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ISSN 2414-3146

# Dicaesium tetramagnesium pentakis(carbonate) decahydrate, $Cs_2Mg_4(CO_3)_5\cdot10H_2O$

Christine Rincke,* Horst Schmidt and Wolfgang Voigt

Institute of Inorganic Chemistry, TU Bergakademie Freiberg, Leipziger Str. 29, D-09599 Freiberg, Germany. *Correspondence e-mail: christine.rincke@chemie.tu-freiberg.de

Received 8 January 2020
Accepted 5 February 2020

Edited by M. Weil, Vienna University of Technology, Austria

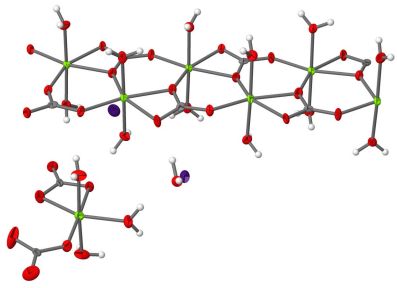
**Keywords:** carbonate; hydrate; magnesium compound; caesium compound; twinning; crystal structure.

**CCDC reference**: 1982137

**Structural data**: full structural data are available from iucrdata.iucr.org

The title carbonate hydrate, $Cs_2Mg_4(CO_3)_5\cdot10H_2O$, was crystallized at room temperature out of aqueous solutions containing caesium bicarbonate and magnesium nitrate. Its monoclinic crystal structure ($P2_1/n$) consists of double chains of composition $^1_\infty[Mg(H_2O)_{2/1}(CO_3)_{3/3}]$, isolated $[Mg(H_2O)(CO_3)_2]^{2-}$ units, two crystallographically distinct $Cs^+$ ions and a free water molecule. The crystal under investigation was twinned by reticular pseudomerohedry.

3D view



## Structure description

Up to now, only two magnesium salts containing hydrogenbiscarbonate anions $[H(CO_3)_2^{3-}]$ were known, *viz*. $KMgH(CO_3)_2\cdot4H_2O$ and $RbMgH(CO_3)_2\cdot4H_2O$. Both can be crystallized at room temperature by combination of an aqueous solution of the alkali metal bicarbonate and an aqueous solution of magnesium chloride or nitrate (Fernandes *et al.*, 1988; Dahm, 2000). The synthesis of the analogous caesium compound was not successful (Gloss, 1937). Tkachev *et al.* (1978) reported on the synthesis of $CsMgH(CO_3)_2\cdot0.5H_2O$, but details about the conditions of formation were missing. In our current investigations on that matter, the title compound was found instead of a hydrogenbiscarbonate.

$Cs_2Mg_4(CO_3)_5\cdot10H_2O$ crystallizes in the space group $P2_1/n$ and contains four slightly distorted $[MgO_6]$ octahedra (Fig. 1). Each of the magnesium cations Mg1, Mg3 and Mg4 forms $[Mg(H_2O)_2(CO_3)_3]^{4-}$ units that are linked by bridging carbonate anions of the carbon atoms C1, C2 and C3 (Fig. 2). Each carbonate anion bonds in a bidentate mode to one and in a monodentate to the other cations (Figs. 1, 2). In each octahedron, the water molecules are located in the *trans*-positions and have no bridging character. In this way, double chains of composition $^1_\infty[Mg(H_2O)_{2/1}(CO_3)_{3/3}]$ are formed, extending parallel to the $[\bar{1}01]$ direction (Fig. 3). Between these double chains, isolated $[Mg(H_2O)_3(CO_3)_2]^{2-}$ units involving the Mg2 cation are located (Fig. 4). The Mg2 cation is also octahedrally

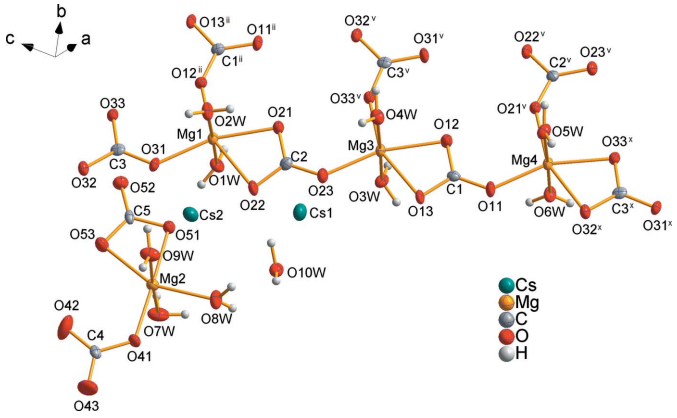



**Figure 1**
The expanded asymmetric unit of $Cs_2Mg_4(CO_3)_5{\cdot}10H_2O$ showing the coordination polyhedra around the four Mg sites. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (x) $x+1, y, z-1$.]

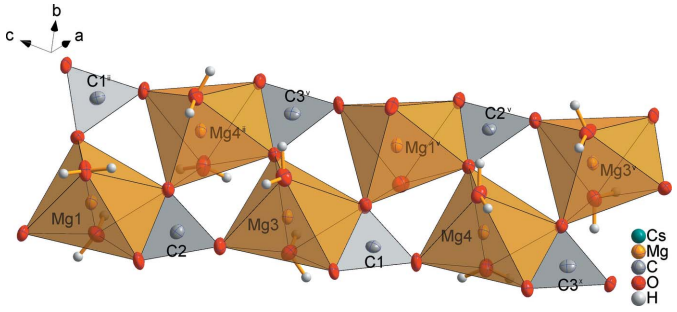



**Figure 2**
Double chain built up from octahedra around Mg1, Mg3 and Mg4 and carbonate units. [Symmetry codes: (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (x) $x+1, y, z-1$.]

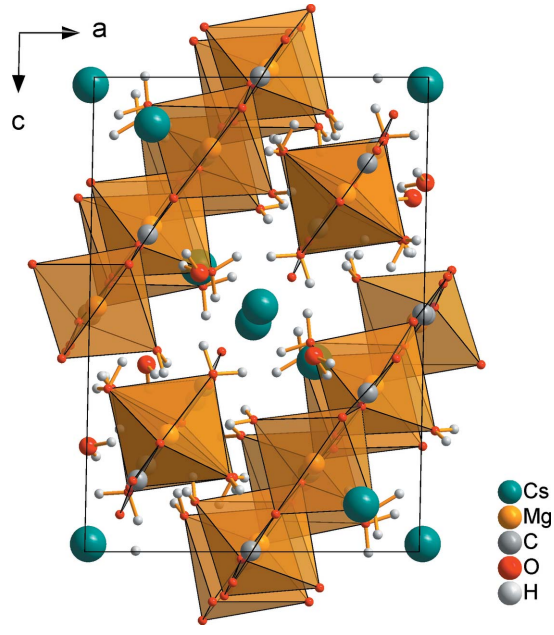



**Figure 3**
The crystal structure of $Cs_2Mg_4(CO_3)_5{\cdot}10H_2O$ in a view along the *b* axis.

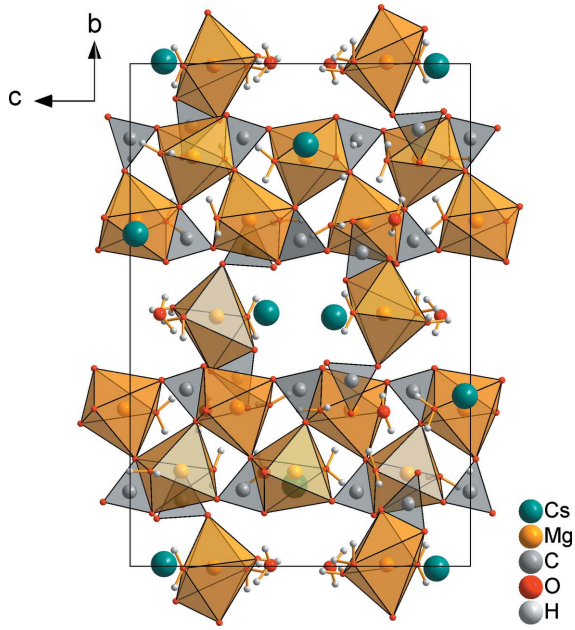



**Figure 4**
The crystal structure of $Cs_2Mg_4(CO_3)_5{\cdot}10H_2O$ in a view along the *a* axis.

coordinated, in this case by three water molecules and two carbonate anions (C4, C5) in a monodentate and a bidentate fashion, respectively (Fig. 1). The $^1_\infty[Mg(H_2O)_{2/1}(CO_3)_{3/3}]$ double chains and the isolated $[Mg(H_2O)_3(CO_3)_2]^{2-}$ units form alternating sheets parallel to (010) (Fig. 4).

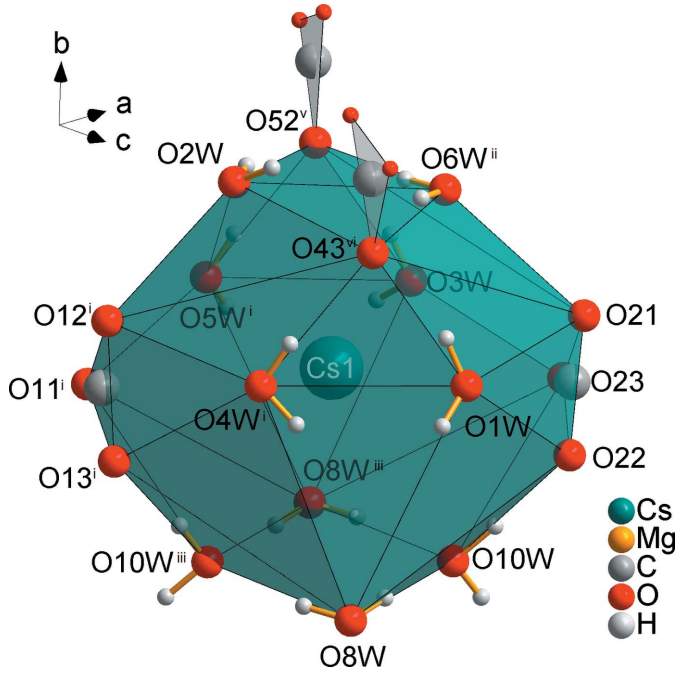



**Figure 5**
Coordination sphere of the Cs1 cation, with all atoms drawn as spheres of arbitrary radii (oxygen atoms not coordinating to Cs with half of the size of other O atoms). [Symmetry codes: (i) $x-1, y, z$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+2, -y+1, -z$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (vi) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.]

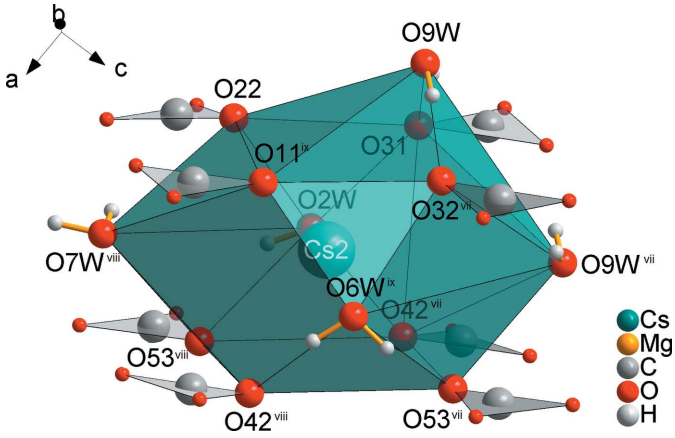



**Figure 6**
Coordination sphere of the Cs2 cation, with all atoms drawn as spheres of arbitrary radii (oxygen atoms not coordinating to Cs with half of the size of other O atoms). [Symmetry codes: (vii) $-x+2, -y+1, -z+1$; (viii) $x+1, y, z$; (ix) $-x+3, -y+1, -z$.]

The C—O bonds of the carbonate units range from 1.252 (12) to 1.316 (11) Å and the O—C—O angles from 114.8 (8) to 124.4 (8)°. In comparison with other crystal structures containing carbonate units and deposited in the Inorganic Structure Database (ICSD; Zagorac *et al.*, 2019), these deviations of the bond lengths and angles from ideal values of a equilateral triangle are not unusual (Cirpus, 1997). As a result, the symmetry of the carbonate anions deviates significantly from ideal $D_{3h}$; however, the sum of all O—C—O angles remains 360° and planarity is kept, which is typical for all carbonate structures (Zemann, 1981; Cirpus, 1997).

The two caesium cations interconnect two adjacent double chains and four (Cs1) and three (Cs2) $[Mg2(H_2O)_3(CO_3)_2]^{2-}$ units, respectively, thereby generating a three-dimensional framework. The coordination numbers of the caesium cations are [6 + 12] for Cs1 and [7 + 6] for Cs2, whereby the first numeral indicates the number of the coordinating O atoms

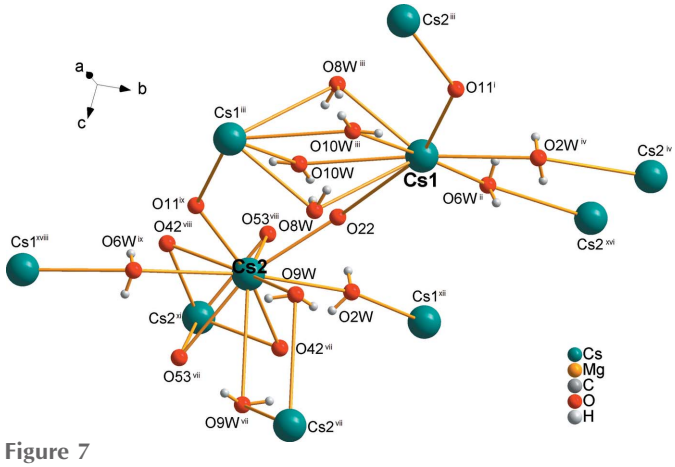



**Figure 7**
Linkage of Cs cations by O atoms, with all atoms drawn as spheres of arbitrary radii (other atoms are left out for clarity). [Symmetry codes: (i) $x-1, y, z$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+2, -y+1, -z$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (vii) $-x+2, -y+1, -z+1$; (viii) $x+1, y, z$; (ix) $-x+3, -y+1, -z$; (xi) $-x+3, -y+1, -z+1$; (xvi) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (xviii) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.]

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$A$···O51 | 0.82 (5) | 1.85 (6) | 2.658 (10) | 172 (12) |
| O1$W$—H1$B$···O43$^{i}$ | 0.83 (5) | 1.89 (6) | 2.686 (11) | 162 (12) |
| O2$W$—H2$A$···O52$^{ii}$ | 0.80 (5) | 2.01 (6) | 2.783 (11) | 160 (12) |
| O2$W$—H2$B$···O42$^{iii}$ | 0.81 (5) | 1.93 (6) | 2.734 (12) | 170 (13) |
| O3$W$—H3$A$···O52$^{iv}$ | 0.82 (5) | 2.23 (6) | 2.993 (12) | 157 (11) |
| O3$W$—H3$B$···O41$^{v}$ | 0.82 (5) | 1.92 (6) | 2.737 (11) | 175 (12) |
| O4$W$—H4$A$···O43$^{vi}$ | 0.82 (5) | 1.93 (6) | 2.724 (11) | 162 (13) |
| O4$W$—H4$B$···O51$^{ii}$ | 0.82 (5) | 1.84 (6) | 2.661 (9) | 174 (14) |
| O5$W$—H5$A$···O52$^{vii}$ | 0.82 (5) | 2.04 (6) | 2.853 (10) | 169 (13) |
| O5$W$—H5$B$···O41$^{viii}$ | 0.80 (5) | 2.05 (6) | 2.831 (10) | 164 (13) |
| O6$W$—H6$A$···O43$^{v}$ | 0.84 (5) | 2.21 (6) | 3.021 (13) | 165 (13) |
| O6$W$—H6$B$···O52$^{ix}$ | 0.81 (5) | 1.98 (6) | 2.783 (10) | 174 (13) |
| O7$W$—H7$B$···O23$^{x}$ | 0.83 (5) | 2.07 (7) | 2.843 (10) | 155 (13) |
| O8$W$—H8$A$···O10$W$ | 0.82 (5) | 2.02 (6) | 2.815 (10) | 165 (13) |
| O8$W$—H8$B$···O10$W^{v}$ | 0.82 (5) | 2.02 (7) | 2.815 (10) | 164 (15) |
| O9$W$—H9$A$···O31 | 0.82 (5) | 2.09 (7) | 2.869 (10) | 161 (13) |
| O9$W$—H9$B$···O32$^{iii}$ | 0.82 (5) | 1.87 (7) | 2.673 (10) | 170 (13) |
| O10$W$—H10$A$···O13$^{viii}$ | 0.81 (5) | 2.01 (6) | 2.798 (9) | 162 (13) |
| O10$W$—H10$B$···O22 | 0.90 (13) | 1.84 (13) | 2.730 (10) | 169 (12) |

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+1, y, z$; (iii) $-x+2, -y+1, -z+1$; (iv) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $-x+2, -y+1, -z$; (vi) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (vii) $x+\frac{3}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (viii) $-x+3, -y+1, -z$; (ix) $x+1, y, z-1$; (x) $x-1, y, z$.

with a distance between 3.06 to 3.44 Å and the second number the number of O atoms with a distance between 3.44 and 4.12 Å. The Cs1 cation is coordinated by ten water molecules and four carbonate units (Fig. 5), the Cs2 cation by five water molecules and eight carbonate units (Fig. 6). The $[Cs1O_{18}]$ polyhedron is connected with another $[Cs1O_{18}]$ polyhedron by face-sharing through O8$W$, O8$W^{iii}$, O10$W$ and O10$W^{iii}$ and is also linked by sharing corners to four $[Cs2O_{13}]$ polyhedra through O2$W^{iv}$, O11$^{i}$, O6$W^{ii}$ and O22. Likewise, a $[Cs2O_{13}]$ polyhedron is linked by face-sharing through O42$^{vii}$, O42$^{viii}$, O53$^{vii}$ and O53$^{viii}$ with another $[Cs2O_{13}]$ polyhedron and by edge-sharing with two $[Cs2O_{13}]$ polyhedra through O9$W$ and O9$W^{vii}$ (Fig. 7).

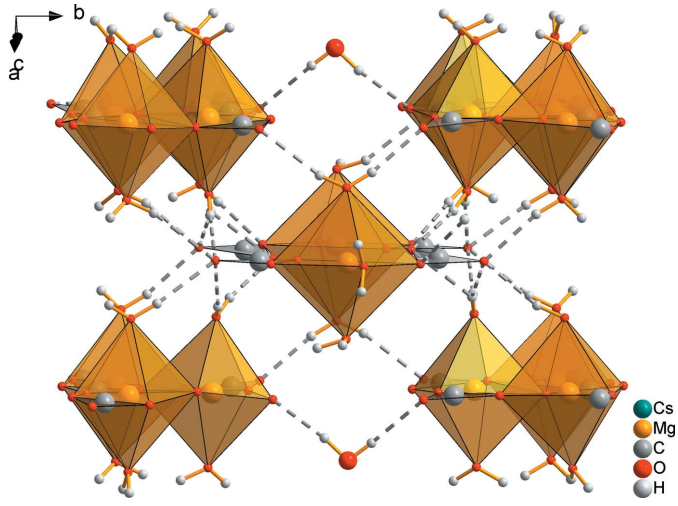



**Figure 8**
Interconnection of double chains (at the corners), the $[Mg2(H_2O)_3(CO_3)_2]^{2-}$ units (in the middle) and the free water molecule *via* hydrogen bonds in the crystal structure of $Cs_2Mg_4(CO_3)_5{\cdot}10H_2O$. Hydrogen bonds are represented by dashed lines; Cs atoms are omitted for clarity.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $Cs_2Mg_4(CO_3)_5{\cdot}10H_2O$ |
| $M_r$ | 843.27 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 200 |
| $a, b, c$ (Å) | 9.1617 (9), 19.233 (3), 13.0065 (13) |
| $\beta$ (°) | 91.136 (8) |
| $V$ (Å$^3$) | 2291.4 (4) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 3.41 |
| Crystal size (mm) | 0.6 × 0.45 × 0.25 |
| Data collection | |
| Diffractometer | STOE *IPDS* 2T |
| Absorption correction | Integration (Coppens, 1970) |
| $T_{min}$, $T_{max}$ | 0.151, 0.439 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 37526, 37526, 31786 |
| $R_{int}$ | 0.086 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.650 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.073, 0.274, 1.22 |
| No. of reflections | 37526 |
| No. of parameters | 386 |
| No. of restraints | 19 |
| H-atom treatment | Only H-atom coordinates refined |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 3.48, −2.86 |

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2017) and *publCIF* (Westrip, 2010).

Additional stability in the crystal structure is accomplished by hydrogen bonds between the water molecules of the double chains, the $[Mg2(H_2O)_3(CO_3)_2]^{2-}$ units and the free water molecule (H25*A*—O25—H25*B*) (Fig. 8, Table 1). The shortest hydrogen bonds are built between O4*W*—H4*B*···O51$^{i}$, O10*W*—H10*B*···O22, O4*W*—H4*A*···O43$^{ii}$ and O6*W*—H6*B*···O52$^{vi}$ with H···O distances < 2.00 Å (Table 1). The bond length correlates with the strength of the hydrogen bonds (Steiner, 2002), and in the present case the strength of the hydrogen bonding is considered to be moderate.

For the crystal structures of other alkali metal magnesium carbonates and hydrogen bis(carbonates), see: $KMgH(CO_3)_2{\cdot}4H_2O$ (Fernandes *et al.*, 1988), $RbMgH(CO_3)_2{\cdot}4H_2O$ (Dahm, 2000), $K_2Mg(CO_3)_2{\cdot}4H_2O$ (Bucat *et al.*, 1977), $Rb_2Mg(CO_3)_2{\cdot}4H_2O$ (Zheng & Adam, 1994), $Cs_2Mg(CO_3)_2{\cdot}4H_2O$ (Zheng & Adam, 1999).

## Synthesis and crystallization

The synthesis was derived from the information for crystallization of $KMgH(CO_3)_2{\cdot}4H_2O$ as reported by Fernandes *et al.* (1988). $CO_2$ was bubbled through a solution of $Cs_2CO_3$ (9.043 g, Merck, > 99.5%) and water (22.120 g) for three h. Afterwards, a solution of $Mg(NO_3)_2{\cdot}6H_2O$ (1.041 g, Merck, p.a.) and water (2.643 g) was added and stored in a sealed bottle for 2 d. A crystalline solid was formed and filtered off. The characterization with powder X-ray diffraction showed that the product was a mixture of $MgCO_3{\cdot}3H_2O$ and the title compound.

After filtration the remaining solution was stored in a sealed bottle for 14 d at room temperature. During this period further acicular crystals (200 *x* 20 µm) were formed. The product was washed with ethanol and characterized by powder X-ray diffraction, thermal analysis, FT–IR spectroscopy and SEM (see: supporting information). Some crystals were kept in the mother solution in a sealed vessel for one month. Afterwards a suitable crystal for the single-crystal determination was selected.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. If twinning is not accounted for, the reflections can be indexed by a large orthorhombic cell, but the subsequent refinement did not result in an useful structure model. Close inspection of the diffraction pattern revealed the presence of two monoclinic cells ($P2_1/n$) with lattice parameters of $a$ = 9.1617 (9), $b$ = 19.233 (3), $c$ = 13.0065 (13) Å, $\beta$ = 91.136 (8)°. Therefore the crystal under investigation exhibited twinning by reticular pseudomerohedry; the matrix that relates the individual diffraction pattern was determined as ($-\frac{1}{3}$ 0 $-\frac{2}{3}$, 0 −1 0, $-\frac{4}{3}$ 0 $\frac{1}{3}$). The reflections of both domains were integrated concurrently, leading to the following numbers. Reflections belonging to domain 1: 16785; reflections belonging to domain 2: 26839; overlaid reflections: 10073; major twin component fraction: 56%.

Structure solution permitted the assignment of all heavy atoms and the subsequent refinement leads to a chemical sensible atomic arrangement. All H atoms were discernable from difference-Fourier maps and refined with an O—H distance restraint of 0.82(2) Å and $U_{iso}$(H) = 1.2$U_{eq}$(O).

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# full crystallographic data

*IUCrData* (2020). **5**, x200165 [https://doi.org/10.1107/S2414314620001650]

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**Christine Rincke, Horst Schmidt and Wolfgang Voigt**

### Dicaesium tetramagnesium pentakis(carbonate) decahydrate

*Crystal data*

$Cs_2Mg_4(CO_3)_5{\cdot}10H_2O$
$M_r$ = 843.27
Monoclinic, $P2_1/n$
$a$ = 9.1617 (9) Å
$b$ = 19.233 (3) Å
$c$ = 13.0065 (13) Å
$\beta$ = 91.136 (8)°
$V$ = 2291.4 (4) Å$^3$
$Z$ = 4
$F(000)$ = 1632
$D_x$ = 2.444 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 11266 reflections
$\theta$ = 10.0–27.5°
$\mu$ = 3.41 mm$^{-1}$
$T$ = 200 K
Needle, colorless
0.6 × 0.45 × 0.25 mm

*Data collection*

STOE IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm$^{-1}$
rotation method scans
Absorption correction: integration (Coppens, 1970)
$T_{min}$ = 0.151, $T_{max}$ = 0.439
37526 measured reflections
37526 independent reflections
31786 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.086
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.7°
$h$ = −11→11
$k$ = −24→24
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.274
$S$ = 1.22
37526 reflections
386 parameters
19 restraints
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 3.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.86 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refined as a two-component twin. All H atoms were discernable from difference Fourier maps. Their $U_{iso}$ values were set at $1.2U_{eq}$(O) using a riding-model approximation, with O—H distance restraint of 0.82 (2) Å.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cs1 | 1.00975 (7) | 0.66121 (4) | −0.01626 (5) | 0.0303 (3) |
| Cs2 | 1.32369 (7) | 0.49560 (3) | 0.40043 (5) | 0.0264 (3) |
| Mg1 | 1.1797 (3) | 0.68437 (15) | 0.3146 (2) | 0.0151 (6) |
| Mg2 | 0.7423 (3) | 0.50315 (14) | 0.2539 (2) | 0.0180 (6) |
| Mg3 | 1.5193 (3) | 0.68707 (16) | −0.0165 (2) | 0.0149 (6) |
| Mg4 | 1.8523 (3) | 0.68950 (15) | −0.3500 (2) | 0.0148 (6) |
| C1 | 1.6693 (10) | 0.6520 (4) | −0.1682 (7) | 0.0151 (17) |
| C2 | 1.3367 (10) | 0.6479 (5) | 0.1655 (7) | 0.0157 (17) |
| C3 | 0.9960 (9) | 0.6486 (5) | 0.4985 (7) | 0.0159 (18) |
| C4 | 0.6528 (9) | 0.3691 (5) | 0.3489 (7) | 0.0159 (15) |
| C5 | 0.6780 (9) | 0.6242 (5) | 0.3186 (6) | 0.0161 (15) |
| O1W | 0.9961 (8) | 0.6901 (4) | 0.2222 (6) | 0.0214 (13) |
| H1A | 0.927 (10) | 0.664 (6) | 0.231 (10) | 0.026* |
| H1B | 0.972 (13) | 0.729 (4) | 0.201 (10) | 0.026* |
| O2W | 1.3628 (8) | 0.6785 (4) | 0.4098 (6) | 0.0226 (14) |
| H2A | 1.437 (9) | 0.678 (7) | 0.378 (8) | 0.027* |
| H2B | 1.375 (14) | 0.658 (6) | 0.464 (6) | 0.027* |
| O31 | 1.0684 (8) | 0.6279 (4) | 0.4208 (5) | 0.0200 (13) |
| O21 | 1.3187 (7) | 0.7114 (3) | 0.1938 (5) | 0.0185 (12) |
| O22 | 1.2623 (8) | 0.6024 (3) | 0.2168 (5) | 0.0211 (13) |
| O23 | 1.4196 (8) | 0.6297 (4) | 0.0929 (5) | 0.0197 (13) |
| O3W | 1.3266 (8) | 0.6867 (4) | −0.1057 (6) | 0.0204 (13) |
| H3B | 1.318 (14) | 0.662 (6) | −0.157 (7) | 0.025* |
| H3A | 1.301 (13) | 0.725 (4) | −0.126 (9) | 0.025* |
| O4W | 1.7042 (8) | 0.6938 (4) | 0.0761 (6) | 0.0220 (14) |
| H4B | 1.726 (14) | 0.667 (6) | 0.123 (8) | 0.026* |
| H4A | 1.734 (14) | 0.731 (4) | 0.102 (9) | 0.026* |
| O5W | 2.0403 (8) | 0.6925 (4) | −0.2549 (6) | 0.0218 (14) |
| H5B | 2.097 (11) | 0.661 (5) | −0.258 (10) | 0.026* |
| H5A | 2.074 (13) | 0.730 (4) | −0.233 (10) | 0.026* |
| O6W | 1.6622 (8) | 0.6890 (4) | −0.4404 (6) | 0.0227 (14) |
| H6A | 1.576 (7) | 0.684 (7) | −0.421 (10) | 0.027* |
| H6B | 1.652 (14) | 0.690 (7) | −0.502 (4) | 0.027* |
| O11 | 1.7447 (8) | 0.6338 (4) | −0.2448 (5) | 0.0220 (14) |
| O12 | 1.6439 (8) | 0.7159 (3) | −0.1449 (5) | 0.0200 (13) |
| O13 | 1.6152 (7) | 0.6063 (3) | −0.1054 (5) | 0.0176 (12) |
| O7W | 0.5600 (9) | 0.5047 (3) | 0.1568 (7) | 0.0302 (16) |
| H7A | 0.601 (15) | 0.512 (8) | 0.100 (7) | 0.036* |
| H7B | 0.527 (14) | 0.545 (4) | 0.156 (11) | 0.036* |
| O8W | 0.8731 (8) | 0.4854 (4) | 0.1256 (5) | 0.0280 (14) |
| H8A | 0.960 (7) | 0.495 (6) | 0.122 (12) | 0.034* |
| H8B | 0.843 (15) | 0.490 (7) | 0.066 (5) | 0.034* |
| O51 | 0.7580 (7) | 0.6121 (3) | 0.2376 (5) | 0.0182 (12) |
| O52 | 0.6504 (8) | 0.6860 (3) | 0.3457 (6) | 0.0231 (13) |
| O41 | 0.7184 (8) | 0.3984 (3) | 0.2720 (5) | 0.0241 (13) |

| | | | | |
|---|---|---|---|---|
| O42 | 0.6027 (12) | 0.4052 (5) | 0.4216 (7) | 0.049 (2) |
| O43 | 0.6392 (11) | 0.3043 (4) | 0.3508 (7) | 0.040 (2) |
| O32 | 0.9441 (7) | 0.6056 (3) | 0.5649 (5) | 0.0186 (13) |
| O33 | 0.9686 (8) | 0.7136 (3) | 0.5157 (5) | 0.0177 (12) |
| O9W | 0.9293 (9) | 0.5041 (3) | 0.3441 (6) | 0.0283 (15) |
| H9B | 0.959 (14) | 0.468 (4) | 0.370 (10) | 0.034* |
| H9A | 0.949 (14) | 0.542 (4) | 0.369 (10) | 0.034* |
| O53 | 0.6312 (7) | 0.5693 (4) | 0.3652 (5) | 0.0261 (14) |
| O10W | 1.1733 (8) | 0.4982 (3) | 0.0876 (5) | 0.0222 (14) |
| H10A | 1.223 (12) | 0.465 (5) | 0.103 (9) | 0.027* |
| H10B | 1.214 (14) | 0.531 (7) | 0.128 (10) | 0.027* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cs1 | 0.0293 (4) | 0.0358 (4) | 0.0260 (4) | −0.0016 (2) | 0.0086 (3) | −0.0031 (2) |
| Cs2 | 0.0259 (4) | 0.0232 (4) | 0.0301 (4) | −0.00246 (19) | 0.0027 (3) | 0.0020 (2) |
| Mg1 | 0.0138 (15) | 0.0184 (14) | 0.0132 (15) | −0.0001 (10) | 0.0024 (11) | −0.0003 (11) |
| Mg2 | 0.0192 (15) | 0.0154 (14) | 0.0195 (14) | −0.0015 (9) | 0.0023 (12) | 0.0001 (10) |
| Mg3 | 0.0136 (14) | 0.0178 (14) | 0.0135 (15) | 0.0011 (10) | 0.0036 (11) | 0.0000 (10) |
| Mg4 | 0.0127 (14) | 0.0188 (14) | 0.0129 (15) | 0.0006 (10) | 0.0027 (11) | 0.0000 (11) |
| C1 | 0.015 (4) | 0.015 (4) | 0.015 (4) | −0.002 (3) | −0.004 (3) | 0.000 (3) |
| C2 | 0.016 (4) | 0.018 (4) | 0.013 (4) | 0.003 (3) | −0.003 (3) | 0.001 (3) |
| C3 | 0.014 (4) | 0.018 (4) | 0.015 (4) | 0.001 (3) | −0.008 (3) | 0.000 (3) |
| C4 | 0.010 (3) | 0.023 (4) | 0.015 (4) | −0.004 (3) | −0.002 (3) | 0.003 (3) |
| C5 | 0.010 (4) | 0.027 (4) | 0.011 (4) | −0.004 (3) | 0.000 (3) | 0.002 (3) |
| O1W | 0.016 (3) | 0.023 (3) | 0.025 (4) | −0.003 (2) | −0.001 (3) | 0.003 (3) |
| O2W | 0.017 (3) | 0.035 (4) | 0.016 (3) | 0.002 (3) | 0.002 (2) | 0.006 (3) |
| O31 | 0.023 (3) | 0.022 (3) | 0.015 (3) | 0.001 (2) | 0.008 (3) | −0.004 (2) |
| O21 | 0.022 (3) | 0.017 (3) | 0.017 (3) | 0.001 (2) | 0.006 (2) | 0.001 (2) |
| O22 | 0.021 (3) | 0.022 (3) | 0.021 (3) | −0.001 (2) | 0.011 (3) | 0.003 (2) |
| O23 | 0.019 (3) | 0.022 (3) | 0.018 (3) | 0.002 (2) | 0.007 (3) | 0.001 (2) |
| O3W | 0.019 (3) | 0.023 (3) | 0.019 (4) | 0.002 (2) | 0.000 (3) | −0.005 (3) |
| O4W | 0.021 (3) | 0.027 (3) | 0.018 (3) | −0.001 (2) | −0.004 (3) | 0.006 (3) |
| O5W | 0.019 (3) | 0.028 (3) | 0.018 (3) | 0.004 (2) | −0.001 (3) | −0.003 (3) |
| O6W | 0.014 (3) | 0.037 (4) | 0.017 (3) | −0.004 (3) | 0.000 (2) | −0.002 (3) |
| O11 | 0.025 (4) | 0.026 (3) | 0.016 (3) | 0.000 (3) | 0.010 (3) | 0.002 (3) |
| O12 | 0.026 (4) | 0.016 (3) | 0.017 (3) | 0.002 (2) | 0.005 (3) | 0.002 (2) |
| O13 | 0.015 (3) | 0.022 (3) | 0.016 (3) | −0.002 (2) | 0.007 (2) | 0.002 (2) |
| O7W | 0.023 (4) | 0.020 (3) | 0.046 (4) | 0.002 (2) | −0.011 (3) | −0.002 (3) |
| O8W | 0.021 (3) | 0.042 (4) | 0.021 (3) | 0.000 (3) | 0.006 (3) | 0.002 (3) |
| O51 | 0.020 (3) | 0.016 (3) | 0.019 (3) | 0.001 (2) | 0.004 (2) | 0.001 (2) |
| O52 | 0.026 (3) | 0.018 (3) | 0.026 (3) | 0.002 (2) | 0.001 (3) | −0.001 (3) |
| O41 | 0.035 (3) | 0.018 (3) | 0.019 (3) | −0.008 (3) | 0.007 (3) | 0.002 (2) |
| O42 | 0.075 (6) | 0.044 (5) | 0.030 (4) | 0.027 (4) | 0.023 (4) | 0.000 (3) |
| O43 | 0.070 (6) | 0.021 (3) | 0.030 (4) | −0.009 (4) | −0.007 (4) | 0.009 (3) |
| O32 | 0.018 (3) | 0.022 (3) | 0.016 (3) | −0.001 (2) | 0.005 (2) | 0.002 (2) |
| O33 | 0.021 (3) | 0.017 (3) | 0.015 (3) | 0.001 (2) | 0.004 (2) | −0.001 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O9W | 0.030 (4) | 0.019 (3) | 0.035 (4) | 0.000 (2) | −0.012 (3) | 0.004 (3) |
| O53 | 0.030 (3) | 0.019 (3) | 0.029 (3) | −0.001 (2) | 0.010 (3) | 0.003 (3) |
| O10W | 0.020 (3) | 0.024 (4) | 0.023 (3) | 0.000 (2) | 0.001 (3) | −0.002 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cs1—O4W$^{i}$ | 3.132 (8) | Mg1—O21 | 2.107 (8) |
| Cs1—O1W | 3.156 (8) | Mg1—O22 | 2.171 (8) |
| Cs1—O5W$^{i}$ | 3.180 (8) | Mg2—O41 | 2.041 (7) |
| Cs1—O3W | 3.187 (8) | Mg2—O9W | 2.057 (9) |
| Cs1—O6W$^{ii}$ | 3.342 (8) | Mg2—O7W | 2.074 (9) |
| Cs1—O8W$^{iii}$ | 3.344 (8) | Mg2—O8W | 2.102 (7) |
| Cs1—O2W$^{iv}$ | 3.492 (8) | Mg2—O51 | 2.111 (7) |
| Cs1—O10W$^{iii}$ | 3.607 (7) | Mg2—O53 | 2.193 (7) |
| Cs1—O52$^{v}$ | 3.689 (7) | Mg3—O33$^{v}$ | 2.012 (8) |
| Cs1—O10W | 3.718 (7) | Mg3—O23 | 2.032 (7) |
| Cs1—O43$^{vi}$ | 3.767 (8) | Mg3—O4W | 2.063 (7) |
| Cs1—O11$^{i}$ | 3.837 (7) | Mg3—O3W | 2.093 (7) |
| Cs1—O12$^{i}$ | 3.862 (7) | Mg3—O12 | 2.116 (8) |
| Cs1—O13$^{i}$ | 3.920 (7) | Mg3—O13 | 2.137 (7) |
| Cs1—O22 | 3.943 (7) | Mg4—O11 | 2.011 (7) |
| Cs1—O21 | 4.013 (7) | Mg4—O21$^{v}$ | 2.015 (7) |
| Cs1—O23 | 4.034 (7) | Mg4—O6W | 2.082 (7) |
| Cs1—O8W | 4.062 (8) | Mg4—O5W | 2.101 (7) |
| Cs2—O42$^{vii}$ | 3.065 (10) | Mg4—O33$^{x}$ | 2.115 (8) |
| Cs2—O42$^{viii}$ | 3.099 (9) | Mg4—O32$^{x}$ | 2.139 (7) |
| Cs2—O32$^{vii}$ | 3.171 (7) | C1—O11 | 1.272 (11) |
| Cs2—O22 | 3.191 (7) | C1—O12 | 1.289 (11) |
| Cs2—O53$^{viii}$ | 3.195 (7) | C1—O13 | 1.305 (11) |
| Cs2—O11$^{ix}$ | 3.261 (7) | C2—O23 | 1.272 (11) |
| Cs2—O53$^{vii}$ | 3.312 (7) | C2—O21 | 1.286 (11) |
| Cs2—O31 | 3.470 (7) | C2—O22 | 1.302 (11) |
| Cs2—O2W | 3.537 (8) | C3—O31 | 1.283 (11) |
| Cs2—O6W$^{ix}$ | 3.590 (8) | C3—O32 | 1.292 (11) |
| Cs2—O9W | 3.676 (8) | C3—O33 | 1.296 (12) |
| Cs2—O7W$^{viii}$ | 3.877 (9) | C4—O43 | 1.252 (12) |
| Cs2—O9W$^{vii}$ | 4.090 (9) | C4—O42 | 1.267 (12) |
| Mg1—O12$^{ii}$ | 2.017 (7) | C4—O41 | 1.305 (11) |
| Mg1—O31 | 2.045 (8) | C5—O52 | 1.266 (12) |
| Mg1—O1W | 2.050 (8) | C5—O53 | 1.296 (11) |
| Mg1—O2W | 2.068 (7) | C5—O51 | 1.316 (11) |
| | | | |
| O4W$^{i}$—Cs1—O1W | 62.25 (18) | O11$^{ix}$—Cs2—O9W$^{vii}$ | 113.60 (15) |
| O4W$^{i}$—Cs1—O5W$^{i}$ | 115.68 (19) | O53$^{vii}$—Cs2—O9W$^{vii}$ | 46.77 (15) |
| O1W—Cs1—O5W$^{i}$ | 158.76 (19) | O31—Cs2—O9W$^{vii}$ | 62.82 (15) |
| O4W$^{i}$—Cs1—O3W | 159.55 (19) | O2W—Cs2—O9W$^{vii}$ | 91.69 (16) |
| O1W—Cs1—O3W | 112.70 (19) | O6W$^{ix}$—Cs2—O9W$^{vii}$ | 84.43 (16) |
| O5W$^{i}$—Cs1—O3W | 61.06 (18) | O9W—Cs2—O9W$^{vii}$ | 65.87 (19) |

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|---|---|---|---|
| O4W$^{i}$—Cs1—O6W$^{ii}$ | 94.90 (19) | O7W$^{viii}$—Cs2—O9W$^{vii}$ | 177.29 (14) |
| O1W—Cs1—O6W$^{ii}$ | 65.32 (18) | O12$^{ii}$—Mg1—O31 | 104.0 (3) |
| O5W$^{i}$—Cs1—O6W$^{ii}$ | 94.64 (19) | O12$^{ii}$—Mg1—O1W | 88.1 (3) |
| O3W—Cs1—O6W$^{ii}$ | 66.23 (17) | O31—Mg1—O1W | 90.6 (3) |
| O4W$^{i}$—Cs1—O8W$^{iii}$ | 128.97 (18) | O12$^{ii}$—Mg1—O2W | 91.7 (3) |
| O1W—Cs1—O8W$^{iii}$ | 125.86 (18) | O31—Mg1—O2W | 88.6 (3) |
| O5W$^{i}$—Cs1—O8W$^{iii}$ | 73.09 (18) | O1W—Mg1—O2W | 179.1 (3) |
| O3W—Cs1—O8W$^{iii}$ | 70.86 (17) | O12$^{ii}$—Mg1—O21 | 93.7 (3) |
| O6W$^{ii}$—Cs1—O8W$^{iii}$ | 135.78 (18) | O31—Mg1—O21 | 162.0 (3) |
| O4W$^{i}$—Cs1—O2W$^{iv}$ | 65.55 (17) | O1W—Mg1—O21 | 92.9 (3) |
| O1W—Cs1—O2W$^{iv}$ | 95.32 (18) | O2W—Mg1—O21 | 88.0 (3) |
| O5W$^{i}$—Cs1—O2W$^{iv}$ | 66.73 (17) | O12$^{ii}$—Mg1—O22 | 154.6 (3) |
| O3W—Cs1—O2W$^{iv}$ | 96.47 (18) | O31—Mg1—O22 | 101.2 (3) |
| O6W$^{ii}$—Cs1—O2W$^{iv}$ | 58.45 (17) | O1W—Mg1—O22 | 89.3 (3) |
| O8W$^{iii}$—Cs1—O2W$^{iv}$ | 138.81 (18) | O2W—Mg1—O22 | 91.3 (3) |
| O4W$^{i}$—Cs1—O10W$^{iii}$ | 81.63 (18) | O21—Mg1—O22 | 61.3 (3) |
| O1W—Cs1—O10W$^{iii}$ | 112.04 (17) | O41—Mg2—O9W | 91.9 (3) |
| O5W$^{i}$—Cs1—O10W$^{iii}$ | 87.65 (17) | O41—Mg2—O7W | 89.9 (3) |
| O3W—Cs1—O10W$^{iii}$ | 117.33 (17) | O9W—Mg2—O7W | 176.9 (4) |
| O6W$^{ii}$—Cs1—O10W$^{iii}$ | 176.43 (18) | O41—Mg2—O8W | 89.7 (3) |
| O8W$^{iii}$—Cs1—O10W$^{iii}$ | 47.59 (17) | O9W—Mg2—O8W | 88.4 (3) |
| O2W$^{iv}$—Cs1—O10W$^{iii}$ | 120.32 (16) | O7W—Mg2—O8W | 89.1 (3) |
| O4W$^{i}$—Cs1—O52$^{v}$ | 110.53 (17) | O41—Mg2—O51 | 177.6 (3) |
| O1W—Cs1—O52$^{v}$ | 111.04 (17) | O9W—Mg2—O51 | 89.5 (3) |
| O5W$^{i}$—Cs1—O52$^{v}$ | 48.39 (17) | O7W—Mg2—O51 | 88.9 (3) |
| O3W—Cs1—O52$^{v}$ | 50.97 (17) | O8W—Mg2—O51 | 92.3 (3) |
| O6W$^{ii}$—Cs1—O52$^{v}$ | 46.30 (17) | O41—Mg2—O53 | 116.4 (3) |
| O8W$^{iii}$—Cs1—O52$^{v}$ | 110.27 (17) | O9W—Mg2—O53 | 90.6 (3) |
| O2W$^{iv}$—Cs1—O52$^{v}$ | 45.51 (17) | O7W—Mg2—O53 | 90.9 (3) |
| O10W$^{iii}$—Cs1—O52$^{v}$ | 135.79 (15) | O8W—Mg2—O53 | 153.9 (3) |
| O4W$^{i}$—Cs1—O10W | 112.73 (17) | O51—Mg2—O53 | 61.6 (3) |
| O1W—Cs1—O10W | 79.33 (17) | O33$^{v}$—Mg3—O23 | 105.2 (3) |
| O5W$^{i}$—Cs1—O10W | 118.15 (17) | O33$^{v}$—Mg3—O4W | 90.5 (3) |
| O3W—Cs1—O10W | 84.19 (17) | O23—Mg3—O4W | 90.0 (3) |
| O6W$^{ii}$—Cs1—O10W | 117.17 (16) | O33$^{v}$—Mg3—O3W | 85.6 (3) |
| O8W$^{iii}$—Cs1—O10W | 46.62 (16) | O23—Mg3—O3W | 90.0 (3) |
| O2W$^{iv}$—Cs1—O10W | 174.40 (16) | O4W—Mg3—O3W | 176.0 (3) |
| O10W$^{iii}$—Cs1—O10W | 63.82 (19) | O33$^{v}$—Mg3—O12 | 92.6 (3) |
| O52$^{v}$—Cs1—O10W | 134.94 (15) | O23—Mg3—O12 | 162.2 (3) |
| O4W$^{i}$—Cs1—O43$^{vi}$ | 45.4 (2) | O4W—Mg3—O12 | 89.7 (3) |
| O1W—Cs1—O43$^{vi}$ | 44.59 (18) | O3W—Mg3—O12 | 91.5 (3) |
| O5W$^{i}$—Cs1—O43$^{vi}$ | 117.36 (19) | O33$^{v}$—Mg3—O13 | 154.5 (3) |
| O3W—Cs1—O43$^{vi}$ | 116.1 (2) | O23—Mg3—O13 | 100.3 (3) |
| O6W$^{ii}$—Cs1—O43$^{vi}$ | 49.9 (2) | O4W—Mg3—O13 | 91.2 (3) |
| O8W$^{iii}$—Cs1—O43$^{vi}$ | 169.12 (19) | O3W—Mg3—O13 | 92.8 (3) |
| O2W$^{iv}$—Cs1—O43$^{vi}$ | 50.96 (18) | O12—Mg3—O13 | 61.9 (3) |
| O10W$^{iii}$—Cs1—O43$^{vi}$ | 126.59 (19) | O11—Mg4—O21$^{v}$ | 103.4 (3) |
| O52$^{v}$—Cs1—O43$^{vi}$ | 80.2 (2) | O11—Mg4—O6W | 88.1 (3) |

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|---|---|---|---|
| O10W—Cs1—O43$^{vi}$ | 123.82 (17) | O21$^{v}$—Mg4—O6W | 91.9 (3) |
| O4W$^{i}$—Cs1—O11$^{i}$ | 76.59 (17) | O11—Mg4—O5W | 91.2 (3) |
| O1W—Cs1—O11$^{i}$ | 138.48 (17) | O21$^{v}$—Mg4—O5W | 86.3 (3) |
| O5W$^{i}$—Cs1—O11$^{i}$ | 48.42 (16) | O6W—Mg4—O5W | 177.9 (3) |
| O3W—Cs1—O11$^{i}$ | 107.78 (16) | O11—Mg4—O33$^{x}$ | 160.1 (3) |
| O6W$^{ii}$—Cs1—O11$^{i}$ | 126.97 (16) | O21$^{v}$—Mg4—O33$^{x}$ | 96.2 (3) |
| O8W$^{iii}$—Cs1—O11$^{i}$ | 76.01 (17) | O6W—Mg4—O33$^{x}$ | 88.0 (3) |
| O2W$^{iv}$—Cs1—O11$^{i}$ | 70.93 (16) | O5W—Mg4—O33$^{x}$ | 93.4 (3) |
| O10W$^{iii}$—Cs1—O11$^{i}$ | 53.13 (15) | O11—Mg4—O32$^{x}$ | 98.8 (3) |
| C1$^{i}$—Cs1—O11$^{i}$ | 19.35 (18) | O21$^{v}$—Mg4—O32$^{x}$ | 157.5 (3) |
| O52$^{v}$—Cs1—O11$^{i}$ | 87.38 (15) | O6W—Mg4—O32$^{x}$ | 92.2 (3) |
| O10W—Cs1—O11$^{i}$ | 114.21 (15) | O5W—Mg4—O32$^{x}$ | 89.9 (3) |
| O43$^{vi}$—Cs1—O11$^{i}$ | 108.19 (17) | O33$^{x}$—Mg4—O32$^{x}$ | 61.9 (3) |
| C2—Cs1—O11$^{i}$ | 162.70 (18) | O11—C1—O12 | 123.4 (9) |
| O4W$^{i}$—Cs1—O12$^{i}$ | 48.47 (17) | O11—C1—O13 | 121.6 (8) |
| O1W—Cs1—O12$^{i}$ | 109.07 (17) | O12—C1—O13 | 115.0 (8) |
| O5W$^{i}$—Cs1—O12$^{i}$ | 67.54 (17) | O23—C2—O21 | 123.8 (9) |
| O3W—Cs1—O12$^{i}$ | 126.08 (17) | O23—C2—O22 | 121.4 (8) |
| O6W$^{ii}$—Cs1—O12$^{i}$ | 104.30 (15) | O21—C2—O22 | 114.8 (8) |
| O8W$^{iii}$—Cs1—O12$^{i}$ | 109.18 (16) | O31—C3—O32 | 122.1 (8) |
| O2W$^{iv}$—Cs1—O12$^{i}$ | 46.65 (15) | O31—C3—O33 | 122.7 (9) |
| O10W$^{iii}$—Cs1—O12$^{i}$ | 74.03 (15) | O32—C3—O33 | 115.3 (8) |
| O52$^{v}$—Cs1—O12$^{i}$ | 83.15 (15) | O43—C4—O42 | 119.5 (9) |
| O10W—Cs1—O12$^{i}$ | 136.66 (15) | O43—C4—O41 | 119.5 (9) |
| O43$^{vi}$—Cs1—O12$^{i}$ | 74.18 (17) | O42—C4—O41 | 121.0 (9) |
| C2—Cs1—O12$^{i}$ | 163.24 (17) | O43—C4—Cs2$^{i}$ | 122.3 (7) |
| O11$^{i}$—Cs1—O12$^{i}$ | 34.05 (15) | O52—C5—O53 | 124.4 (8) |
| O4W$^{i}$—Cs1—O13$^{i}$ | 48.80 (16) | O52—C5—O51 | 120.5 (8) |
| O1W—Cs1—O13$^{i}$ | 106.49 (16) | O53—C5—O51 | 115.1 (8) |
| O5W$^{i}$—Cs1—O13$^{i}$ | 82.00 (16) | Mg1—O1W—Cs1 | 121.2 (3) |
| O3W—Cs1—O13$^{i}$ | 140.80 (16) | Mg1—O2W—Cs1$^{xi}$ | 114.8 (3) |
| O6W$^{ii}$—Cs1—O13$^{i}$ | 134.21 (16) | Mg1—O2W—Cs2 | 87.3 (3) |
| O8W$^{iii}$—Cs1—O13$^{i}$ | 87.06 (16) | Cs1$^{xi}$—O2W—Cs2 | 157.8 (2) |
| O2W$^{iv}$—Cs1—O13$^{i}$ | 78.95 (15) | Mg1—O2W—Cs2$^{xii}$ | 141.2 (3) |
| O10W$^{iii}$—Cs1—O13$^{i}$ | 43.39 (15) | Cs1$^{xi}$—O2W—Cs2$^{xii}$ | 103.85 (15) |
| O52$^{v}$—Cs1—O13$^{i}$ | 113.57 (14) | Cs2—O2W—Cs2$^{xii}$ | 53.93 (10) |
| O10W—Cs1—O13$^{i}$ | 104.06 (14) | C3—O31—Mg1 | 129.8 (6) |
| O43$^{vi}$—Cs1—O13$^{i}$ | 91.34 (18) | C3—O31—Cs2 | 130.3 (6) |
| O11$^{i}$—Cs1—O13$^{i}$ | 33.70 (13) | Mg1—O31—Cs2 | 89.5 (2) |
| O12$^{i}$—Cs1—O13$^{i}$ | 32.64 (14) | C3—O31—Cs2$^{vii}$ | 52.0 (5) |
| O4W$^{i}$—Cs1—O22 | 106.13 (16) | Mg1—O31—Cs2$^{vii}$ | 162.3 (3) |
| O1W—Cs1—O22 | 47.85 (16) | Cs2—O31—Cs2$^{vii}$ | 100.45 (15) |
| O5W$^{i}$—Cs1—O22 | 138.01 (16) | C2—O21—Mg4$^{ii}$ | 142.7 (7) |
| O3W—Cs1—O22 | 78.46 (16) | C2—O21—Mg1 | 93.6 (6) |
| O6W$^{ii}$—Cs1—O22 | 77.57 (15) | Mg4$^{ii}$—O21—Mg1 | 122.8 (4) |
| O8W$^{iii}$—Cs1—O22 | 84.08 (16) | C2—O21—Cs1 | 70.7 (5) |
| O2W$^{iv}$—Cs1—O22 | 133.02 (15) | Mg4$^{ii}$—O21—Cs1 | 98.3 (2) |
| O10W$^{iii}$—Cs1—O22 | 102.53 (15) | Mg1—O21—Cs1 | 91.1 (2) |

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| O52$^{v}$—Cs1—O22 | 113.41 (14) | C2—O21—Cs1$^{xi}$ | 131.5 (5) |
| O10W—Cs1—O22 | 41.62 (14) | Mg4$^{ii}$—O21—Cs1$^{xi}$ | 71.6 (2) |
| O43$^{vi}$—Cs1—O22 | 89.08 (16) | Mg1—O21—Cs1$^{xi}$ | 75.9 (2) |
| O11$^{i}$—Cs1—O22 | 155.36 (15) | Cs1—O21—Cs1$^{xi}$ | 154.06 (17) |
| O12$^{i}$—Cs1—O22 | 154.45 (14) | C2—O21—Cs2 | 50.1 (5) |
| O13$^{i}$—Cs1—O22 | 132.37 (15) | Mg4$^{ii}$—O21—Cs2 | 161.5 (3) |
| O4W$^{i}$—Cs1—O21 | 108.32 (16) | Mg1—O21—Cs2 | 52.20 (17) |
| O1W—Cs1—O21 | 47.90 (16) | Cs1—O21—Cs2 | 99.62 (13) |
| O5W$^{i}$—Cs1—O21 | 123.01 (17) | Cs1$^{xi}$—O21—Cs2 | 90.13 (11) |
| O3W—Cs1—O21 | 64.93 (16) | C2—O22—Mg1 | 90.2 (5) |
| O6W$^{ii}$—Cs1—O21 | 46.11 (15) | C2—O22—Cs2 | 136.9 (5) |
| O8W$^{iii}$—Cs1—O21 | 105.33 (16) | Mg1—O22—Cs2 | 95.0 (2) |
| O2W$^{iv}$—Cs1—O21 | 103.78 (15) | C2—O22—Cs1 | 73.7 (5) |
| O10W$^{iii}$—Cs1—O21 | 134.24 (15) | Mg1—O22—Cs1 | 92.1 (2) |
| O52$^{v}$—Cs1—O21 | 83.76 (14) | Cs2—O22—Cs1 | 148.4 (2) |
| O10W—Cs1—O21 | 71.43 (14) | C2—O23—Mg3 | 130.8 (6) |
| O43$^{vi}$—Cs1—O21 | 72.18 (17) | C2—O23—Cs1 | 69.8 (5) |
| O11$^{i}$—Cs1—O21 | 170.94 (14) | Mg3—O23—Cs1 | 95.7 (2) |
| O12$^{i}$—Cs1—O21 | 145.47 (16) | C2—O23—Cs2 | 54.2 (5) |
| O13$^{i}$—Cs1—O21 | 154.19 (14) | Mg3—O23—Cs2 | 163.1 (3) |
| O22—Cs1—O21 | 31.80 (13) | Cs1—O23—Cs2 | 100.81 (14) |
| O4W$^{i}$—Cs1—O23 | 136.71 (16) | Mg3—O3W—Cs1 | 124.2 (3) |
| O1W—Cs1—O23 | 74.65 (16) | Mg3—O4W—Cs1$^{viii}$ | 119.6 (3) |
| O5W$^{i}$—Cs1—O23 | 105.83 (16) | Mg4—O5W—Cs1$^{viii}$ | 118.8 (3) |
| O3W—Cs1—O23 | 45.84 (16) | Mg4—O5W—Cs2$^{ix}$ | 42.37 (17) |
| O6W$^{ii}$—Cs1—O23 | 69.21 (16) | Cs1$^{viii}$—O5W—Cs2$^{ix}$ | 98.86 (18) |
| O8W$^{iii}$—Cs1—O23 | 73.66 (16) | Mg4—O6W—Cs1$^{v}$ | 120.2 (3) |
| O2W$^{iv}$—Cs1—O23 | 125.51 (15) | Mg4—O6W—Cs2$^{ix}$ | 84.0 (2) |
| O10W$^{iii}$—Cs1—O23 | 112.81 (15) | Cs1$^{v}$—O6W—Cs2$^{ix}$ | 155.4 (2) |
| O52$^{v}$—Cs1—O23 | 87.67 (14) | Mg4—O6W—Cs2$^{xiii}$ | 135.1 (3) |
| O10W—Cs1—O23 | 51.65 (15) | Cs1$^{v}$—O6W—Cs2$^{xiii}$ | 104.75 (15) |
| O43$^{vi}$—Cs1—O23 | 104.71 (17) | Cs2$^{ix}$—O6W—Cs2$^{xiii}$ | 51.31 (9) |
| O11$^{i}$—Cs1—O23 | 145.33 (16) | C1—O11—Mg4 | 131.9 (6) |
| O12$^{i}$—Cs1—O23 | 170.81 (14) | C1—O11—Cs2$^{ix}$ | 126.5 (6) |
| O13$^{i}$—Cs1—O23 | 155.54 (14) | Mg4—O11—Cs2$^{ix}$ | 94.3 (2) |
| O22—Cs1—O23 | 32.67 (13) | C1—O11—Cs1$^{viii}$ | 72.6 (5) |
| O21—Cs1—O23 | 32.57 (14) | Mg4—O11—Cs1$^{viii}$ | 98.2 (3) |
| O4W$^{i}$—Cs1—O8W | 72.94 (17) | Cs2$^{ix}$—O11—Cs1$^{viii}$ | 134.2 (2) |
| O1W—Cs1—O8W | 71.44 (16) | C1—O12—Mg1$^{v}$ | 144.5 (7) |
| O5W$^{i}$—Cs1—O8W | 129.40 (17) | C1—O12—Mg3 | 92.2 (6) |
| O3W—Cs1—O8W | 125.80 (17) | Mg1$^{v}$—O12—Mg3 | 123.3 (4) |
| O6W$^{ii}$—Cs1—O8W | 135.59 (17) | C1—O12—Cs1$^{viii}$ | 71.5 (5) |
| O8W$^{iii}$—Cs1—O8W | 66.15 (18) | Mg1$^{v}$—O12—Cs1$^{viii}$ | 103.2 (3) |
| O2W$^{iv}$—Cs1—O8W | 137.70 (16) | Mg3—O12—Cs1$^{viii}$ | 93.7 (2) |
| O10W$^{iii}$—Cs1—O8W | 42.56 (15) | C1—O12—Cs2$^{ix}$ | 26.0 (5) |
| O52$^{v}$—Cs1—O8W | 176.33 (16) | Mg1$^{v}$—O12—Cs2$^{ix}$ | 123.9 (3) |
| O10W—Cs1—O8W | 42.13 (15) | Mg3—O12—Cs2$^{ix}$ | 109.5 (2) |
| O43$^{vi}$—Cs1—O8W | 103.32 (18) | Cs1$^{viii}$—O12—Cs2$^{ix}$ | 90.21 (13) |

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| O11$^{i}$—Cs1—O8W | 92.38 (15) | C1—O13—Mg3 | 90.8 (5) |
| O12$^{i}$—Cs1—O8W | 98.68 (15) | C1—O13—Cs1$^{viii}$ | 69.1 (5) |
| O13$^{i}$—Cs1—O8W | 67.61 (14) | Mg3—O13—Cs1$^{viii}$ | 91.7 (2) |
| O22—Cs1—O8W | 66.01 (14) | C1—O13—Cs2$^{ix}$ | 72.2 (5) |
| O21—Cs1—O8W | 96.34 (14) | Mg3—O13—Cs2$^{ix}$ | 150.0 (3) |
| O23—Cs1—O8W | 90.46 (14) | Cs1$^{viii}$—O13—Cs2$^{ix}$ | 104.35 (14) |
| O42$^{vii}$—Cs2—O42$^{viii}$ | 96.5 (2) | Mg2—O7W—Cs2$^{i}$ | 87.6 (3) |
| O42$^{vii}$—Cs2—O32$^{vii}$ | 115.7 (2) | Mg2—O8W—Cs1$^{iii}$ | 131.9 (3) |
| O42$^{viii}$—Cs2—O32$^{vii}$ | 106.4 (2) | Mg2—O8W—Cs1 | 114.3 (3) |
| O42$^{vii}$—Cs2—O22 | 101.4 (2) | Cs1$^{iii}$—O8W—Cs1 | 113.85 (18) |
| O42$^{viii}$—Cs2—O22 | 124.1 (2) | C5—O51—Mg2 | 93.2 (5) |
| O32$^{vii}$—Cs2—O22 | 112.10 (17) | C5—O51—Cs1 | 156.7 (5) |
| O42$^{vii}$—Cs2—O53$^{viii}$ | 69.5 (2) | Mg2—O51—Cs1 | 110.1 (2) |
| O42$^{viii}$—Cs2—O53$^{viii}$ | 62.2 (2) | C5—O51—Cs2$^{i}$ | 44.7 (4) |
| O32$^{vii}$—Cs2—O53$^{viii}$ | 168.44 (17) | Mg2—O51—Cs2$^{i}$ | 57.54 (17) |
| O22—Cs2—O53$^{viii}$ | 75.52 (18) | Cs1—O51—Cs2$^{i}$ | 151.86 (15) |
| O42$^{vii}$—Cs2—O11$^{ix}$ | 168.8 (2) | C5—O51—Cs2$^{vii}$ | 41.9 (5) |
| O42$^{viii}$—Cs2—O11$^{ix}$ | 77.0 (2) | Mg2—O51—Cs2$^{vii}$ | 60.22 (17) |
| O32$^{vii}$—Cs2—O11$^{ix}$ | 58.68 (17) | Cs1—O51—Cs2$^{vii}$ | 153.67 (15) |
| O22—Cs2—O11$^{ix}$ | 89.88 (17) | Cs2$^{i}$—O51—Cs2$^{vii}$ | 47.04 (6) |
| O53$^{viii}$—Cs2—O11$^{ix}$ | 114.14 (17) | C5—O52—Cs1$^{ii}$ | 163.0 (6) |
| O42$^{vii}$—Cs2—O53$^{vii}$ | 61.2 (2) | C5—O52—Cs2$^{i}$ | 56.8 (5) |
| O42$^{viii}$—Cs2—O53$^{vii}$ | 67.60 (19) | Cs1$^{ii}$—O52—Cs2$^{i}$ | 108.13 (17) |
| O32$^{vii}$—Cs2—O53$^{vii}$ | 73.77 (17) | C5—O52—Cs2$^{vii}$ | 60.2 (5) |
| O22—Cs2—O53$^{vii}$ | 161.46 (17) | Cs1$^{ii}$—O52—Cs2$^{vii}$ | 104.91 (17) |
| O53$^{viii}$—Cs2—O53$^{vii}$ | 101.82 (15) | Cs2$^{i}$—O52—Cs2$^{vii}$ | 50.61 (7) |
| O11$^{ix}$—Cs2—O53$^{vii}$ | 107.61 (17) | C4—O41—Mg2 | 124.5 (6) |
| O42$^{vii}$—Cs2—O31 | 67.9 (2) | C4—O41—Cs1$^{iii}$ | 138.8 (5) |
| O42$^{viii}$—Cs2—O31 | 163.9 (2) | Mg2—O41—Cs1$^{iii}$ | 96.2 (2) |
| O32$^{vii}$—Cs2—O31 | 85.09 (17) | C4—O41—Cs2$^{i}$ | 60.1 (5) |
| O22—Cs2—O31 | 58.40 (16) | Mg2—O41—Cs2$^{i}$ | 73.5 (2) |
| O53$^{viii}$—Cs2—O31 | 106.45 (17) | Cs1$^{iii}$—O41—Cs2$^{i}$ | 152.17 (18) |
| O11$^{ix}$—Cs2—O31 | 119.04 (16) | C4—O41—Cs2$^{vii}$ | 56.7 (5) |
| O53$^{vii}$—Cs2—O31 | 106.15 (16) | Mg2—O41—Cs2$^{vii}$ | 71.9 (2) |
| O42$^{vii}$—Cs2—O2W | 48.3 (2) | Cs1$^{iii}$—O41—Cs2$^{vii}$ | 149.07 (17) |
| O42$^{viii}$—Cs2—O2W | 118.2 (2) | Cs2$^{i}$—O41—Cs2$^{vii}$ | 53.02 (8) |
| O32$^{vii}$—Cs2—O2W | 133.11 (17) | C4—O42—Cs2$^{vii}$ | 145.8 (8) |
| O22—Cs2—O2W | 53.27 (17) | C4—O42—Cs2$^{i}$ | 123.5 (7) |
| O53$^{viii}$—Cs2—O2W | 58.31 (17) | Cs2$^{vii}$—O42—Cs2$^{i}$ | 83.5 (2) |
| O11$^{ix}$—Cs2—O2W | 142.97 (17) | C4—O42—Cs1$^{xiv}$ | 75.4 (6) |
| O53$^{vii}$—Cs2—O2W | 109.42 (17) | Cs2$^{vii}$—O42—Cs1$^{xiv}$ | 116.4 (2) |
| O31—Cs2—O2W | 48.41 (17) | Cs2$^{i}$—O42—Cs1$^{xiv}$ | 112.2 (3) |
| O42$^{vii}$—Cs2—O6W$^{ix}$ | 120.0 (2) | C4—O43—Cs1$^{xiv}$ | 140.8 (7) |
| O42$^{viii}$—Cs2—O6W$^{ix}$ | 53.5 (2) | C4—O43—Cs2$^{i}$ | 44.8 (6) |
| O32$^{vii}$—Cs2—O6W$^{ix}$ | 53.01 (17) | Cs1$^{xiv}$—O43—Cs2$^{i}$ | 105.1 (2) |
| O22—Cs2—O6W$^{ix}$ | 138.61 (17) | C4—O43—Cs2$^{vii}$ | 41.1 (5) |
| O53$^{viii}$—Cs2—O6W$^{ix}$ | 115.48 (17) | Cs1$^{xiv}$—O43—Cs2$^{vii}$ | 102.23 (19) |
| O11$^{ix}$—Cs2—O6W$^{ix}$ | 48.78 (17) | Cs2$^{i}$—O43—Cs2$^{vii}$ | 49.58 (9) |

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| O53$^{vii}$—Cs2—O6W$^{ix}$ | 59.37 (17) | C3—O32—Mg4$^{xv}$ | 91.0 (6) |
| O31—Cs2—O6W$^{ix}$ | 137.44 (17) | C3—O32—Cs2$^{vii}$ | 141.6 (5) |
| O2W—Cs2—O6W$^{ix}$ | 167.16 (17) | Mg4$^{xv}$—O32—Cs2$^{vii}$ | 94.4 (2) |
| O42$^{vii}$—Cs2—O9W | 108.9 (2) | C3—O32—Cs2 | 72.2 (5) |
| O42$^{viii}$—Cs2—O9W | 148.0 (2) | Mg4$^{xv}$—O32—Cs2 | 152.9 (3) |
| O32$^{vii}$—Cs2—O9W | 45.22 (16) | Cs2$^{vii}$—O32—Cs2 | 112.07 (17) |
| O22—Cs2—O9W | 70.37 (17) | C3—O33—Mg3$^{ii}$ | 146.5 (7) |
| O53$^{viii}$—Cs2—O9W | 144.84 (16) | C3—O33—Mg4$^{xv}$ | 91.9 (6) |
| O11$^{ix}$—Cs2—O9W | 74.59 (17) | Mg3$^{ii}$—O33—Mg4$^{xv}$ | 120.1 (3) |
| O53$^{vii}$—Cs2—O9W | 107.74 (17) | C3—O33—Cs1$^{ii}$ | 129.4 (5) |
| O31—Cs2—O9W | 47.24 (16) | Mg3$^{ii}$—O33—Cs1$^{ii}$ | 73.4 (2) |
| O2W—Cs2—O9W | 93.49 (15) | Mg4$^{xv}$—O33—Cs1$^{ii}$ | 74.3 (2) |
| O6W$^{ix}$—Cs2—O9W | 96.06 (15) | C3—O33—Cs2$^{vii}$ | 50.4 (5) |
| O42$^{vii}$—Cs2—O7W$^{viii}$ | 118.1 (2) | Mg3$^{ii}$—O33—Cs2$^{vii}$ | 160.5 (3) |
| O42$^{viii}$—Cs2—O7W$^{viii}$ | 67.99 (19) | Mg4$^{xv}$—O33—Cs2$^{vii}$ | 50.09 (17) |
| O32$^{vii}$—Cs2—O7W$^{viii}$ | 126.18 (17) | Cs1$^{ii}$—O33—Cs2$^{vii}$ | 87.18 (11) |
| O22—Cs2—O7W$^{viii}$ | 56.80 (16) | Mg2—O9W—Cs2 | 156.6 (4) |
| O53$^{viii}$—Cs2—O7W$^{viii}$ | 49.80 (17) | Mg2—O9W—Cs2$^{vii}$ | 89.1 (3) |
| O11$^{ix}$—Cs2—O7W$^{viii}$ | 68.33 (16) | Cs2—O9W—Cs2$^{vii}$ | 114.13 (19) |
| O53$^{vii}$—Cs2—O7W$^{viii}$ | 135.04 (16) | C5—O53—Mg2 | 90.1 (5) |
| O31—Cs2—O7W$^{viii}$ | 114.68 (15) | C5—O53—Cs2$^{i}$ | 136.9 (5) |
| O2W—Cs2—O7W$^{viii}$ | 85.72 (16) | Mg2—O53—Cs2$^{i}$ | 105.0 (3) |
| O6W$^{ix}$—Cs2—O7W$^{viii}$ | 98.27 (16) | C5—O53—Cs2$^{vii}$ | 134.6 (5) |
| O9W—Cs2—O7W$^{viii}$ | 113.43 (18) | Mg2—O53—Cs2$^{vii}$ | 109.7 (3) |
| O42$^{vii}$—Cs2—O9W$^{vii}$ | 60.4 (2) | Cs2$^{i}$—O53—Cs2$^{vii}$ | 78.18 (15) |
| O42$^{viii}$—Cs2—O9W$^{vii}$ | 114.08 (19) | Cs1$^{iii}$—O10W—Cs1 | 116.18 (19) |
| O32$^{vii}$—Cs2—O9W$^{vii}$ | 55.41 (16) | Cs1$^{iii}$—O10W—Cs2 | 112.02 (16) |
| O22—Cs2—O9W$^{vii}$ | 120.86 (16) | Cs1—O10W—Cs2 | 118.44 (16) |
| O53$^{viii}$—Cs2—O9W$^{vii}$ | 129.17 (16) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O51 | 0.82 (5) | 1.85 (6) | 2.658 (10) | 172 (12) |
| O1*W*—H1*B*···O43$^{vi}$ | 0.83 (5) | 1.89 (6) | 2.686 (11) | 162 (12) |
| O2*W*—H2*A*···O52$^{viii}$ | 0.80 (5) | 2.01 (6) | 2.783 (11) | 160 (12) |
| O2*W*—H2*B*···O42$^{vii}$ | 0.81 (5) | 1.93 (6) | 2.734 (12) | 170 (13) |
| O3*W*—H3*A*···O52$^{v}$ | 0.82 (5) | 2.23 (6) | 2.993 (12) | 157 (11) |
| O3*W*—H3*B*···O41$^{iii}$ | 0.82 (5) | 1.92 (6) | 2.737 (11) | 175 (12) |
| O4*W*—H4*A*···O43$^{xvi}$ | 0.82 (5) | 1.93 (6) | 2.724 (11) | 162 (13) |
| O4*W*—H4*B*···O51$^{viii}$ | 0.82 (5) | 1.84 (6) | 2.661 (9) | 174 (14) |
| O5*W*—H5*A*···O52$^{xvii}$ | 0.82 (5) | 2.04 (6) | 2.853 (10) | 169 (13) |
| O5*W*—H5*B*···O41$^{ix}$ | 0.80 (5) | 2.05 (6) | 2.831 (10) | 164 (13) |
| O6*W*—H6*A*···O43$^{iii}$ | 0.84 (5) | 2.21 (6) | 3.021 (13) | 165 (13) |
| O6*W*—H6*B*···O52$^{x}$ | 0.81 (5) | 1.98 (6) | 2.783 (10) | 174 (13) |

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| O7*W*—H7*B*···O23$^{i}$ | 0.83 (5) | 2.07 (7) | 2.843 (10) | 155 (13) |
| O8*W*—H8*A*···O10*W* | 0.82 (5) | 2.02 (6) | 2.815 (10) | 165 (13) |
| O8*W*—H8*B*···O10*W*$^{iii}$ | 0.82 (5) | 2.02 (7) | 2.815 (10) | 164 (15) |
| O9*W*—H9*A*···O31 | 0.82 (5) | 2.09 (7) | 2.869 (10) | 161 (13) |
| O9*W*—H9*B*···O32$^{vii}$ | 0.82 (5) | 1.87 (7) | 2.673 (10) | 170 (13) |
| O10*W*—H10*A*···O13$^{ix}$ | 0.81 (5) | 2.01 (6) | 2.798 (9) | 162 (13) |
| O10*W*—H10*B*···O22 | 0.90 (13) | 1.84 (13) | 2.730 (10) | 169 (12) |

Symmetry codes: (i) *x*−1, *y*, *z*; (iii) −*x*+2, −*y*+1, −*z*; (v) *x*+1/2, −*y*+3/2, *z*−1/2; (vi) −*x*+3/2, *y*+1/2, −*z*+1/2; (vii) −*x*+2, −*y*+1, −*z*+1; (viii) *x*+1, *y*, *z*; (ix) −*x*+3, −*y*+1, −*z*; (x) *x*+1, *y*, *z*−1; (xvi) −*x*+5/2, *y*+1/2, −*z*+1/2; (xvii) *x*+3/2, −*y*+3/2, *z*−1/2.