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$CsMgPO_4$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(P–O) = 0.001 Å; R factor = 0.021; wR factor = 0.047; data-to-parameter ratio = 27.7.

Caesium magnesium orthophosphate is built up from MgO_4 and PO_4 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 $A^{I}B^{II}PO_4$ (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 $CsZnPO_4$. In contrast, $CsMnPO_4$ occurs in only one type, see: Yakubovich *et al.* (1990). The title compound is isotypic with the *Pnma* form of $CsZnPO_4$. For related structures, see: Yakubovich *et al.* (1990); Blum *et al.* (1986); Zaripov *et al.* (2008).

Experimental

Crystal data

$CsMgPO_4$
M_r = 252.19
Orthorhombic, *Pnma*
a = 8.9327 (2) Å
b = 5.5277 (2) Å
c = 9.6487 (3) Å
V = 476.43 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.13 mm^{-1}
T = 293 K
0.12 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur-3 diffractometer
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_{int} = 0.027

Refinement

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

Table 1
Selected bond lengths (Å).

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^{ii}	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) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (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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$CsMgPO_4$

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S1. Comment

Double phosphates $A^IB^{II}PO_4$ (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, $CsZnPO_4$ occurs in a monoclinic (space group $P2_1/a$) and two orthorhombic types (space groups $Pna2_1$ and *Pnma*) (Blum *et al.*, 1986). In contrast, $CsMnPO_4$ occurs in only one type (space group $Pna2_1$) (Yakubovich *et al.*, 1990). $CsMgPO_4$, reported here, is isotypic with the *Pnma* form of $CsZnPO_4$.

Except for O2 (8d), all atoms are in special positions (4c) (Fig. 1). Each MgO_4 tetrahedron is linked with four PO_4 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 $Cs*M*^{II}PO_4$ ($*M*^{II}$ = Mn, Zn) (Yakubovich *et al.*, 1990; Blum *et al.*, 1986) and $CsLi_{0.5}Al_{0.5}PO_4$ (Zapirov *et al.*, 2008).

S2. Experimental

In the course of investigating the Cs_2O–MgO–Bi_2O_3–P_2O_5 system, the starting components $CsPO_3$ (3.0 g), MgO (0.113 g) and Bi_2O_3 (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 $CsMgPO_4$ is the only crystalline product.

S3. Refinement

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

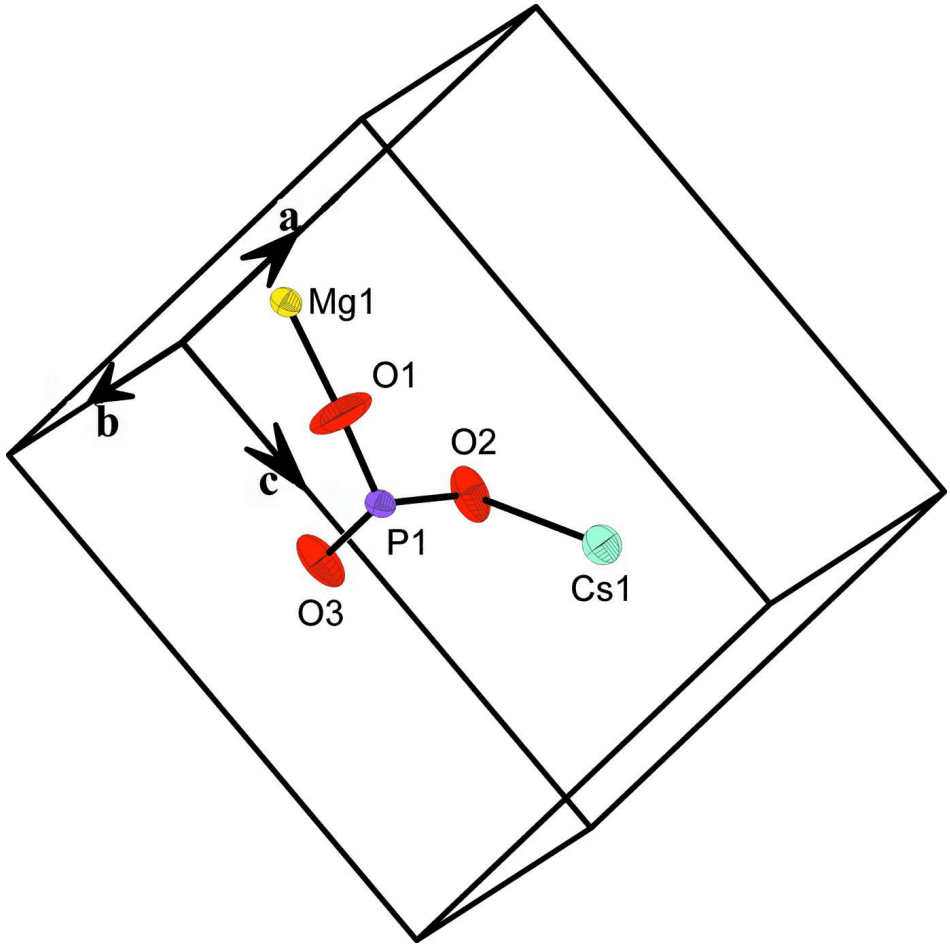

Figure 1

View of $CsMgPO_4$ with displacement ellipsoids at the 50% probability level.

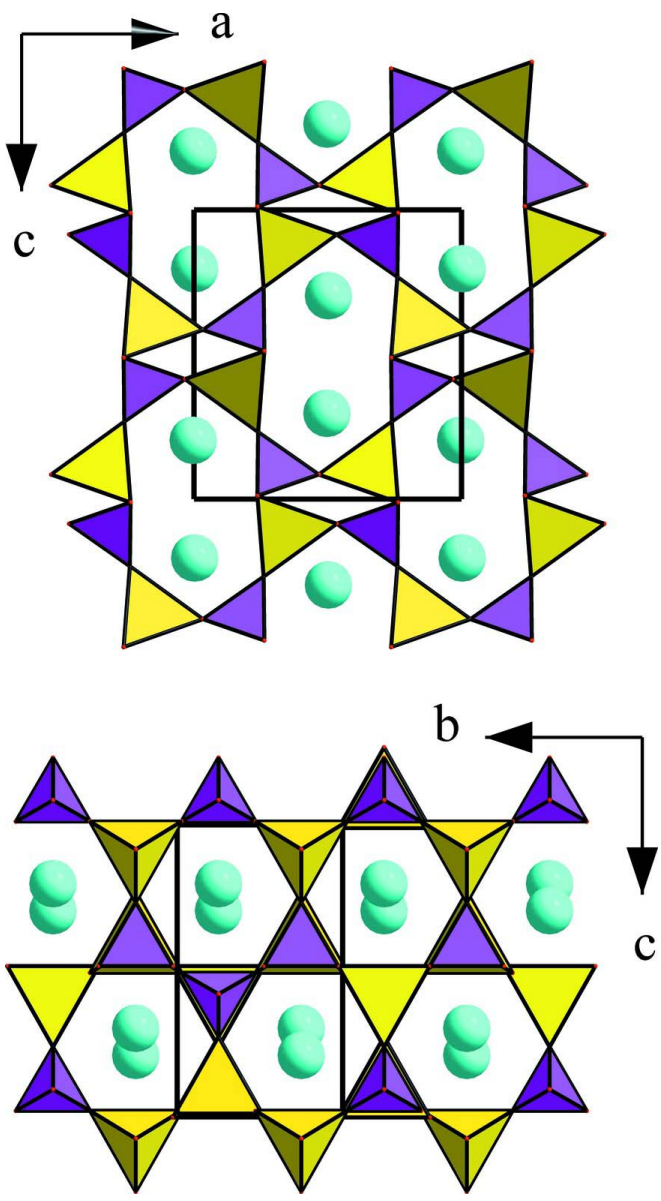

Figure 2

Formation of hexagonal channels along a and b directions in $CsMgPO_4$ (PO_4, pink; MgO_4, yellow; Cs, blue).

Caesium magnesium orthophosphate

Crystal data

$CsMgPO_4$
$M_r = 252.19$
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
$a = 8.9327$ (2) Å
$b = 5.5277$ (2) Å
$c = 9.6487$ (3) Å
$V = 476.43$ (3) Å^3
$Z = 4$
$F(000) = 456$
$D_x = 3.516$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8753 reflections
$\theta = 3.1$–$35.0°$
$\mu = 8.13$ mm^{-1}
$T = 293$ K
Prism, colorless
0.12 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur-3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
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_{int} = 0.027
θ_{max} = 35.0°, θ_{min} = 3.1°
h = −14→14
k = −8→8
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.047
S = 1.00
1137 reflections
41 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.018
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 e 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 (Å²)

	x	y	z	U_{iso}*/U_{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 (Å²)

	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, º)

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)
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)
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, $-z+3/2$.