$—Mg2—O2 | 88.82 (6) | O3$^{iii}$—Mg4—O1 | 171.78 (7) |
| O7$^{iv}$—Mg2—O2$^{v}$ | 88.82 (6) | O3—P1—O1 | 111.79 (9) |
| O7$^{ii}$—Mg2—O2$^{v}$ | 91.18 (6) | O3—P1—O2 | 114.92 (9) |
| O2—Mg2—O2$^{v}$ | 180.00 (7) | O1—P1—O2 | 110.31 (9) |
| O7$^{iv}$—Mg2—O11$^{vi}$ | 90.17 (6) | O3—P1—O4 | 106.96 (9) |
| O7$^{ii}$—Mg2—O11$^{vi}$ | 89.83 (6) | O1—P1—O4 | 107.87 (9) |
| O2—Mg2—O11$^{vi}$ | 85.85 (6) | O2—P1—O4 | 104.43 (9) |
| O2$^{v}$—Mg2—O11$^{vi}$ | 94.15 (6) | O5—P2—O6 | 109.03 (9) |
| O7$^{iv}$—Mg2—O11$^{vii}$ | 89.83 (6) | O5—P2—O8 | 111.40 (9) |
| O7$^{ii}$—Mg2—O11$^{vii}$ | 90.17 (6) | O6—P2—O8 | 109.62 (9) |
| O2—Mg2—O11$^{vii}$ | 94.15 (6) | O5—P2—O7 | 109.95 (9) |
| O2$^{v}$—Mg2—O11$^{vii}$ | 85.85 (6) | O6—P2—O7 | 108.49 (9) |
| O11$^{vi}$—Mg2—O11$^{vii}$ | 180.00 (8) | O8—P2—O7 | 108.30 (9) |
| O4$^{viii}$—Mg3—O1 | 104.92 (7) | O10—P3—O11 | 112.06 (9) |

| | | | |
|---|---|---|---|
| O4$^{viii}$—Mg3—O6 | 165.27 (8) | O10—P3—O9 | 112.08 (9) |
| O1—Mg3—O6 | 89.19 (7) | O11—P3—O9 | 111.85 (9) |
| O4$^{viii}$—Mg3—O6$^{ix}$ | 87.80 (7) | O10—P3—O12 | 107.28 (9) |
| O1—Mg3—O6$^{ix}$ | 165.83 (8) | O11—P3—O12 | 109.21 (9) |
| O6—Mg3—O6$^{ix}$ | 78.70 (7) | O9—P3—O12 | 103.90 (9) |
| O4$^{viii}$—Mg3—O12$^{x}$ | 89.06 (7) | | |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4···O7$^{iv}$ | 0.86 | 1.61 | 2.460 (2) | 172. |
| O12—H12···O10$^{i}$ | 0.86 | 1.80 | 2.656 (2) | 171. |

Symmetry codes: (iv) *x*, *y*−1, *z*; (i) −*x*−1, −*y*+1, −*z*−1.

**Fig. 1**

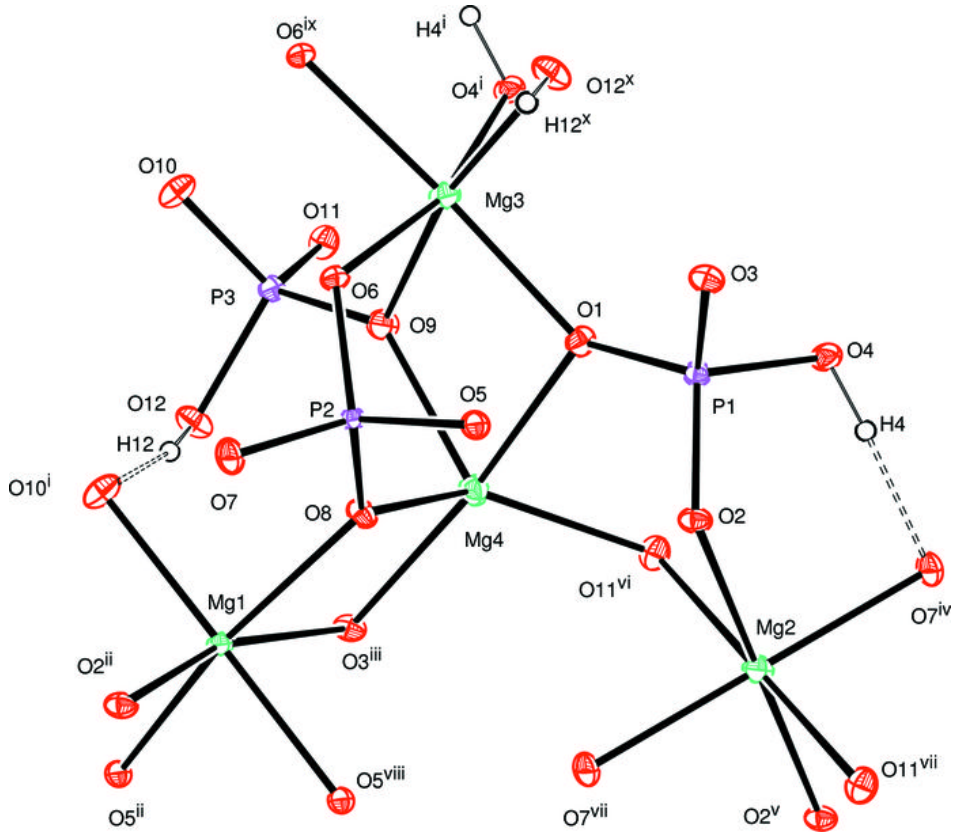
O6ix
H4i
O4i
O12x
H12x
O10
Mg3
O11
O3
P3
O6
O1
O9
O4
O12
P2
O5
P1
H12
H4
O10i
O7
O8
O2
Mg4
O11vi
Mg1
O7iv
Mg2
O2ii
O3iii
O5viii
O11vii
O5ii
O7vii
O2v

**Fig. 2**