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Redetermination of $MgCrO_4 \cdot 5H_2O$

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ(Mg–O) = 0.001 Å; R factor = 0.031; wR factor = 0.069; data-to-parameter ratio = 28.1.

The CCD-data based redetermination of the crystal structure of the title compound, magnesium chromate(VI) pentahydrate, confirms in principle the previous study based on precession film data [Bertrand *et al.* (1971). *C. R. Hebd. Seances Acad. Sci. Serie C*, **272**, 530–533.], but with all atoms refined with anisotropic displacement parameters and with all H atoms localized. This allowed an unambiguous assignment of the hydrogen-bonding pattern. $MgCrO_4 \cdot 5H_2O$ adopts the $MgSO_4 \cdot 5H_2O$ structure type. It contains two Mg^{2+} sites on special positions with site symmetry $\overline{1}$, one tetrahedral CrO_4 group and five water molecules. Four of them coordinate to the Mg^{2+} cation, and one is an uncoordinating lattice water molecule. The octahedral environment of the Mg^{2+} cation is completed by two axial O atoms of CrO_4 tetrahedra. This arrangement leads to the formation of chains parallel to [011]. Adjacent chains are linked through O—H⋯O hydrogen bonds (one of them bifurcated), involving both the coordinating and lattice water molecules, into a three-dimensional network.

Related literature

For the original structure determination of the title compound, see: Bertrand *et al.* (1971). For hydrogen-bonding pattern in the structures of $MXO_4 \cdot 5H_2O$ compounds (M = Mg, Cu; X = S, Cr), see: Baur & Rolin (1972). For Cr—O bond length distributions in chromates(VI), see: Pressprich *et al.* (1988). For bond lengths and angles in the related structure of $MgCrO_4 \cdot 11H_2O$, see: Fortes *et al.* (2013). For standardization of structure data, see: Gelato & Parthé (1987).

Experimental

Crystal data

$MgCrO_4 \cdot 5H_2O$
M_r = 230.39
Triclinic, $P\overline{1}$
a = 6.1467 (3) Å
b = 6.3742 (4) Å
c = 10.7048 (6) Å
α = 75.919 (4)°
β = 81.603 (3)°
γ = 71.134 (3)°
V = 383.92 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 296 K
0.10 × 0.08 × 0.01 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
T_{min} = 0.594, T_{max} = 0.748
10569 measured reflections
4019 independent reflections
3340 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.069
S = 1.02
4019 reflections
143 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mg1—*O*W3	2.0505 (9)	Mg2—O1	2.1099 (9)
Mg1—*O*W2^{i}	2.0656 (9)	Cr1—O3^{iii}	1.6357 (9)
Mg1—O4^{ii}	2.0952 (9)	Cr1—O4^{iii}	1.6554 (9)
Mg2—*O*W5	2.0265 (10)	Cr1—O1	1.6568 (9)
Mg2—*O*W1	2.0467 (8)	Cr1—O2	1.6579 (8)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y, -z$; (iii) $-x+1, -y, -z+1$.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
*O*W1—HW1*A*⋯O2^{iv}	0.81 (2)	1.96 (2)	2.7702 (13)	174 (2)
*O*W1—HW1*B*⋯O3	0.80 (2)	1.97 (2)	2.7598 (13)	169 (2)
*O*W2—HW2*A*⋯O1^{v}	0.79 (2)	2.19 (2)	2.9014 (13)	150 (2)
*O*W2—HW2*A*⋯*O*W1	0.79 (2)	2.52 (2)	3.1008 (14)	132 (2)
*O*W2—HW2*B*⋯*O*W4	0.80 (2)	2.02 (2)	2.8173 (12)	171 (2)
*O*W3—HW3*A*⋯O2^{iii}	0.82 (2)	1.97 (2)	2.7891 (13)	170 (2)
*O*W3—HW3*B*⋯*O*W4^{vi}	0.81 (2)	1.99 (2)	2.7906 (14)	172 (2)
*O*W4—HW4*B*⋯O1^{iv}	0.83 (2)	2.32 (2)	3.1205 (14)	163 (2)
*O*W4—HW4*A*⋯O4	0.80 (2)	2.06 (2)	2.8535 (14)	170 (2)
*O*W5—HW5*B*⋯O2^{iii}	0.80 (2)	1.93 (2)	2.7262 (13)	173 (2)
*O*W5—HW5*A*⋯O3^{vii}	0.79 (2)	1.96 (2)	2.7409 (12)	174 (2)

Symmetry codes: (iii) $-x+1, -y, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $-x, -y+1, -z+1$; (vi) $-x+1, -y+1, -z$; (vii) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS for Windows* (Dowty, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2229).

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supporting information

Acta Cryst. (2013). E**69**, i48–i49 [doi:10.1107/S1600536813018588]

Redetermination of $MgCrO_4{\cdot}5H_2O$

Matthias Weil

S1. Comment

In the current study $MgCrO_4.5H_2O$ was prepared as a precursor for preparation of anhydrous $MgCrO_4$. The structure of $MgCrO_4.5H_2O$ has already been determined from film data (precession camera) by Bertrand *et al.* (1971), revealing isotypism with $MgSO_4.5H_2O$, $CuSO_4.5H_2O$ and other $MXO_4.5H_2O$ structures (M = Mg or a divalent first row transition metal; X = S, Se, Cr). The original refinement of $MgCrO_4.5H_2O$ did not report any standard uncertainties on lattice parameters and atomic coordinates. It converged with a R value of 0.095, with the displacement parameters of all atoms refined isotropically and with no H-atoms localized. The geometric parameters (bond lengths, bond angles, hydrogen bonding pattern) of the crystal structures of the three isotypic salts $MgSO_4.5H_2O$, $CuSO_4.5H_2O$ and $MgCrO_4.5H_2O$ were compared by Baur & Rolin (1972), using the original $MgCrO_4.5H_2O$ data by Bertrand *et al.* (1971) under assumption of geometrically calculated hydrogen positions for the water molecules. Therefore a redetermination of the $MgCrO_4.5H_2O$ structure based on modern CCD-based intensity data seemed appropriate. The current study revealed all non-H atoms with anisotropic displacement parameters and with all H atoms localized, allowing an unambiguous assignment of the hydrogen-bonding pattern, together with more accurate bond lengths.

In a crystal chemical sense, $MgCrO_4.5H_2O$ is better represented by the formula $[Mg(H_2O)_4]CrO_4.H_2O$. Its structure contains two Mg^{2+} cations, each located on an inversion centre, one CrO_4^{2-} anion and five water molecules. The Mg^{2+} cations are octahedrally surrounded by four water molecules in equatorial sites and by O atoms of CrO_4 tetrahedra in axial sites. The bridging character of the CrO_4 tetrahedra leads to the formation of chains extending parallel to [011] (Fig. 1). The two $[MgO_2(H_2O)_4]$ octahedra are slightly distorted (Table 1), with average Mg—O bond lengths of 2.070 for Mg1 and 2.061 for Mg2. The CrO_4 tetrahedron is likewise slightly distorted and has a mean Cr—O bond lengths of 1.658 Å, typical for chromates(VI) with isolated CrO_4 anions (1.646 (25) Å; Pressprich *et al.* 1988). The values of bond lengths and angles of the MgO_6 octahedron and the CrO_4 tetrahedron in the title structure are in the same range as in the related undecahydrate $MgCrO_4.11H_2O$ (Fortes *et al.*, 2013).

Neighbouring chains are linked through O—H···O hydrogen bonds, involving the coordinating water molecules as well as the lattice water molecule (OW4). The strength of most of the hydrogen bonds can be considered as medium-strong, with O···O separations between 2.7262 (13) and 2.7906 (14) Å. Somewhat weaker hydrogen bonds are also present, with O···O separations > 2.80 Å, and the longest O···O separation being 3.1205 (14) Å. It is interesting to note that HW2A protons are involved in a bifurcated hydrogen bond (Table 1).

The experimentally determined hydrogen bonding scheme of $[Mg(H_2O)_4]CrO_4.H_2O$ is in good agreement with the one calculated and discussed previously by Baur & Rolin (1972).

S2. Experimental

Half-concentrated chromic acid, prepared by dissolving CrO_3 in water, was neutralized with $MgCO_3$. This solution was evaporated until dryness and the resulting solid recrystallized in water. Yellow crystals with a platy habit and edge length up to 1 mm were obtained.

S3. Refinement

In the original study (Bertrand *et al.*, 1971) a non-reduced setting in space group $P\bar{1}$ has been used, with lattice parameters $a = 6.384$, $b = 10.702$, $c = 6.115$ Å, $\alpha = 81.55$, $\beta = 108.75$, $\gamma = 104.333$ °. For the present study the unit-cell parameters were transformed into the reduced cell using the transformation matrix ($0\ 0\ \bar{1}$, $1\ 0\ 0$, $0\ \bar{1}\ 0$). For refinement, the atomic coordinates of the original determination were used as starting parameters. They were finally standardized with *STRUCTURE TIDY* (Gelato & Parthé, 1987). All H atoms were discernible from difference maps. Their coordinates were refined with distance restraints of d(O—H) = 0.82 (5) Å, with individual U_{iso} parameters for each H atom. One reflection (0 0 1) was affected by the beam stop and was omitted from the refinement.

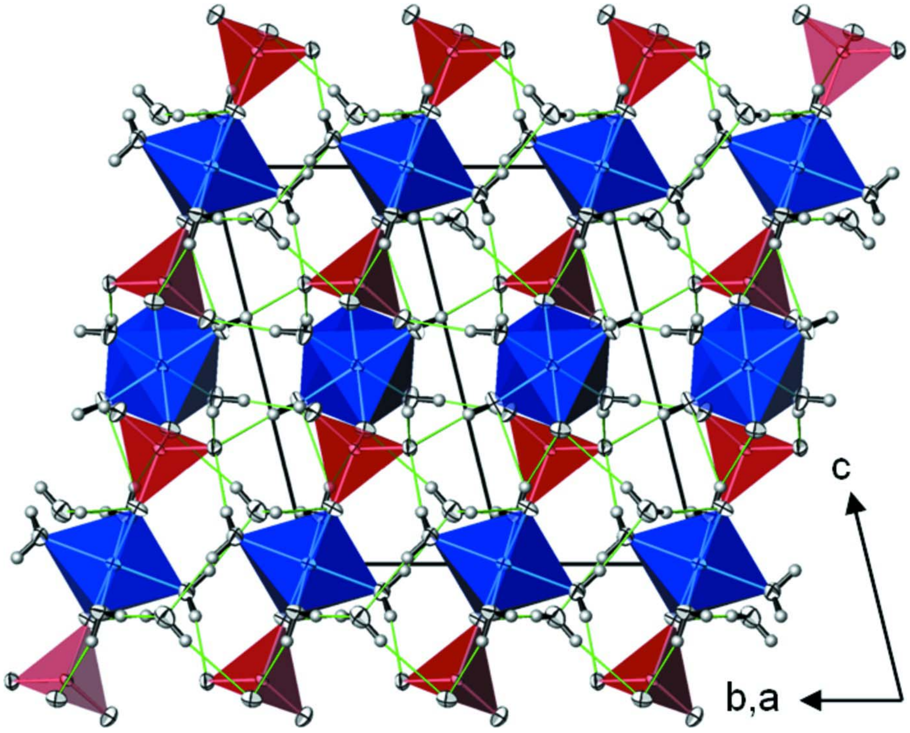

Figure 1

Projection of the structure of $MgCrO_4.5H_2O$ along [$\bar{1}$10]. MgO_6 octahedra are blue, CrO_4 tetrahedra are red, O atoms are colourless. For non-H atoms, displacement parameters are given at the 90% probability level. O—H···O hydrogen bonds are indicated by green lines.

Magnesium chromate(VI) pentahydrate

Crystal data

$MgCrO_4\cdot 5H_2O$
$M_r = 230.39$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a = 6.1467$ (3) Å
$b = 6.3742$ (4) Å
$c = 10.7048$ (6) Å
$\alpha = 75.919$ (4)°
$\beta = 81.603$ (3)°
$\gamma = 71.134$ (3)°
$V = 383.92$ (4) Å^3
$Z = 2$
$F(000) = 236$
$D_x = 1.993$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3623 reflections
$\theta = 3.5$–39.7°
$\mu = 1.59$ mm^{-1}

T = 296 K	0.10 × 0.08 × 0.01 mm
Plate, yellow	

Data collection

Bruker APEXII CCD diffractometer	10569 measured reflections
Radiation source: fine-focus sealed tube	4019 independent reflections
Graphite monochromator	3340 reflections with $I > 2\sigma(I)$
ω– and φ–scans	$R_{\rm int}$ = 0.031
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)	$\theta_{\rm max}$ = 37.5°, $\theta_{\rm min}$ = 3.5°
$T_{\rm min}$ = 0.594, $T_{\rm max}$ = 0.748	$h = -10 \rightarrow 10$
	$k = -10 \rightarrow 10$
	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: isomorphous structure methods
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.069	$w = 1/[\sigma^2(F_o^2) + (0.0263P)^2 + 0.1663P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{\rm max} < 0.001$
4019 reflections	$\Delta\rho_{\rm max}$ = 1.17 e Å^{-3}
143 parameters	$\Delta\rho_{\rm min}$ = −0.72 e Å^{-3}
10 restraints	

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	$U_{\rm iso}$*/$U_{\rm eq}$
Mg1	0.0000	0.0000	0.0000	0.00672 (11)
Mg2	0.0000	0.5000	0.5000	0.00587 (10)
Cr1	0.35414 (3)	0.02843 (3)	0.709355 (18)	0.00508 (4)
O1	0.17472 (14)	0.28496 (15)	0.66131 (9)	0.00919 (15)
O2	0.61762 (13)	0.04795 (15)	0.70554 (9)	0.00825 (15)
O3	0.64389 (14)	0.14163 (16)	0.38351 (9)	0.00978 (16)
O4	0.72867 (14)	0.07678 (16)	0.14081 (9)	0.00919 (15)
OW1	0.30276 (14)	0.54057 (17)	0.40541 (10)	0.01038 (16)
HW1A	0.331 (4)	0.660 (3)	0.378 (2)	0.029 (6)*
HW1B	0.413 (3)	0.435 (3)	0.397 (2)	0.032 (6)*
OW2	0.16925 (14)	0.70426 (17)	0.12175 (9)	0.01025 (16)
HW2A	0.118 (4)	0.675 (4)	0.1938 (16)	0.027 (6)*
HW2B	0.305 (3)	0.669 (4)	0.130 (2)	0.026 (5)*
OW3	0.16025 (16)	0.18082 (17)	0.06898 (10)	0.01161 (17)

HW3A	0.240 (3)	0.115 (3)	0.1307 (17)	0.024 (5)*
HW3B	0.221 (4)	0.263 (4)	0.016 (2)	0.038 (7)*
OW4	0.65171 (16)	0.54576 (17)	0.13300 (10)	0.01237 (17)
HW4A	0.689 (4)	0.414 (3)	0.130 (2)	0.036 (7)*
HW4B	0.714 (4)	0.560 (4)	0.1924 (18)	0.030 (6)*
OW5	0.03331 (14)	0.23596 (17)	0.41734 (10)	0.01081 (16)
HW5A	−0.076 (3)	0.201 (4)	0.413 (2)	0.023 (5)*
HW5B	0.143 (3)	0.156 (3)	0.384 (2)	0.029 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0071 (2)	0.0069 (3)	0.0059 (3)	−0.00218 (18)	−0.00012 (17)	−0.0010 (2)
Mg2	0.0065 (2)	0.0051 (3)	0.0058 (3)	−0.00195 (18)	−0.00013 (17)	−0.0007 (2)
Cr1	0.00505 (6)	0.00478 (8)	0.00506 (8)	−0.00132 (5)	−0.00015 (5)	−0.00072 (6)
O1	0.0101 (3)	0.0067 (4)	0.0085 (4)	−0.0003 (3)	−0.0012 (3)	−0.0001 (3)
O2	0.0072 (3)	0.0092 (4)	0.0093 (4)	−0.0038 (3)	−0.0002 (3)	−0.0021 (3)
O3	0.0102 (3)	0.0092 (4)	0.0113 (4)	−0.0021 (3)	−0.0015 (3)	−0.0054 (3)
O4	0.0100 (3)	0.0084 (4)	0.0071 (4)	−0.0023 (3)	0.0017 (3)	0.0004 (3)
OW1	0.0078 (3)	0.0071 (4)	0.0147 (4)	−0.0024 (3)	0.0022 (3)	−0.0010 (3)
OW2	0.0094 (3)	0.0116 (4)	0.0074 (4)	−0.0020 (3)	−0.0003 (3)	0.0006 (3)
OW3	0.0143 (4)	0.0125 (4)	0.0099 (4)	−0.0075 (3)	−0.0038 (3)	0.0007 (3)
OW4	0.0140 (4)	0.0081 (4)	0.0141 (5)	−0.0029 (3)	0.0001 (3)	−0.0018 (3)
OW5	0.0078 (3)	0.0105 (4)	0.0162 (5)	−0.0024 (3)	0.0002 (3)	−0.0075 (3)

Geometric parameters (Å, º)

Mg1—OW3$^{\text{i}}$	2.0505 (9)	Mg2—OW1	2.0467 (8)
Mg1—OW3	2.0505 (9)	Mg2—OW1$^{\text{vi}}$	2.0467 (8)
Mg1—OW2$^{\text{ii}}$	2.0656 (9)	Mg2—O1	2.1099 (9)
Mg1—OW2$^{\text{iii}}$	2.0656 (9)	Mg2—O1$^{\text{vi}}$	2.1099 (9)
Mg1—O4$^{\text{iv}}$	2.0952 (9)	Cr1—O3$^{\text{vii}}$	1.6357 (9)
Mg1—O4$^{\text{v}}$	2.0952 (9)	Cr1—O4$^{\text{vii}}$	1.6554 (9)
Mg2—OW5	2.0265 (10)	Cr1—O1	1.6568 (9)
Mg2—OW5$^{\text{vi}}$	2.0265 (10)	Cr1—O2	1.6579 (8)
OW3$^{\text{i}}$—Mg1—OW3	180.00 (5)	OW5$^{\text{vi}}$—Mg2—O1$^{\text{vi}}$	92.35 (4)
OW3$^{\text{i}}$—Mg1—OW2$^{\text{ii}}$	90.97 (4)	OW1—Mg2—O1$^{\text{vi}}$	88.90 (4)
OW3—Mg1—OW2$^{\text{ii}}$	89.03 (4)	OW1$^{\text{vi}}$—Mg2—O1$^{\text{vi}}$	91.10 (4)
OW3$^{\text{i}}$—Mg1—OW2$^{\text{iii}}$	89.03 (4)	O1—Mg2—O1$^{\text{vi}}$	180.00 (3)
OW3—Mg1—OW2$^{\text{iii}}$	90.97 (4)	O3$^{\text{vii}}$—Cr1—O4$^{\text{vii}}$	109.01 (5)
OW2$^{\text{ii}}$—Mg1—OW2$^{\text{iii}}$	180.00 (7)	O3$^{\text{vii}}$—Cr1—O1	111.25 (5)
OW3$^{\text{i}}$—Mg1—O4$^{\text{iv}}$	91.55 (4)	O4$^{\text{vii}}$—Cr1—O1	108.90 (5)
OW3—Mg1—O4$^{\text{iv}}$	88.45 (4)	O3$^{\text{vii}}$—Cr1—O2	109.30 (4)
OW2$^{\text{ii}}$—Mg1—O4$^{\text{iv}}$	88.19 (4)	O4$^{\text{vii}}$—Cr1—O2	109.31 (4)
OW2$^{\text{iii}}$—Mg1—O4$^{\text{iv}}$	91.81 (4)	O1—Cr1—O2	109.05 (4)
OW3$^{\text{i}}$—Mg1—O4$^{\text{v}}$	88.45 (4)	Cr1—O1—Mg2	142.08 (6)
OW3—Mg1—O4$^{\text{v}}$	91.55 (4)	Cr1$^{\text{vii}}$—O4—Mg1$^{\text{viii}}$	140.12 (5)

OW2$^{\rm ii}$—Mg1—O4$^{\rm v}$	91.81 (4)
OW2$^{\rm iii}$—Mg1—O4$^{\rm v}$	88.19 (4)
O4$^{\rm iv}$—Mg1—O4$^{\rm v}$	180.00 (5)
OW5—Mg2—OW5$^{\rm vi}$	180.00 (5)
OW5—Mg2—OW1	90.91 (4)
OW5$^{\rm vi}$—Mg2—OW1	89.09 (4)
OW5—Mg2—OW1$^{\rm vi}$	89.09 (4)
OW5$^{\rm vi}$—Mg2—OW1$^{\rm vi}$	90.91 (4)
OW1—Mg2—OW1$^{\rm vi}$	180.0
OW5—Mg2—O1	92.35 (4)
OW5$^{\rm vi}$—Mg2—O1	87.65 (4)
OW1—Mg2—O1	91.10 (4)
OW1$^{\rm vi}$—Mg2—O1	88.90 (4)
OW5—Mg2—O1$^{\rm vi}$	87.65 (4)
Mg2—OW1—HW1A	126.4 (16)
Mg2—OW1—HW1B	121.9 (17)
HW1A—OW1—HW1B	111 (2)
Mg1$^{\rm ix}$—OW2—HW2A	119.3 (16)
Mg1$^{\rm ix}$—OW2—HW2B	122.2 (15)
HW2A—OW2—HW2B	102 (2)
Mg1—OW3—HW3A	118.2 (15)
Mg1—OW3—HW3B	117.0 (18)
HW3A—OW3—HW3B	111 (2)
HW4A—OW4—HW4B	109 (2)
Mg2—OW5—HW5A	119.5 (16)
Mg2—OW5—HW5B	131.6 (16)
HW5A—OW5—HW5B	109 (2)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*, −*y*+1, −*z*; (iii) *x*, *y*−1, *z*; (iv) *x*−1, *y*, *z*; (v) −*x*+1, −*y*, −*z*; (vi) −*x*, −*y*+1, −*z*+1; (vii) −*x*+1, −*y*, −*z*+1; (viii) *x*+1, *y*, *z*; (ix) *x*, *y*+1, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*1—H*W*1*A*···O2$^{\rm x}$	0.81 (2)	1.96 (2)	2.7702 (13)	174 (2)
O*W*1—H*W*1*B*···O3	0.80 (2)	1.97 (2)	2.7598 (13)	169 (2)
O*W*2—H*W*2*A*···O1$^{\rm vi}$	0.79 (2)	2.19 (2)	2.9014 (13)	150 (2)
O*W*2—H*W*2*A*···O*W*1	0.79 (2)	2.52 (2)	3.1008 (14)	132 (2)
O*W*2—H*W*2*B*···O*W*4	0.80 (2)	2.02 (2)	2.8173 (12)	171 (2)
O*W*3—H*W*3*A*···O2$^{\rm vii}$	0.82 (2)	1.97 (2)	2.7891 (13)	170 (2)
O*W*3—H*W*3*B*···O*W*4$^{\rm xi}$	0.81 (2)	1.99 (2)	2.7906 (14)	172 (2)
O*W*4—H*W*4*B*···O1$^{\rm x}$	0.83 (2)	2.32 (2)	3.1205 (14)	163 (2)
O*W*4—H*W*4*A*···O4	0.80 (2)	2.06 (2)	2.8535 (14)	170 (2)
O*W*5—H*W*5*B*···O2$^{\rm vii}$	0.80 (2)	1.93 (2)	2.7262 (13)	173 (2)
O*W*5—H*W*5*A*···O3$^{\rm iv}$	0.79 (2)	1.96 (2)	2.7409 (12)	174 (2)

Symmetry codes: (iv) *x*−1, *y*, *z*; (vi) −*x*, −*y*+1, −*z*+1; (vii) −*x*+1, −*y*, −*z*+1; (x) −*x*+1, −*y*+1, −*z*+1; (xi) −*x*+1, −*y*+1, −*z*.