Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# Redetermination of the cubic struvite analogue $Cs[Mg(OH_2)_6](AsO_4)$

**Matthias Weil**

Institute for Chemical Technologies and Analytics, Division of Structural Chemistry, Vienna University of Technology, Getreidemarkt 9/164-SC, A-1060 Vienna, Austria
Correspondence e-mail: mweil@mail.zserv.tuwien.ac.at

Received 18 December 2008; accepted 18 December 2008

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(Mg–O) = 0.003 Å; $R$ factor = 0.016; $wR$ factor = 0.038; data-to-parameter ratio = 13.9.

In contrast to the previous refinement from photographic data [Ferrari *et al.* (1955). *Gazz. Chim. Ital.* **84**, 169–174], the present redetermination of the title compound, caesium hexaaquamagnesium arsenate(V), revealed the Cs atom to be on Wyckoff position 4*d* instead of Wyckoff position 4*b* of space group $F\overline{4}3m$. The structure can be derived from the halite structure. The centres of the complex $[Mg(OH_2)_6]$ octahedra and the $AsO_4$ tetrahedra (both with $\overline{4}3m$ symmetry) are on the respective Na and Cl positions. The building units are connected to each other by O—H$\cdots$O hydrogen bonds. The $Cs^+$ cations ($\overline{4}3m$ symmetry) are located in the voids of this arrangement and exhibit a regular cuboctahedral 12-coordination to the O atoms of the water molecules. The O atom bonded to As has 2*mm* site symmetry (Wyckoff position 24*f*) and the water-molecule O atom has *m* site symmetry (Wyckoff position 48*h*).

## Related literature

The crystal structure of struvite, $NH_4[Mg(OH_2)_6](PO_4)$, was reported by Whitaker & Jeffery (1970*a*,*b*). Crystal growth of struvite-type compounds using the gel diffusion technique was reported by Banks *et al.* (1975). For isotypic structures, see: Carver *et al.* (2006) for $Cs[Fe(OH_2)_6](PO_4)$ and Massa *et al.* (2003) for the cubic form of dimorphic $Cs[Mg(OH_2)_6](PO_4)$. Isotypic struvite-type phases as well as analogues were recently surveyed by Weil (2008).

## Experimental

### *Crystal data*

$Cs[Mg(OH_2)_6](AsO_4)$
$M_r$ = 404.24
Cubic, $F\overline{4}3m$
$a$ = 10.1609 (5) Å
$V$ = 1049.05 (9) Å$^3$

$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 6.75 mm$^{-1}$
$T$ = 293 (2) K
0.18 × 0.18 × 0.18 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: integration (*SHELXTL*; Sheldrick, 2008)
$T_{min}$ = 0.341, $T_{max}$ = 0.382
3332 measured reflections

208 independent reflections
207 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
3 standard reflections
frequency: 200 min
intensity decay: none

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.038
$S$ = 1.14
208 reflections
15 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$
Absolute structure: Flack (1983), 90 Friedel pairs
Flack parameter: 0.01 (4)

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cs1—O1$^i$ | 3.6239 (5) | As1—O2 | 1.681 (3) |
| Mg1—O1 | 2.064 (3) | | |

Symmetry code: (i) $-x+1, -y+1, z+1$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O1—H1$\cdots$O2$^{ii}$ | 0.79 (2) | 1.86 (2) | 2.650 (2) | 176 (4) |

Symmetry code: (ii) $x, -y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *HELENA* implemented in *PLATON* (Spek, 2003); method used to solve structure: coordinates taken from an isotypic compound; program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2004); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2885).

## References

Banks, E., Chianelli, R. & Korenstein, R. (1975). *Inorg. Chem.* **14**, 1634–1639.
Carver, G., Dobe, C., Jensen, T. B., Tregenna-Piggott, P. L. W., Janssen, S., Bill, E., McIntyre, G. J. & Barra, A. L. (2006). *Inorg. Chem.* **45**, 4695–4705.
Dowty, E. (2004). *ATOMS for Windows*. Shape Software, Kingsport, Tennessee, USA.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Ferrari, A., Calvaca, L. & Nardelli, M. (1955). *Gazz. Chim. Ital.* **84**, 169–174.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Massa, W., Yakubovich, O. V. & Dimitrova, O. V. (2003). *Acta Cryst.* C**59**, i83–i85.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Weil, M. (2008). *Cryst. Res. Technol.* **43**, 1286–1291.
Whitaker, A. & Jeffery, J. W. (1970*a*). *Acta Cryst.* B**26**, 1429–1440.
Whitaker, A. & Jeffery, J. W. (1970*b*). *Acta Cryst.* B**26**, 1440–1444.

# supplementary materials

*Acta Cryst.* (2009). E**65**, i2 [ **doi:10.1107/S1600536808043171** ]

# Redetermination of the cubic struvite analogue Cs[Mg($OH_2$)$_6$]($AsO_4$)

**M. Weil**

## Comment

Numerous compounds with general formula $A[B(OH_2)_6]XO_4$, where $A$ = alkali metal, $NH_4$ or Tl, $B$ = Mg or first row transition metal, and $X$ = P or As, are known to crystallize in the orthorhombic struvite ($NH_4[Mg(OH_2)_6](PO_4)$) structure in space group *Pmn*2$_1$ (Whitaker & Jeffrey, 1970*a*, *b*). The title compound, (I), $Cs[Mg(OH_2)_6](AsO_4)$, is an isoformular analogue of struvite, but crystallizes in the cubic crystal system. All these structures can be described in terms of closed-packed layers with different stacking sequences (Massa *et al.*, 2003). Phases that are isotypes of struvite, as well as struvite analogues were recently surveyed by Weil (2008). In comparison with the previous refinement from photographic data (Ferrari *et al.*, 1955), the present redetermination of $Cs[Mg(OH_2)_6](AsO_4)$ revealed a different location of the Cs atom, the localization of the H atom and anisotropic displacement parameters for all non H-atoms.

The structure can be described as a derivative of the NaCl structure type (Massa *et al.*, 2003). The centres of the regular complex $[Mg(H_2O)_6]$ octahedra are situated on the respective Na positions, and the centres of the regular $AsO_4$ tetrahedra are situated on the Cl positions (Fig. 1). Thus one $[Mg(H_2O)_6]$ octahedron is surrounded by six $AsO_4$ tetrahedra in an octahedral arrangement, and *vice versa*. The corresponding Mg—O and As—O distances are in the normal range (Table 1). These building units are linked *via* medium-strong hydrogen bonds (Table 2). Details and differences of the hydrogen bonding schemes in cubic, hexagonal and orthorhombic struvite-type structures were discussed in detail by Massa *et al.* (2003). The $Cs^+$ cations are located in the voids of this arrangement and exhibit a regular cuboctahedral 12-coordination to the oxygen atoms of the water molecules (Table 1).

## Experimental

Colourless octahedral crystals of $Cs[Mg(OH_2)_6](AsO_4)$ with an edge-length up to 1 mm were grown by means of the gel diffusion technique, following a slightly modified procedure as that given by Banks *et al.* (1975). Aqueous solutions of 0.025 *M* $MgSO_4$ and 0.02 *M* $Na_4$edta (edta = ethylenediaminetetraacetate) were adjusted to pH 10 with NaOH. Commercially available gelatine foils (5 g) were dissolved in the hot resulting 100 ml solution and allowed to form a gel inside a large test tube overnight. When the gel had set, an equivalent amount of a solution of 0.025 *M* $CsH_2AsO_4$ (50 ml) was carefully poured over the gel. This solution was then adjusted to pH 9 with NaOH. The test tube was covered with parafilm and the crystal growth proceeded at the gel-liquid interface and into the gel. Crystals large enough for conventional *x*-ray analysis grew within one week at room temperature. They were separated mechanically from the gel and were washed with a water/ethanol/acetone (1/3/1) mixture.

## Refinement

The coordinates of the isotypic compound $Cs[Fe(OH_2)_6](PO_4)$ (Carver *et al.*, 2006) were taken as starting parameters. The Cs atom in the original structure determination (Ferrari *et al.*, 1955) was positioned on Wyckoff site 4*b* (1/2, 1/2, 1/2), whereas in the present refinement Cs is on position 4*d* (3/4, 3/4, 3/4). The position of the H atom was found from difference Fourier maps and was refined with a soft distance restraint of O—H = 0.85 (3) Å.

## Figures

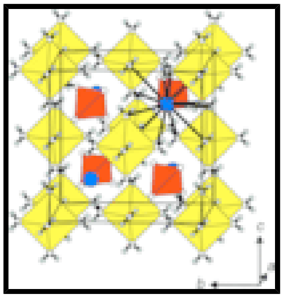

Fig. 1. The crystal structure of $Cs[Mg(H_2O)_6](AsO_4)$ projected approximately along $[00\bar{1}]$. $[Mg(OH_2)_6]$ octahedra are yellow, $PO_4$ tetrahedra are red, Cs atoms are blue O atoms are white and H atoms are grey. For one of the $Cs^+$ cations the Cs–O bonds are indicated.

## Caesium hexaquamagnesium orthoarsenate(V)

### *Crystal data*

$Cs[Mg(H_2O)_6](AsO_4)$
$M_r = 404.24$
Cubic, $F\bar{4}3m$
Hall symbol: F -4 2 3
$a = 10.1609$ (5) Å
$b = 10.1609$ (5) Å
$c = 10.1609$ (5) Å
$\alpha = 90°$
$\beta = 90°$
$\gamma = 90°$
$V = 1049.05$ (9) Å$^3$

$Z = 4$
$F_{000} = 768$
$D_x = 2.559$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 11.4$–12.7°
$\mu = 6.75$ mm$^{-1}$
$T = 293$ (2) K
Octahedron, colourless
0.18 × 0.18 × 0.18 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
$T = 293(2)$ K
$\omega/2\theta$ scans
Absorption correction: integration (SHELXTL; Sheldrick, 2008)
$T_{min} = 0.341$, $T_{max} = 0.382$
3332 measured reflections
208 independent reflections
207 reflections with $I > 2\sigma(I)$

$R_{int} = 0.037$
$\theta_{max} = 30.9°$
$\theta_{min} = 3.5°$
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$
3 standard reflections
every 200 min
intensity decay: none

### *Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.038$

$S = 1.14$

208 reflections

15 parameters

1 restraint

Primary atom site location: isomorphous structure methods

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + 5.0469P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.50$ e Å$^{-3}$

$\Delta\rho_{\min} = -0.48$ e Å$^{-3}$

Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00144 (17)

Absolute structure: Flack (1983), 90 Friedel pairs

Flack parameter: 0.01 (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$^2$)*

| | $x$ | $y$ | $z$ | $U_{\rm iso}*/U_{\rm eq}$ |
|---|---|---|---|---|
| Cs1 | 0.7500 | 0.7500 | 0.7500 | 0.0599 (3) |
| Mg1 | 0.0000 | 0.0000 | 0.0000 | 0.0250 (6) |
| As1 | 0.2500 | 0.2500 | 0.2500 | 0.0201 (2) |
| O1 | 0.2031 (3) | 0.0000 | 0.0000 | 0.0508 (8) |
| O2 | 0.34550 (19) | 0.34550 (19) | 0.34550 (19) | 0.0269 (7) |
| H1 | 0.249 (3) | 0.045 (2) | 0.045 (2) | 0.053 (12)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cs1 | 0.0599 (3) | 0.0599 (3) | 0.0599 (3) | 0.000 | 0.000 | 0.000 |
| Mg1 | 0.0250 (6) | 0.0250 (6) | 0.0250 (6) | 0.000 | 0.000 | 0.000 |
| As1 | 0.0201 (2) | 0.0201 (2) | 0.0201 (2) | 0.000 | 0.000 | 0.000 |
| O1 | 0.0259 (13) | 0.0632 (13) | 0.0632 (13) | 0.000 | 0.000 | −0.033 (2) |
| O2 | 0.0269 (7) | 0.0269 (7) | 0.0269 (7) | −0.0036 (7) | −0.0036 (7) | −0.0036 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cs1—O1$^{i}$ | 3.6239 (5) | Mg1—O1$^{xiii}$ | 2.064 (3) |
| Cs1—O1$^{ii}$ | 3.6239 (5) | Mg1—O1$^{xiv}$ | 2.064 (3) |
| Cs1—O1$^{iii}$ | 3.6239 (5) | Mg1—O1$^{xv}$ | 2.064 (3) |
| Cs1—O1$^{iv}$ | 3.6239 (5) | Mg1—O1$^{xvi}$ | 2.064 (3) |
| Cs1—O1$^{v}$ | 3.6239 (5) | Mg1—O1$^{xvii}$ | 2.064 (3) |
| Cs1—O1$^{vi}$ | 3.6239 (5) | Mg1—O1 | 2.064 (3) |
| Cs1—O1$^{vii}$ | 3.6239 (5) | As1—O2 | 1.681 (3) |
| Cs1—O1$^{viii}$ | 3.6239 (5) | As1—O2$^{xviii}$ | 1.681 (3) |
| Cs1—O1$^{ix}$ | 3.6239 (5) | As1—O2$^{xix}$ | 1.681 (3) |
| Cs1—O1$^{x}$ | 3.6239 (5) | As1—O2$^{xx}$ | 1.681 (3) |
| Cs1—O1$^{xi}$ | 3.6239 (5) | O1—H1 | 0.79 (2) |
| Cs1—O1$^{xii}$ | 3.6239 (5) | | |
| O1$^{i}$—Cs1—O1$^{ii}$ | 47.49 (8) | O1$^{iii}$—Cs1—O1$^{xi}$ | 72.12 (8) |
| O1$^{i}$—Cs1—O1$^{iii}$ | 47.49 (8) | O1$^{iv}$—Cs1—O1$^{xi}$ | 47.49 (8) |
| O1$^{ii}$—Cs1—O1$^{iii}$ | 47.49 (8) | O1$^{v}$—Cs1—O1$^{xi}$ | 90.991 (13) |
| O1$^{i}$—Cs1—O1$^{iv}$ | 164.89 (10) | O1$^{vi}$—Cs1—O1$^{xi}$ | 119.429 (8) |
| O1$^{ii}$—Cs1—O1$^{iv}$ | 119.430 (7) | O1$^{vii}$—Cs1—O1$^{xi}$ | 72.12 (8) |
| O1$^{iii}$—Cs1—O1$^{iv}$ | 119.429 (7) | O1$^{viii}$—Cs1—O1$^{xi}$ | 119.429 (7) |
| O1$^{i}$—Cs1—O1$^{v}$ | 119.429 (8) | O1$^{ix}$—Cs1—O1$^{xi}$ | 47.49 (8) |
| O1$^{ii}$—Cs1—O1$^{v}$ | 164.89 (10) | O1$^{x}$—Cs1—O1$^{xi}$ | 164.89 (10) |
| O1$^{iii}$—Cs1—O1$^{v}$ | 119.429 (7) | O1$^{i}$—Cs1—O1$^{xii}$ | 72.12 (8) |
| O1$^{iv}$—Cs1—O1$^{v}$ | 72.12 (8) | O1$^{ii}$—Cs1—O1$^{xii}$ | 119.429 (7) |
| O1$^{i}$—Cs1—O1$^{vi}$ | 119.429 (8) | O1$^{iii}$—Cs1—O1$^{xii}$ | 90.991 (13) |
| O1$^{ii}$—Cs1—O1$^{vi}$ | 119.429 (8) | O1$^{iv}$—Cs1—O1$^{xii}$ | 119.429 (8) |
| O1$^{iii}$—Cs1—O1$^{vi}$ | 164.89 (10) | O1$^{v}$—Cs1—O1$^{xii}$ | 47.49 (8) |
| O1$^{iv}$—Cs1—O1$^{vi}$ | 72.12 (8) | O1$^{vi}$—Cs1—O1$^{xii}$ | 90.991 (13) |
| O1$^{v}$—Cs1—O1$^{vi}$ | 72.12 (8) | O1$^{vii}$—Cs1—O1$^{xii}$ | 47.49 (8) |
| O1$^{i}$—Cs1—O1$^{vii}$ | 90.991 (13) | O1$^{viii}$—Cs1—O1$^{xii}$ | 119.429 (7) |
| O1$^{ii}$—Cs1—O1$^{vii}$ | 119.430 (7) | O1$^{ix}$—Cs1—O1$^{xii}$ | 164.89 (10) |
| O1$^{iii}$—Cs1—O1$^{vii}$ | 72.12 (8) | O1$^{x}$—Cs1—O1$^{xii}$ | 72.12 (8) |
| O1$^{iv}$—Cs1—O1$^{vii}$ | 90.991 (13) | O1$^{xi}$—Cs1—O1$^{xii}$ | 119.429 (8) |
| O1$^{v}$—Cs1—O1$^{vii}$ | 47.49 (8) | O1$^{xiii}$—Mg1—O1$^{xiv}$ | 180.0 |
| O1$^{vi}$—Cs1—O1$^{vii}$ | 119.429 (8) | O1$^{xiii}$—Mg1—O1$^{xv}$ | 90.0 |
| O1$^{i}$—Cs1—O1$^{viii}$ | 90.991 (13) | O1$^{xiv}$—Mg1—O1$^{xv}$ | 90.0 |
| O1$^{ii}$—Cs1—O1$^{viii}$ | 72.12 (8) | O1$^{xiii}$—Mg1—O1$^{xvi}$ | 90.0 |
| O1$^{iii}$—Cs1—O1$^{viii}$ | 119.430 (7) | O1$^{xiv}$—Mg1—O1$^{xvi}$ | 90.0 |
| O1$^{iv}$—Cs1—O1$^{viii}$ | 90.991 (13) | O1$^{xv}$—Mg1—O1$^{xvi}$ | 180.0 |
| O1$^{v}$—Cs1—O1$^{viii}$ | 119.429 (8) | O1$^{xiii}$—Mg1—O1$^{xvii}$ | 90.0 |

| | |
|---|---|
| O1$^{\text{vi}}$—Cs1—O1$^{\text{viii}}$ | 47.49 (8) |
| O1$^{\text{vii}}$—Cs1—O1$^{\text{viii}}$ | 164.89 (10) |
| O1$^{\text{i}}$—Cs1—O1$^{\text{ix}}$ | 119.429 (7) |
| O1$^{\text{ii}}$—Cs1—O1$^{\text{ix}}$ | 72.12 (8) |
| O1$^{\text{iii}}$—Cs1—O1$^{\text{ix}}$ | 90.991 (13) |
| O1$^{\text{iv}}$—Cs1—O1$^{\text{ix}}$ | 47.49 (8) |
| O1$^{\text{v}}$—Cs1—O1$^{\text{ix}}$ | 119.429 (8) |
| O1$^{\text{vi}}$—Cs1—O1$^{\text{ix}}$ | 90.991 (13) |
| O1$^{\text{vii}}$—Cs1—O1$^{\text{ix}}$ | 119.429 (8) |
| O1$^{\text{viii}}$—Cs1—O1$^{\text{ix}}$ | 72.12 (8) |
| O1$^{\text{i}}$—Cs1—O1$^{\text{x}}$ | 72.12 (8) |
| O1$^{\text{ii}}$—Cs1—O1$^{\text{x}}$ | 90.991 (13) |
| O1$^{\text{iii}}$—Cs1—O1$^{\text{x}}$ | 119.430 (7) |
| O1$^{\text{iv}}$—Cs1—O1$^{\text{x}}$ | 119.429 (8) |
| O1$^{\text{v}}$—Cs1—O1$^{\text{x}}$ | 90.991 (13) |
| O1$^{\text{vi}}$—Cs1—O1$^{\text{x}}$ | 47.49 (8) |
| O1$^{\text{vii}}$—Cs1—O1$^{\text{x}}$ | 119.429 (7) |
| O1$^{\text{viii}}$—Cs1—O1$^{\text{x}}$ | 47.49 (8) |
| O1$^{\text{ix}}$—Cs1—O1$^{\text{x}}$ | 119.429 (7) |
| O1$^{\text{i}}$—Cs1—O1$^{\text{xi}}$ | 119.430 (7) |
| O1$^{\text{ii}}$—Cs1—O1$^{\text{xi}}$ | 90.991 (13) |
| O1$^{\text{xiv}}$—Mg1—O1$^{\text{xvii}}$ | 90.0 |
| O1$^{\text{xv}}$—Mg1—O1$^{\text{xvii}}$ | 90.0 |
| O1$^{\text{xvi}}$—Mg1—O1$^{\text{xvii}}$ | 90.0 |
| O1$^{\text{xiii}}$—Mg1—O1 | 90.0 |
| O1$^{\text{xiv}}$—Mg1—O1 | 90.0 |
| O1$^{\text{xv}}$—Mg1—O1 | 90.0 |
| O1$^{\text{xvi}}$—Mg1—O1 | 90.0 |
| O1$^{\text{xvii}}$—Mg1—O1 | 180.0 |
| O2—As1—O2$^{\text{xviii}}$ | 109.5 |
| O2—As1—O2$^{\text{xix}}$ | 109.471 (1) |
| O2$^{\text{xviii}}$—As1—O2$^{\text{xix}}$ | 109.5 |
| O2—As1—O2$^{\text{xx}}$ | 109.5 |
| O2$^{\text{xviii}}$—As1—O2$^{\text{xx}}$ | 109.5 |
| O2$^{\text{xix}}$—As1—O2$^{\text{xx}}$ | 109.5 |
| Mg1—O1—Cs1$^{\text{xxi}}$ | 97.56 (5) |
| Mg1—O1—Cs1$^{\text{xxii}}$ | 97.56 (5) |
| Cs1$^{\text{xxi}}$—O1—Cs1$^{\text{xxii}}$ | 164.89 (10) |
| Mg1—O1—H1 | 126 (3) |
| Cs1$^{\text{xxi}}$—O1—H1 | 85.6 (3) |
| Cs1$^{\text{xxii}}$—O1—H1 | 85.6 (3) |

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

### *Hydrogen-bond geometry (Å, °)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2$^{\text{xix}}$ | 0.79 (2) | 1.86 (2) | 2.650 (2) | 176 (4) |

Symmetry codes: (xix) $x, -y+1/2, -z+1/2$.

**Fig. 1**