

CsMgPO₄Nataliya Yu. Strutynska,^{a*} Igor V. Zatovsky,^a
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Key indicators: single-crystal X-ray study; *T* = 293 K; mean $\sigma(\text{P}-\text{O}) = 0.001 \text{ \AA}$; *R* factor = 0.021; *wR* factor = 0.047; data-to-parameter ratio = 27.7.

Caesium magnesium orthophosphate is built up from MgO₄ and PO₄ tetrahedra (both with *m*. symmetry) linked together by corners, forming a three-dimensional framework. The Cs atoms have *m*. site symmetry and are located in hexagonal channels running along the *a*- and *b*-axis directions.

Related literature

For the properties of double phosphates $A^I B^{II} \text{PO}_4$ ($A^I =$ alkali metal; $B^{II} =$ Ca, Sr, Ba, Zn, Cd, Pb) such as ferroelectric and non-linear optical behaviour, see: Blum *et al.* (1984); Elouadi *et al.* (1984); Sawada *et al.* (2003). Several polymorphs have been found among orthophosphates containing Cs and divalent metals, see: Blum *et al.* (1986) for CsZnPO₄. In contrast, CsMnPO₄ occurs in only one type, see: Yakubovich *et al.* (1990). The title compound is isotypic with the *Pnma* form of CsZnPO₄. For related structures, see: Yakubovich *et al.* (1990); Blum *et al.* (1986); Zaripov *et al.* (2008).

Experimental

Crystal data

| | |
|------------------------------|---|
| CsMgPO ₄ | $V = 476.43 (3) \text{ \AA}^3$ |
| $M_r = 252.19$ | $Z = 4$ |
| Orthorhombic, <i>Pnma</i> | Mo $K\alpha$ radiation |
| $a = 8.9327 (2) \text{ \AA}$ | $\mu = 8.13 \text{ mm}^{-1}$ |
| $b = 5.5277 (2) \text{ \AA}$ | $T = 293 \text{ K}$ |
| $c = 9.6487 (3) \text{ \AA}$ | $0.12 \times 0.10 \times 0.08 \text{ mm}$ |

Data collection

| | |
|--|---------------------------------------|
| Oxford Diffraction Xcalibur-3 diffractometer | 8753 measured reflections |
| Absorption correction: multi-scan (Blessing, 1995) | 1137 independent reflections |
| $T_{\min} = 0.413$, $T_{\max} = 0.503$ | 874 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.027$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.021$ | 41 parameters |
| $wR(F^2) = 0.047$ | $\Delta\rho_{\text{max}} = 1.23 \text{ e \AA}^{-3}$ |
| $S = 1.00$ | $\Delta\rho_{\text{min}} = -1.02 \text{ e \AA}^{-3}$ |
| 1137 reflections | |

Table 1

Selected bond lengths (\AA).

| | | | |
|-----------------------|-------------|----------------------|-------------|
| Cs1—O2 | 3.1951 (9) | Mg1—O1 | 1.8847 (13) |
| Cs1—O2 ⁱ | 3.2166 (9) | Mg1—O3 ^{iv} | 1.8932 (13) |
| Cs1—O3 ⁱⁱ | 3.4476 (11) | Mg1—O2 ^v | 1.9228 (8) |
| Cs1—O1 ⁱ | 3.5224 (11) | P1—O1 | 1.5056 (13) |
| Cs1—O1 ⁱⁱⁱ | 3.6496 (11) | P1—O3 | 1.5138 (13) |
| Cs1—O3 ⁱⁱⁱ | 3.6968 (18) | P1—O2 | 1.5249 (8) |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2075).

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supplementary materials

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CsMgPO₄

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Comment

Double phosphates A^IB^{II}PO₄ (A^I = alkali metal; B^{II} = Ca, Sr, Ba, Zn, Cd, Pb) exhibit important properties such as ferroelectric and nonlinear optical behaviour (Blum *et al.*, 1984; Elouadi *et al.*, 1984; Sawada *et al.*, 2003). Among some orthophosphates containing Cs and divalent metals, several polymorphs have been found. For instance, CsZnPO₄ occurs in a monoclinic (space group *P2₁/a*) and two orthorhombic types (space groups *Pna2₁* and *Pnma*) (Blum *et al.*, 1986). In contrast, CsMnPO₄ occurs in only one type (space group *Pna2₁*) (Yakubovich *et al.*, 1990). CsMgPO₄, reported here, is isotopic with the *Pnma* form of CsZnPO₄.

Except for O2 (8d), all atoms are in special positions (4c) (Fig. 1). Each MgO₄ tetrahedron is linked with four PO₄ tetrahedra *via* common vertices, resulting in a three-dimensional framework with two types of hexagonal channels, filled by Cs atoms, along the a and b directions (Fig. 2). With a cut-off distance of 3.7 Å, the Cs atoms are 11-coordinate. In general, the principles of crystal structure building are equivalent to those in CsM^{II}PO₄ (M^{II} = Mn, Zn) (Yakubovich *et al.*, 1990; Blum *et al.*, 1986) and CsLi_{0.5}Al_{0.5}PO₄ (Zapirov *et al.*, 2008).

Experimental

In the course of investigating the Cs₂O–MgO–Bi₂O₃–P₂O₅ system, the starting components CsPO₃ (3.0 g), MgO (0.113 g) and Bi₂O₃ (0.652 g) were finely ground and melted in a platinum crucible at 1273 K. The melt was kept at this temperature over 2 h to reach homogeneity and then cooled at a rate of 30 K h⁻¹ to 993 K. After the melt was cooled to room temperature and treated with a small amount of deionized water, colorless needle-shaped crystals were isolated. X-ray powder diffraction showed that CsMgPO₄ is the only crystalline product.

Refinement

The deepest hole and the highest peak are 0.67 Å and 0.65 Å, respectively, from Cs1.

Figures

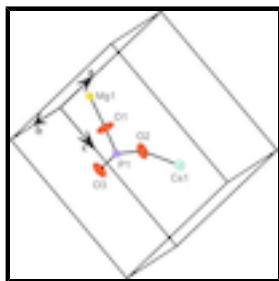


Fig. 1. View of CsMgPO₄ with displacement ellipsoids at the 50% probability level.

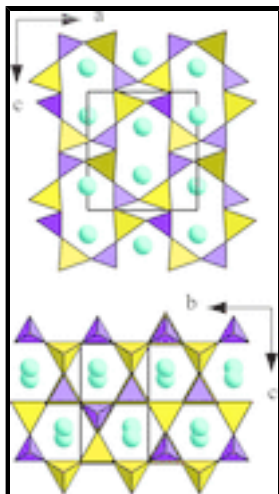


Fig. 2. Formation of hexagonal channels along a and b directions in CsMgPO₄ (PO₄, pink; MgO₄, yellow; Cs, blue).

Caesium magnesium orthophosphate

Crystal data

CsMgPO₄

$M_r = 252.19$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 8.9327(2) \text{ \AA}$

$b = 5.5277(2) \text{ \AA}$

$c = 9.6487(3) \text{ \AA}$

$V = 476.43(3) \text{ \AA}^3$

$Z = 4$

$F_{000} = 456$

$D_x = 3.516 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 8753 reflections

$\theta = 3.1\text{--}35.0^\circ$

$\mu = 8.13 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Prism, colorless

$0.12 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur-3 diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293 \text{ K}$

φ and ω scans

Absorption correction: multi-scan (Blessing, 1995)

$T_{\min} = 0.413$, $T_{\max} = 0.503$

8753 measured reflections

1137 independent reflections

874 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 35.0^\circ$

$\theta_{\min} = 3.1^\circ$

$h = -14 \rightarrow 14$

$k = -8 \rightarrow 8$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$$R[F^2 > 2\sigma(F^2)] = 0.021$$

$$wR(F^2) = 0.047$$

$$S = 1.00$$

1137 reflections

41 parameters

Primary atom site location: structure-invariant direct methods

$$(\Delta/\sigma)_{\max} = 0.018$$

$$\Delta\rho_{\max} = 1.23 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -1.02 \text{ e } \text{Å}^{-3}$$

Extinction correction: SHELXL97 (Sheldrick, 2008)

Extinction coefficient: 0.0211 (4)

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.

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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|---------------|----------------------------------|
| Cs1 | 0.497176 (11) | 0.25 | 0.703332 (10) | 0.02472 (2) |
| Mg1 | 0.32166 (5) | 0.25 | 0.08109 (5) | 0.01434 (11) |
| P1 | 0.20302 (4) | 0.25 | 0.41474 (4) | 0.01345 (7) |
| O1 | 0.26034 (19) | 0.25 | 0.26799 (13) | 0.0590 (6) |
| O2 | 0.26291 (11) | 0.02604 (13) | 0.48850 (9) | 0.0328 (2) |
| O3 | 0.03356 (14) | 0.25 | 0.41501 (19) | 0.0345 (4) |

Atomic displacement parameters (Å^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|-------------|--------------|------------|
| Cs1 | 0.02161 (4) | 0.02632 (5) | 0.02623 (4) | 0 | -0.00031 (4) | 0 |
| Mg1 | 0.01301 (19) | 0.0133 (2) | 0.0168 (2) | 0 | 0.00166 (17) | 0 |
| P1 | 0.01272 (13) | 0.01259 (14) | 0.01505 (14) | 0 | 0.00207 (12) | 0 |
| O1 | 0.0594 (11) | 0.1014 (17) | 0.0162 (7) | 0 | 0.0121 (7) | 0 |
| O2 | 0.0239 (4) | 0.0190 (4) | 0.0555 (6) | -0.0002 (3) | -0.0016 (4) | 0.0156 (4) |
| O3 | 0.0121 (4) | 0.0286 (6) | 0.0629 (10) | 0 | -0.0003 (6) | 0 |

Geometric parameters (Å , $^\circ$)

| | | | |
|-----------------------|-------------|-------------------------|-------------|
| Cs1—O2 | 3.1951 (9) | Mg1—Cs1 ^{xiii} | 4.1402 (4) |
| Cs1—O2 ⁱ | 3.1951 (9) | P1—O1 | 1.5056 (13) |
| Cs1—O2 ⁱⁱ | 3.2166 (9) | P1—O3 | 1.5138 (13) |
| Cs1—O2 ⁱⁱⁱ | 3.2166 (9) | P1—O2 ⁱ | 1.5249 (8) |
| Cs1—O3 ^{iv} | 3.4476 (11) | P1—O2 | 1.5249 (8) |

supplementary materials

| | | | |
|---|--------------|---|--------------|
| Cs1—O3 ^v | 3.4476 (11) | P1—Cs1 ^{ix} | 3.8727 (3) |
| Cs1—O1 ^{vi} | 3.5224 (11) | P1—Cs1 ^{xiii} | 3.8727 (3) |
| Cs1—O1 ⁱⁱ | 3.5224 (11) | P1—Cs1 ^{vi} | 4.0136 (3) |
| Cs1—O1 ^v | 3.6496 (11) | P1—Cs1 ⁱⁱ | 4.0136 (3) |
| Cs1—O1 ^{iv} | 3.6496 (11) | P1—Cs1 ^{xiv} | 4.1184 (4) |
| Cs1—O3 ^{vii} | 3.6968 (18) | O1—Cs1 ^{vi} | 3.5224 (11) |
| Cs1—Mg1 ^{vi} | 3.8189 (4) | O1—Cs1 ⁱⁱ | 3.5224 (11) |
| Mg1—O1 | 1.8847 (13) | O1—Cs1 ^{ix} | 3.6496 (11) |
| Mg1—O3 ^{viii} | 1.8932 (13) | O1—Cs1 ^{xiii} | 3.6496 (11) |
| Mg1—O2 ^{ix} | 1.9228 (8) | O2—Mg1 ^v | 1.9228 (8) |
| Mg1—O2 ^x | 1.9228 (8) | O2—Cs1 ⁱⁱ | 3.2166 (9) |
| Mg1—Cs1 ^{vi} | 3.8189 (4) | O3—Mg1 ^{xii} | 1.8932 (13) |
| Mg1—Cs1 ⁱⁱ | 3.8189 (4) | O3—Cs1 ^{ix} | 3.4476 (11) |
| Mg1—Cs1 ^{xi} | 3.9678 (5) | O3—Cs1 ^{xiii} | 3.4476 (11) |
| Mg1—Cs1 ^{xii} | 3.9916 (5) | O3—Cs1 ^{xiv} | 3.6968 (18) |
| Mg1—Cs1 ^{ix} | 4.1402 (4) | | |
| O2—Cs1—O2 ⁱ | 45.59 (3) | O1—Mg1—Cs1 ^{ix} | 61.80 (3) |
| O2—Cs1—O2 ⁱⁱ | 83.06 (3) | O3 ^{viii} —Mg1—Cs1 ^{ix} | 133.01 (2) |
| O2 ⁱ —Cs1—O2 ⁱⁱ | 104.291 (19) | O2 ^{ix} —Mg1—Cs1 ^{ix} | 48.11 (3) |
| O2—Cs1—O2 ⁱⁱⁱ | 104.291 (19) | O2 ^x —Mg1—Cs1 ^{ix} | 113.07 (3) |
| O2 ⁱ —Cs1—O2 ⁱⁱⁱ | 83.06 (3) | Cs1 ^{vi} —Mg1—Cs1 ^{ix} | 128.277 (13) |
| O2 ⁱⁱ —Cs1—O2 ⁱⁱⁱ | 56.64 (3) | Cs1 ⁱⁱ —Mg1—Cs1 ^{ix} | 69.709 (5) |
| O2—Cs1—O3 ^{iv} | 130.00 (3) | Cs1 ^{xi} —Mg1—Cs1 ^{ix} | 122.243 (9) |
| O2 ⁱ —Cs1—O3 ^{iv} | 91.24 (3) | Cs1 ^{xii} —Mg1—Cs1 ^{ix} | 72.323 (7) |
| O2 ⁱⁱ —Cs1—O3 ^{iv} | 140.73 (3) | O1—Mg1—Cs1 ^{xiii} | 61.80 (3) |
| O2 ⁱⁱⁱ —Cs1—O3 ^{iv} | 90.78 (3) | O3 ^{viii} —Mg1—Cs1 ^{xiii} | 133.01 (2) |
| O2—Cs1—O3 ^v | 91.24 (3) | O2 ^{ix} —Mg1—Cs1 ^{xiii} | 113.07 (3) |
| O2 ⁱ —Cs1—O3 ^v | 130.00 (3) | O2 ^x —Mg1—Cs1 ^{xiii} | 48.11 (3) |
| O2 ⁱⁱ —Cs1—O3 ^v | 90.78 (3) | Cs1 ^{vi} —Mg1—Cs1 ^{xiii} | 69.709 (5) |
| O2 ⁱⁱⁱ —Cs1—O3 ^v | 140.73 (3) | Cs1 ⁱⁱ —Mg1—Cs1 ^{xiii} | 128.277 (14) |
| O3 ^{iv} —Cs1—O3 ^v | 106.58 (5) | Cs1 ^{xi} —Mg1—Cs1 ^{xiii} | 122.243 (9) |
| O2—Cs1—O1 ^{vi} | 139.27 (2) | Cs1 ^{xii} —Mg1—Cs1 ^{xiii} | 72.323 (7) |
| O2 ⁱ —Cs1—O1 ^{vi} | 98.61 (3) | Cs1 ^{ix} —Mg1—Cs1 ^{xiii} | 83.758 (9) |
| O2 ⁱⁱ —Cs1—O1 ^{vi} | 90.44 (3) | O1—P1—O3 | 109.98 (10) |
| O2 ⁱⁱⁱ —Cs1—O1 ^{vi} | 42.55 (2) | O1—P1—O2 ⁱ | 108.64 (5) |
| O3 ^{iv} —Cs1—O1 ^{vi} | 51.20 (3) | O3—P1—O2 ⁱ | 110.49 (5) |
| O3 ^v —Cs1—O1 ^{vi} | 129.16 (3) | O1—P1—O2 | 108.64 (5) |
| O2—Cs1—O1 ⁱⁱ | 98.61 (3) | O3—P1—O2 | 110.49 (5) |
| O2 ⁱ —Cs1—O1 ⁱⁱ | 139.27 (2) | O2 ⁱ —P1—O2 | 108.56 (7) |
| O2 ⁱⁱ —Cs1—O1 ⁱⁱ | 42.55 (2) | O1—P1—Cs1 | 116.78 (7) |

| | | | |
|--|--------------|--|--------------|
| O2 ⁱⁱⁱ —Cs1—O1 ⁱⁱ | 90.44 (3) | O3—P1—Cs1 | 133.24 (7) |
| O3 ^{iv} —Cs1—O1 ⁱⁱ | 129.16 (3) | O2 ⁱ —P1—Cs1 | 54.54 (3) |
| O3 ^v —Cs1—O1 ⁱⁱ | 51.20 (3) | O2—P1—Cs1 | 54.54 (3) |
| O1 ^{vi} —Cs1—O1 ⁱⁱ | 103.38 (4) | O1—P1—Cs1 ^{ix} | 70.23 (4) |
| O2—Cs1—O1 ^v | 53.46 (2) | O3—P1—Cs1 ^{ix} | 62.56 (4) |
| O2 ⁱ —Cs1—O1 ^v | 89.52 (3) | O2 ⁱ —P1—Cs1 ^{ix} | 170.83 (4) |
| O2 ⁱⁱ —Cs1—O1 ^v | 99.15 (2) | O2—P1—Cs1 ^{ix} | 80.12 (3) |
| O2 ⁱⁱⁱ —Cs1—O1 ^v | 151.35 (2) | Cs1—P1—Cs1 ^{ix} | 134.428 (4) |
| O3 ^{iv} —Cs1—O1 ^v | 117.11 (3) | O1—P1—Cs1 ^{xiii} | 70.23 (4) |
| O3 ^v —Cs1—O1 ^v | 40.66 (3) | O3—P1—Cs1 ^{xiii} | 62.56 (4) |
| O1 ^{vi} —Cs1—O1 ^v | 165.554 (5) | O2 ⁱ —P1—Cs1 ^{xiii} | 80.12 (3) |
| O1 ⁱⁱ —Cs1—O1 ^v | 77.288 (3) | O2—P1—Cs1 ^{xiii} | 170.83 (4) |
| O2—Cs1—O1 ^{iv} | 89.52 (3) | Cs1—P1—Cs1 ^{xiii} | 134.428 (4) |
| O2 ⁱ —Cs1—O1 ^{iv} | 53.46 (2) | Cs1 ^{ix} —P1—Cs1 ^{xiii} | 91.069 (8) |
| O2 ⁱⁱ —Cs1—O1 ^{iv} | 151.35 (2) | O1—P1—Cs1 ^{vi} | 60.41 (4) |
| O2 ⁱⁱⁱ —Cs1—O1 ^{iv} | 99.15 (2) | O3—P1—Cs1 ^{vi} | 131.89 (3) |
| O3 ^{iv} —Cs1—O1 ^{iv} | 40.66 (3) | O2 ⁱ —P1—Cs1 ^{vi} | 48.65 (4) |
| O3 ^v —Cs1—O1 ^{iv} | 117.11 (3) | O2—P1—Cs1 ^{vi} | 117.22 (4) |
| O1 ^{vi} —Cs1—O1 ^{iv} | 77.288 (3) | Cs1—P1—Cs1 ^{vi} | 75.434 (6) |
| O1 ⁱⁱ —Cs1—O1 ^{iv} | 165.554 (5) | Cs1 ^{ix} —P1—Cs1 ^{vi} | 130.546 (10) |
| O1 ^v —Cs1—O1 ^{iv} | 98.45 (4) | Cs1 ^{xiii} —P1—Cs1 ^{vi} | 70.558 (4) |
| O2—Cs1—O3 ^{vii} | 134.74 (2) | O1—P1—Cs1 ⁱⁱ | 60.41 (4) |
| O2 ⁱ —Cs1—O3 ^{vii} | 134.74 (2) | O3—P1—Cs1 ⁱⁱ | 131.89 (3) |
| O2 ⁱⁱ —Cs1—O3 ^{vii} | 120.97 (2) | O2 ⁱ —P1—Cs1 ⁱⁱ | 117.22 (4) |
| O2 ⁱⁱⁱ —Cs1—O3 ^{vii} | 120.97 (2) | O2—P1—Cs1 ⁱⁱ | 48.65 (4) |
| O3 ^{iv} —Cs1—O3 ^{vii} | 54.33 (3) | Cs1—P1—Cs1 ⁱⁱ | 75.434 (6) |
| O3 ^v —Cs1—O3 ^{vii} | 54.33 (3) | Cs1 ^{ix} —P1—Cs1 ⁱⁱ | 70.558 (4) |
| O1 ^{vi} —Cs1—O3 ^{vii} | 82.40 (2) | Cs1 ^{xiii} —P1—Cs1 ⁱⁱ | 130.546 (10) |
| O1 ⁱⁱ —Cs1—O3 ^{vii} | 82.40 (2) | Cs1 ^{vi} —P1—Cs1 ⁱⁱ | 87.043 (8) |
| O1 ^v —Cs1—O3 ^{vii} | 83.40 (2) | O1—P1—Cs1 ^{xiv} | 173.36 (7) |
| O1 ^{iv} —Cs1—O3 ^{vii} | 83.40 (2) | O3—P1—Cs1 ^{xiv} | 63.38 (7) |
| O2—Cs1—Mg1 ^{vi} | 155.689 (15) | O2 ⁱ —P1—Cs1 ^{xiv} | 74.87 (4) |
| O2 ⁱ —Cs1—Mg1 ^{vi} | 110.517 (14) | O2—P1—Cs1 ^{xiv} | 74.87 (4) |
| O2 ⁱⁱ —Cs1—Mg1 ^{vi} | 111.987 (18) | Cs1—P1—Cs1 ^{xiv} | 69.857 (6) |
| O2 ⁱⁱⁱ —Cs1—Mg1 ^{vi} | 71.807 (16) | Cs1 ^{ix} —P1—Cs1 ^{xiv} | 105.375 (7) |
| O3 ^{iv} —Cs1—Mg1 ^{vi} | 29.64 (2) | Cs1 ^{xiii} —P1—Cs1 ^{xiv} | 105.375 (7) |
| O3 ^v —Cs1—Mg1 ^{vi} | 106.93 (3) | Cs1 ^{vi} —P1—Cs1 ^{xiv} | 123.498 (7) |
| O1 ^{vi} —Cs1—Mg1 ^{vi} | 29.40 (2) | Cs1 ⁱⁱ —P1—Cs1 ^{xiv} | 123.498 (7) |
| O1 ⁱⁱ —Cs1—Mg1 ^{vi} | 105.34 (2) | P1—O1—Mg1 | 177.02 (12) |
| O1 ^v —Cs1—Mg1 ^{vi} | 136.22 (2) | P1—O1—Cs1 ^{vi} | 97.77 (4) |
| O1 ^{iv} —Cs1—Mg1 ^{vi} | 68.03 (2) | Mg1—O1—Cs1 ^{vi} | 84.06 (4) |

supplementary materials

| | | | |
|--|-------------|--|-------------|
| O3 ^{vii} —Cs1—Mg1 ^{vi} | 54.563 (11) | P1—O1—Cs1 ⁱⁱ | 97.77 (4) |
| O1—Mg1—O3 ^{viii} | 105.76 (8) | Mg1—O1—Cs1 ⁱⁱ | 84.06 (4) |
| O1—Mg1—O2 ^{ix} | 109.29 (4) | Cs1 ^{vi} —O1—Cs1 ⁱⁱ | 103.38 (4) |
| O3 ^{viii} —Mg1—O2 ^{ix} | 113.71 (4) | P1—O1—Cs1 ^{ix} | 86.93 (5) |
| O1—Mg1—O2 ^x | 109.29 (4) | Mg1—O1—Cs1 ^{ix} | 91.12 (4) |
| O3 ^{viii} —Mg1—O2 ^x | 113.71 (4) | Cs1 ^{vi} —O1—Cs1 ^{ix} | 174.41 (4) |
| O2 ^{ix} —Mg1—O2 ^x | 105.04 (6) | Cs1 ⁱⁱ —O1—Cs1 ^{ix} | 78.860 (3) |
| O1—Mg1—Cs1 ^{vi} | 66.55 (3) | P1—O1—Cs1 ^{xiii} | 86.93 (5) |
| O3 ^{viii} —Mg1—Cs1 ^{vi} | 64.25 (3) | Mg1—O1—Cs1 ^{xiii} | 91.12 (4) |
| O2 ^{ix} —Mg1—Cs1 ^{vi} | 173.66 (3) | Cs1 ^{vi} —O1—Cs1 ^{xiii} | 78.860 (3) |
| O2 ^x —Mg1—Cs1 ^{vi} | 81.10 (3) | Cs1 ⁱⁱ —O1—Cs1 ^{xiii} | 174.41 (4) |
| O1—Mg1—Cs1 ⁱⁱ | 66.55 (3) | Cs1 ^{ix} —O1—Cs1 ^{xiii} | 98.45 (4) |
| O3 ^{viii} —Mg1—Cs1 ⁱⁱ | 64.25 (3) | P1—O2—Mg1 ^v | 136.32 (7) |
| O2 ^{ix} —Mg1—Cs1 ⁱⁱ | 81.10 (3) | P1—O2—Cs1 | 102.59 (4) |
| O2 ^x —Mg1—Cs1 ⁱⁱ | 173.66 (3) | Mg1 ^v —O2—Cs1 | 105.27 (4) |
| Cs1 ^{vi} —Mg1—Cs1 ⁱⁱ | 92.725 (11) | P1—O2—Cs1 ⁱⁱ | 110.51 (4) |
| O1—Mg1—Cs1 ^{xi} | 173.62 (6) | Mg1 ^v —O2—Cs1 ⁱⁱ | 98.78 (3) |
| O3 ^{viii} —Mg1—Cs1 ^{xi} | 67.86 (6) | Cs1—O2—Cs1 ⁱⁱ | 96.94 (3) |
| O2 ^{ix} —Mg1—Cs1 ^{xi} | 74.24 (3) | P1—O3—Mg1 ^{xii} | 178.96 (13) |
| O2 ^x —Mg1—Cs1 ^{xi} | 74.24 (3) | P1—O3—Cs1 ^{ix} | 94.51 (5) |
| Cs1 ^{vi} —Mg1—Cs1 ^{xi} | 109.444 (9) | Mg1 ^{xii} —O3—Cs1 ^{ix} | 86.11 (4) |
| Cs1 ⁱⁱ —Mg1—Cs1 ^{xi} | 109.444 (9) | P1—O3—Cs1 ^{xiii} | 94.51 (5) |
| O1—Mg1—Cs1 ^{xii} | 116.54 (5) | Mg1 ^{xii} —O3—Cs1 ^{xiii} | 86.11 (4) |
| O3 ^{viii} —Mg1—Cs1 ^{xii} | 137.70 (6) | Cs1 ^{ix} —O3—Cs1 ^{xiii} | 106.58 (5) |
| O2 ^{ix} —Mg1—Cs1 ^{xii} | 52.79 (3) | P1—O3—Cs1 ^{xiv} | 95.14 (8) |
| O2 ^x —Mg1—Cs1 ^{xii} | 52.79 (3) | Mg1 ^{xii} —O3—Cs1 ^{xiv} | 83.82 (6) |
| Cs1 ^{vi} —Mg1—Cs1 ^{xii} | 133.015 (6) | Cs1 ^{ix} —O3—Cs1 ^{xiv} | 125.67 (3) |
| Cs1 ⁱⁱ —Mg1—Cs1 ^{xii} | 133.015 (6) | Cs1 ^{xiii} —O3—Cs1 ^{xiv} | 125.67 (3) |
| Cs1 ^{xi} —Mg1—Cs1 ^{xii} | 69.840 (9) | | |

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

Fig. 1

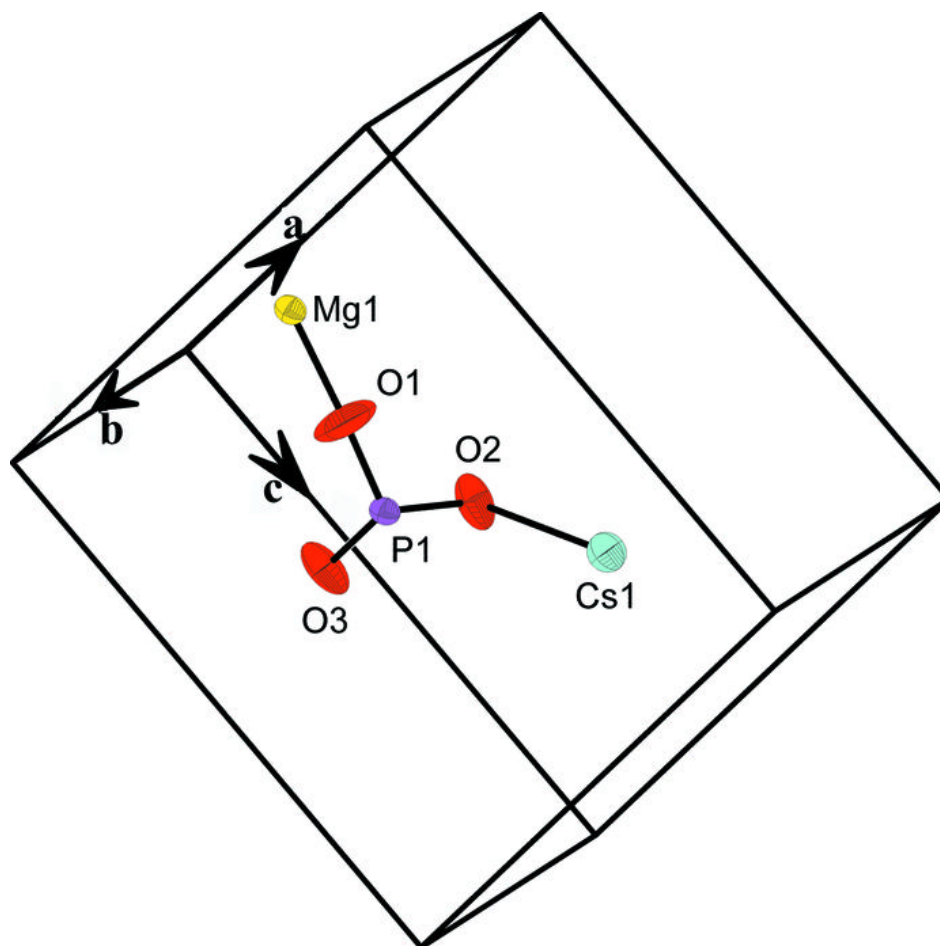


Fig. 2

