

CsMgPO₄

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

Caesium magnesium orthophosphate is built up from 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) Å ³
$M_r = 252.19$	$Z = 4$
Orthorhombic, <i>Pnma</i>	Mo $K\alpha$ radiation
$a = 8.9327$ (2) Å	$\mu = 8.13$ mm ⁻¹
$b = 5.5277$ (2) Å	$T = 293$ K
$c = 9.6487$ (3) Å	$0.12 \times 0.10 \times 0.08$ 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
$wR(F^2) = 0.047$	$\Delta\rho_{\text{max}} = 1.23$ e Å ⁻³
$S = 1.00$	$\Delta\rho_{\text{min}} = -1.02$ e Å ⁻³
1137 reflections	

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 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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