# inorganic compounds

## Redetermination of the hexagonal struvite analogue Cs[Mg(OH$_2$)$_6$](PO$_4$)

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The structure of the hexagonal modification of caesium hexaaquamagnesium phosphate has been redetermined from single-crystal X-ray data. The previous refinement from photographic data [Ferrari, Calvaca & Nardelli (1955). *Gazz. Chim. Ital.* **85**, 1232–1238] was basically confirmed, but with all H atoms located and with all non H-atoms refined with anisotropic displacement parameters. The structure can be derived from the NiAs structure type: the PO$_4$ tetrahedra ($3m$. symmetry) are on the Ni positions and the complex [Mg(OH$_2$)$_6$] octahedra ($3m$. symmetry) are on the As positions. The building units are connected to each other by hydrogen bonds. The Cs$^+$ cations ($3m$. symmetry) are located in the voids of this arrangement and exhibit a distorted cuboctahedral 12-coordination by the O atoms of the water molecules.

## Related literature

The crystal structure of struvite, NH$_4$[Mg(OH$_2$)$_6$](PO$_4$), was reported by Whitaker & Jeffery (1970*a*,*b*). Structure determinations of the hexagonal and cubic forms of Cs[Mg(OH$_2$)$_6$](PO$_4$) were performed by Ferrari *et al.* (1955) and Massa *et al.* (2003), respectively. Crystal growth of struvite-like compounds using the gel diffusion technique was reported by Banks *et al.* (1975). For general background, see: Flack (1983).

## Experimental

### Crystal data

| | |
|---|---|
| Cs[Mg(H$_2$O)$_6$](PO$_4$) | $Z = 2$ |
| $M_r = 360.29$ | Mo $K\alpha$ radiation |
| Hexagonal, $P6_3mc$ | $\mu = 4.04$ mm$^{-1}$ |
| $a = 6.8827$ (8) Å | $T = 293$ (2) K |
| $c = 11.9188$ (16) Å | $0.46 \times 0.38 \times 0.38$ mm |
| $V = 488.97$ (10) Å$^3$ | |

### Data collection

| | |
|---|---|
| Stoe IPDS diffractometer | 5412 measured reflections |
| Absorption correction: numerical (*HABITUS*; Herrendorf, 1997) | 368 independent reflections |
| $T_{min} = 0.213$, $T_{max} = 0.327$ | 367 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.025$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.016$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.034$ | |
| $S = 1.29$ | $\Delta\rho_{max} = 0.40$ e Å$^{-3}$ |
| 368 reflections | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |
| 39 parameters | Absolute structure: Flack (1983), with 164 Friedel pairs |
| 4 restraints | Flack parameter: $-0.01$ (3) |

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

| | | | |
|---|---|---|---|
| Cs—O3$^{i}$ | 3.469 (5) | Mg—O4 | 2.082 (3) |
| Cs—O4$^{i}$ | 3.470 (4) | P—O1 | 1.536 (3) |
| Cs—O4$^{ii}$ | 3.742 (4) | P—O2 | 1.539 (6) |
| Mg—O3 | 2.054 (4) | | |

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

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O3—H1$\cdots$O2 | 0.93 (4) | 1.71 (4) | 2.643 (5) | 180 (6) |
| O3—H2$\cdots$O1$^{iii}$ | 0.88 (4) | 1.76 (5) | 2.630 (5) | 168 (7) |
| O4—H3$\cdots$O1$^{iv}$ | 0.83 (4) | 1.85 (4) | 2.672 (3) | 177 (8) |

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

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 1998); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2004); software used to prepare material for publication: *SHELXL97*.

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**supplementary materials**

## Redetermination of the hexagonal struvite analogue Cs[Mg(OH$_2$)$_6$](PO$_4$)

## M. Weil

### Comment

Numerous compounds with general formula $A$[$B$(OH$_2$)$_6$]$X$O$_4$, 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 & Jeffery, 1979*a,b*). However, for the isoformular compounds Cs[Mg(OH$_2$)$_6$]($X$O$_4$), where $X$ = P and As, cubic and hexagonal forms were reported and structurally characterized (Ferrari *et al.*, 1955; Massa *et al.*, 2003). The cubic polymorph forms under hydrothermal conditions, whereas the hexagonal form is obtained under normal pressure and temperatures. All these structures can be described in terms of closed-packed layers with different stacking sequences (Massa *et al.*, 2003).

In this communication the redetermination of hexagonal Cs[Mg(OH$_2$)$_6$](PO$_4$) is reported. The previous refinement from photographic data (Ferrari *et al.*, 1955) was basically confirmed, but with all H atoms located and with all non H-atoms refined with anisotropic displacement parameters.

In addition to the description of the hexagonal Cs[Mg(OH$_2$)$_6$](PO$_4$) structure in terms of closed-packed layers (Massa *et al.*, 2003), the structure can be described as a derivative of the NiAs structure type. The centres of the slightly distorted PO$_4$ tetrahedra (3*m*. symmetry) are situated on the Ni positions, whereas the centres of the likewise slightly distorted complex [Mg(H$_2$O)$_6$] octahedra (3*m*. symmetry) are situated on the As positions (Fig. 1). Thus one [Mg(H$_2$O)$_6$] octahedron is surrounded by six PO$_4$ tetrahedra in a distorted trigonal–prismatic arrangement, whereas one PO$_4$ tetrahedron is surrounded by six [Mg(H$_2$O)$_6$] octahedra in a distorted octahedral arrangement. The corresponding P—O and Mg—O distances are in the normal range (Table 1). These building units are linked *via* medium-strong hydrogen bonds (Table 2, Fig. 2). Details and differences of the hydrogen bonding schemes in cubic, hexagonal and struvite-type structures were discussed by Massa *et al.* (2003). The Cs$^+$ cations are located in the voids of this arrangement and exhibit a distorted cuboctahedral 12-coordination [9+3] to the oxygen atoms of the water molecules (Table 1).

### Experimental

Colourless crystals of Cs[Mg(OH$_2$)$_6$](PO$_4$) with an edge-length up to 2 mm and mostly spherical habit 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$_2$PO$_4$ (50 ml) was carefully poured over the gel. This solution was then adjusted to pH 8.5 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.

# supplementary materials

**Refinement**

The positions of the H atoms were found from difference Fourier maps and were refined with soft distance restraints ($d$(O—H) = 0.90 (5) Å) and a common $U_{iso}$ parameter.

**Figures**
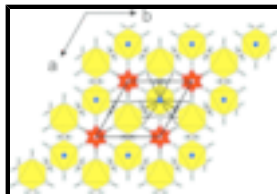


Fig. 1. Projection of the crystal structure of Cs[Mg(H$_2$O)$_6$](PO$_4$) along [00$\bar{1}$]. [Mg(OH$_2$)$_6$] octahedra are yellow, PO$_4$ tetrahedra are red, Cs atoms are blue, O atoms are white and H atoms are grey. For one of the Cs$^+$ cations the Cs—O bonds are indicated.
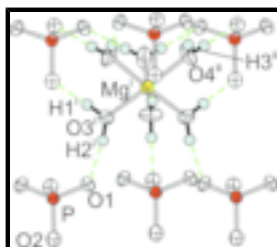


Fig. 2. The [Mg(OH$_2$)$_6$] octahedron with six surrounding PO$_4$ tetrahedra emphasizing the hydrogen bonding scheme (green dashed lines). The anisotropic displacement parameters are given at the 74% probability level. H atoms are given as spheres of arbitrary radius. [Symmetry codes: (i) $y$, $x$, $z$+1/2; (ii) -$x$+1, -$y$+1, -$z$+1.]

**Caesium hexaaquamagnesium orthophosphate**

*Crystal data*

| | |
|---|---|
| Cs[Mg(H$_2$O$_1$)$_6$](PO$_4$) | $Z = 2$ |
| $M_r = 360.29$ | $F_{000} = 348$ |
| Hexagonal, $P6_3mc$ | $D_x = 2.447$ Mg m$^{-3}$ |
| Hall symbol: P 6c -2c | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 6.8827$ (8) Å | Cell parameters from 1544 reflections |
| $b = 6.8827$ (8) Å | $\theta = 3.4–25.9º$ |
| $c = 11.9188$ (16) Å | $\mu = 4.04$ mm$^{-1}$ |
| $\alpha = 90º$ | $T = 293$ (2) K |
| $\beta = 90º$ | Block, colourless |
| $\gamma = 120º$ | $0.46 \times 0.38 \times 0.38$ mm |
| $V = 488.97$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Stoe IPDS diffractometer | 368 independent reflections |
| Radiation source: fine-focus sealed tube | 367 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.025$ |
| $T = 293(2)$ K | $\theta_{max} = 25.7º$ |
| $\omega$ scans | $\theta_{min} = 3.4º$ |
| Absorption correction: numerical | $h = -8\rightarrow8$ |

(HABITUS; Herrendorf, 1997)

$T_{min} = 0.213$, $T_{max} = 0.327$            $k = -8 \rightarrow 8$

5412 measured reflections            $l = -12 \rightarrow 13$

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: difference Fourier map |
| Least-squares matrix: full | H atoms treated by a mixture of independent and constrained refinement |
| $R[F^2 > 2\sigma(F^2)] = 0.016$ | $w = 1/[\sigma^2(F_o^2) + (0.0029P)^2 + 0.8141P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.034$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.29$ | $\Delta\rho_{max} = 0.40$ e Å$^{-3}$ |
| 368 reflections | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |
| 39 parameters | Extinction correction: none |
| 4 restraints | Absolute structure: Flack (1983), with 164 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: −0.01 (3) |
| Secondary atom site location: difference Fourier map | |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Cs | 0.3333 | 0.6667 | 0.02181 (4) | 0.03126 (15) |
| Mg | 0.6667 | 0.3333 | 0.1436 (2) | 0.0159 (5) |
| P | 0.0000 | 0.0000 | 0.29985 (14) | 0.0137 (5) |
| O1 | 0.1220 (2) | 0.2440 (4) | 0.3413 (3) | 0.0173 (6) |
| O2 | 0.0000 | 0.0000 | 0.1707 (5) | 0.0189 (13) |
| O3 | 0.3747 (6) | 0.1873 (3) | 0.0521 (3) | 0.0265 (9) |
| O4 | 0.5229 (3) | 0.0458 (5) | 0.2427 (3) | 0.0282 (8) |
| H1 | 0.243 (8) | 0.122 (4) | 0.094 (5) | 0.048 (9)* |
| H2 | 0.350 (12) | 0.175 (6) | −0.021 (4) | 0.048 (9)* |
| H3 | 0.397 (8) | −0.010 (14) | 0.272 (5) | 0.048 (9)* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cs | 0.02671 (16) | 0.02671 (16) | 0.0404 (3) | 0.01335 (8) | 0.000 | 0.000 |
| Mg | 0.0158 (8) | 0.0158 (8) | 0.0160 (16) | 0.0079 (4) | 0.000 | 0.000 |
| P | 0.0139 (5) | 0.0139 (5) | 0.0134 (13) | 0.0069 (2) | 0.000 | 0.000 |
| O1 | 0.0172 (9) | 0.0139 (13) | 0.0195 (17) | 0.0070 (7) | −0.0023 (6) | −0.0046 (12) |
| O2 | 0.0177 (19) | 0.0177 (19) | 0.021 (4) | 0.0089 (10) | 0.000 | 0.000 |
| O3 | 0.0142 (14) | 0.0406 (14) | 0.016 (3) | 0.0071 (7) | −0.0023 (11) | −0.0012 (5) |
| O4 | 0.0191 (11) | 0.0252 (19) | 0.042 (2) | 0.0126 (10) | 0.0096 (7) | 0.0191 (15) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cs—O3$^i$ | 3.469 (5) | Mg—O3 | 2.054 (4) |
| Cs—O3$^{ii}$ | 3.469 (5) | Mg—O3$^v$ | 2.054 (4) |
| Cs—O3$^{iii}$ | 3.469 (5) | Mg—O4$^{ix}$ | 2.082 (3) |
| Cs—O3$^{iv}$ | 3.469 (5) | Mg—O4 | 2.082 (3) |
| Cs—O3$^v$ | 3.469 (5) | Mg—O4$^v$ | 2.082 (3) |
| Cs—O3 | 3.469 (5) | Mg—Cs$^x$ | 4.2306 (10) |
| Cs—O4$^i$ | 3.470 (4) | Mg—Cs$^{xi}$ | 4.2306 (10) |
| Cs—O4$^{iv}$ | 3.470 (4) | Mg—Cs$^{xii}$ | 4.508 (3) |
| Cs—O4$^v$ | 3.470 (4) | P—O1 | 1.536 (3) |
| Cs—O4$^{vi}$ | 3.742 (4) | P—O1$^{iv}$ | 1.536 (3) |
| Cs—O4$^{vii}$ | 3.742 (4) | P—O1$^{xiii}$ | 1.536 (3) |
| Cs—O4$^{viii}$ | 3.742 (4) | P—O2 | 1.539 (6) |
| Mg—O3$^{ix}$ | 2.054 (4) | | |
| O3$^i$—Cs—O3$^{ii}$ | 51.51 (11) | O3$^v$—Cs—O4$^{vii}$ | 97.18 (5) |
| O3$^i$—Cs—O3$^{iii}$ | 67.77 (11) | O3—Cs—O4$^{vii}$ | 118.02 (7) |
| O3$^{ii}$—Cs—O3$^{iii}$ | 118.93 (2) | O4$^i$—Cs—O4$^{vii}$ | 112.101 (19) |
| O3$^i$—Cs—O3$^{iv}$ | 118.93 (2) | O4$^{iv}$—Cs—O4$^{vii}$ | 145.46 (3) |
| O3$^{ii}$—Cs—O3$^{iv}$ | 165.52 (11) | O4$^v$—Cs—O4$^{vii}$ | 145.46 (3) |
| O3$^{iii}$—Cs—O3$^{iv}$ | 51.51 (11) | O4$^{vi}$—Cs—O4$^{vii}$ | 46.74 (8) |
| O3$^i$—Cs—O3$^v$ | 118.93 (2) | O3$^i$—Cs—O4$^{viii}$ | 118.02 (7) |
| O3$^{ii}$—Cs—O3$^v$ | 67.77 (11) | O3$^{ii}$—Cs—O4$^{viii}$ | 97.18 (5) |
| O3$^{iii}$—Cs—O3$^v$ | 165.52 (11) | O3$^{iii}$—Cs—O4$^{viii}$ | 118.02 (7) |
| O3$^{iv}$—Cs—O3$^v$ | 118.93 (2) | O3$^{iv}$—Cs—O4$^{viii}$ | 97.18 (5) |
| O3$^i$—Cs—O3 | 165.52 (11) | O3$^v$—Cs—O4$^{viii}$ | 71.50 (7) |
| O3$^{ii}$—Cs—O3 | 118.93 (2) | O3—Cs—O4$^{viii}$ | 71.50 (7) |
| O3$^{iii}$—Cs—O3 | 118.93 (2) | O4$^i$—Cs—O4$^{viii}$ | 145.46 (3) |
| O3$^{iv}$—Cs—O3 | 67.77 (11) | O4$^{iv}$—Cs—O4$^{viii}$ | 145.46 (3) |
| O3$^v$—Cs—O3 | 51.51 (11) | O4$^v$—Cs—O4$^{viii}$ | 112.101 (19) |
| O3$^i$—Cs—O4$^i$ | 48.58 (7) | O4$^{vi}$—Cs—O4$^{viii}$ | 46.74 (8) |

| | | | |
|---|---|---|---|
| O3$^{ii}$—Cs—O4$^{i}$ | 48.58 (7) | O4$^{vii}$—Cs—O4$^{viii}$ | 46.74 (8) |
| O3$^{iii}$—Cs—O4$^{i}$ | 88.12 (6) | O3$^{ix}$—Mg—O3 | 94.42 (16) |
| O3$^{iv}$—Cs—O4$^{i}$ | 117.22 (7) | O3$^{ix}$—Mg—O3$^{v}$ | 94.42 (16) |
| O3$^{v}$—Cs—O4$^{i}$ | 88.12 (6) | O3—Mg—O3$^{v}$ | 94.42 (16) |
| O3—Cs—O4$^{i}$ | 117.22 (7) | O3$^{ix}$—Mg—O4$^{ix}$ | 87.27 (10) |
| O3$^{i}$—Cs—O4$^{iv}$ | 88.12 (6) | O3—Mg—O4$^{ix}$ | 177.5 (2) |
| O3$^{ii}$—Cs—O4$^{iv}$ | 117.22 (7) | O3$^{v}$—Mg—O4$^{ix}$ | 87.27 (10) |
| O3$^{iii}$—Cs—O4$^{iv}$ | 48.58 (7) | O3$^{ix}$—Mg—O4 | 87.27 (10) |
| O3$^{iv}$—Cs—O4$^{iv}$ | 48.58 (7) | O3—Mg—O4 | 87.27 (10) |
| O3$^{v}$—Cs—O4$^{iv}$ | 117.22 (7) | O3$^{v}$—Mg—O4 | 177.5 (2) |
| O3—Cs—O4$^{iv}$ | 88.12 (6) | O4$^{ix}$—Mg—O4 | 90.98 (19) |
| O4$^{i}$—Cs—O4$^{iv}$ | 68.67 (8) | O3$^{ix}$—Mg—O4$^{v}$ | 177.5 (2) |
| O3$^{i}$—Cs—O4$^{v}$ | 117.22 (7) | O3—Mg—O4$^{v}$ | 87.27 (10) |
| O3$^{ii}$—Cs—O4$^{v}$ | 88.12 (6) | O3$^{v}$—Mg—O4$^{v}$ | 87.27 (10) |
| O3$^{iii}$—Cs—O4$^{v}$ | 117.22 (7) | O4$^{ix}$—Mg—O4$^{v}$ | 90.98 (19) |
| O3$^{iv}$—Cs—O4$^{v}$ | 88.12 (6) | O4—Mg—O4$^{v}$ | 90.98 (19) |
| O3$^{v}$—Cs—O4$^{v}$ | 48.58 (7) | O1—P—O1$^{iv}$ | 110.17 (14) |
| O3—Cs—O4$^{v}$ | 48.58 (7) | O1—P—O1$^{xiii}$ | 110.17 (14) |
| O4$^{i}$—Cs—O4$^{v}$ | 68.67 (8) | O1$^{iv}$—P—O1$^{xiii}$ | 110.17 (14) |
| O4$^{iv}$—Cs—O4$^{v}$ | 68.67 (8) | O1—P—O2 | 108.76 (14) |
| O3$^{i}$—Cs—O4$^{vi}$ | 97.18 (5) | O1$^{iv}$—P—O2 | 108.76 (14) |
| O3$^{ii}$—Cs—O4$^{vi}$ | 118.02 (7) | O1$^{xiii}$—P—O2 | 108.76 (14) |
| O3$^{iii}$—Cs—O4$^{vi}$ | 71.50 (7) | Mg—O3—Cs$^{x}$ | 96.63 (6) |
| O3$^{iv}$—Cs—O4$^{vi}$ | 71.50 (7) | Mg—O3—Cs | 96.63 (6) |
| O3$^{v}$—Cs—O4$^{vi}$ | 118.02 (7) | Cs$^{x}$—O3—Cs | 165.52 (11) |
| O3—Cs—O4$^{vi}$ | 97.18 (5) | Mg—O3—H1 | 116 (4) |
| O4$^{i}$—Cs—O4$^{vi}$ | 145.46 (3) | Mg—O3—H2 | 132 (5) |
| O4$^{iv}$—Cs—O4$^{vi}$ | 112.101 (19) | H1—O3—H2 | 113 (6) |
| O4$^{v}$—Cs—O4$^{vi}$ | 145.46 (3) | Mg—O4—Cs$^{x}$ | 96.07 (16) |
| O3$^{i}$—Cs—O4$^{vii}$ | 71.50 (7) | Mg—O4—Cs$^{xii}$ | 97.31 (14) |
| O3$^{ii}$—Cs—O4$^{vii}$ | 71.50 (7) | Cs$^{x}$—O4—Cs$^{xii}$ | 166.63 (10) |
| O3$^{iii}$—Cs—O4$^{vii}$ | 97.18 (5) | Mg—O4—H3 | 125 (4) |
| O3$^{iv}$—Cs—O4$^{vii}$ | 118.02 (7) | | |

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


*Hydrogen-bond geometry (Å, °)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H1···O2 | 0.93 (4) | 1.71 (4) | 2.643 (5) | 180 (6) |
| O3—H2···O1$^{xiv}$ | 0.88 (4) | 1.76 (5) | 2.630 (5) | 168 (7) |
| O4—H3···O1$^{xiii}$ | 0.83 (4) | 1.85 (4) | 2.672 (3) | 177 (8) |

Symmetry codes: (xiv) *y*, −*x*+*y*, *z*−1/2; (xiii) −*x*+*y*, −*x*, *z*.

**Fig. 1**

**Fig. 2**