

Poly[disodium [diaquatri- μ_2 -oxalato-dimagnesium(II)]]

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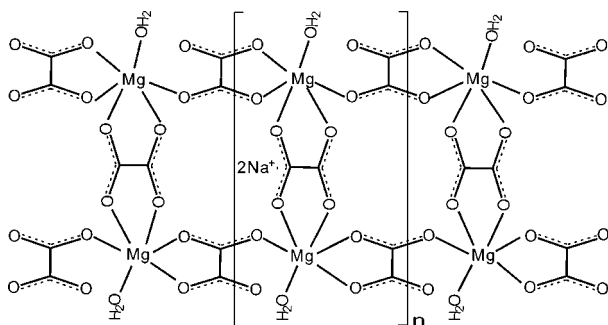
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.034; wR factor = 0.096; data-to-parameter ratio = 19.3.

The title compound, $[\text{Na}_2[\text{Mg}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]]_n$, is isotypic with its Co analogue. There are two crystallographically independent oxalate groups in the asymmetric unit, one lying on an inversion center and the other on a general position. Mg^{2+} ions are ligated by H_2O molecules and bridged by tri- and tetradentate oxalate ligands, forming ladder-like double chains that are held together via $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, with Na^+ cations located between the chains to balance the charge.

Related literature

For related literature, see: Audebrand *et al.* (2003); Brown & Altermatt (1985); Dean *et al.* (2004); Kolitsch (2004); Lethbridge *et al.* (2003); Lu *et al.* (2004); Miessen & Hoppe (1987); Price *et al.* (2000); Schefer & Grube (1995); Shannon (1976).



Experimental

Crystal data

$\text{Na}_2[\text{Mg}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]$
 $M_r = 394.70$
 Monoclinic, $P2_1/c$
 $a = 5.8460$ (12) Å
 $b = 15.726$ (3) Å
 $c = 7.0190$ (14) Å
 $\beta = 101.11$ (3)°
 $V = 633.2$ (2) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.34$ mm⁻¹

$T = 290$ K
 $0.4 \times 0.2 \times 0.2$ mm

Data collection

Rigaku AFC-7R diffractometer
 Absorption correction: ψ scan
 (Kopfmann & Huber, 1968)
 $T_{\min} = 0.912$, $T_{\max} = 0.943$
 2457 measured reflections
 2280 independent reflections

2027 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 3 standard reflections
 every 150 reflections
 intensity decay: 1.2%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.095$
 $S = 1.11$
 2280 reflections

118 parameters
 All H-atom parameters refined
 $\Delta\rho_{\text{max}} = 0.54$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O7}-\text{H7a}\cdots\text{O4}^i$	0.78 (3)	2.06 (3)	2.8335 (13)	170 (2)
$\text{O7}-\text{H7b}\cdots\text{O6}^{ii}$	0.84 (3)	1.89 (3)	2.6952 (13)	162 (3)

Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $x - 1, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *AFC Diffractometer Control Software* (Rigaku, 1994); cell refinement: *AFC Diffractometer Control Software*; data reduction: *AFC Diffractometer Control Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2084).

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supplementary materials

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Poly[disodium [diaquatri- μ_2 -oxalato-dimagnesium(II)]]

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Comment

Oxalates are of considerable interest because many of them are natural minerals and in addition, the oxalate anion can adopt different coordination modes to bind metals to form infinite chains, sheets and networks, leading to the rich structural chemistry (Lu *et al.*, 2004; Dean *et al.*, 2004; Audebrand *et al.*, 2003). In the system of mixed oxalates, $A_xB_y(C_2O_4)_z \cdot nH_2O$, combining alkali-metal elements (A) and alkali-earth-metal cations (B), only one compound, $Cs_2Mg(C_2O_4)_2 \cdot 4H_2O$, has been previously found, and it has a layered structure character in which layers of $MgO_4(H_2O)_2$ octahedra parallel to (10–1) are separated by corrugated layers of nine-coordinated Cs atoms (Kolitsch, 2004). During our exploratory syntheses of novel hydrated borate materials, we have obtained a new member of the $A_xB_y(C_2O_4)_z \cdot nH_2O$ family of compounds, $Na_2Mg_2(C_2O_4)_3 \cdot 2H_2O$. It has a one-dimensional character consisting of $[Mg_2(C_2O_4)_3(H_2O)_2]_n^{2n-}$ infinite chains. We describe its synthesis and crystal structure here for the first time.

The title compound is isotypic with its Co analogue (Price *et al.*, 2000) and the crystal structure consists of Na^+ and Mg^{2+} cations, $[C_2O_4]^{2-}$ groups, and H_2O molecules as the fundamental structural building units (Fig. 1). Mg^{2+} ions are ligated by H_2O molecules and bridged by tri-dentate oxalate ligands to generate a one-dimensional infinite polymeric chain, $[Mg(C_2O_4)(H_2O)]_n$. Two neighboring *inversion-center-related* $[Mg(C_2O_4)(H_2O)]_n$ chains are further bridged by tetra-dentate oxalate ligands to complete the octahedral coordination sphere of Mg^{2+} and to form a ladder-like double chain with the composition $[Mg_2(C_2O_4)_3(H_2O)_2]_n^{2n-}$ (Fig. 2 b). $Mg \cdots Mg$ distances along the double chain are 5.846 (1) Å, slightly longer than those across the chain (5.390 (1) Å). The $[Mg_2(C_2O_4)_3(H_2O)_2]_n^{2n-}$ chains extend along the [100] direction and pack in two orientations in a herringbone pattern, as illustrated in Fig.2a. These chains are held together *via* medium-to-weak $O-H \cdots O$ hydrogen bonds existing between the coordinated H_2O molecules and the O atoms from tri-dentate oxalate ligands (Table 1). Na^+ cations are located in the void space between the chains to balance charge.

There is one crystallographically independent Na^+ cation, which is coordinated to seven O atoms, forming an irregular coordination polyhedral geometry. The Na—O distances range from 2.2952 (10) to 2.8074 (10) Å, with an average of 2.510 Å, which is comparable to the value 2.46 Å computed from crystal radii for a 7-coordinated Na^+ ion (Shannon, 1976) and the distances 2.409 (3)–2.606 (3) Å (average 2.505 Å, CN = 7) in $NaLi_2BO_3$ (Miessen & Hoppe, 1987). Bond valence sum (BVS) calculations using Brown's formula (Brown & Altermatt, 1985) produced a BVS value of 1.15 for Na, in good agreement with its expected formal valence. The Mg atom also occupies one crystallographically distinct site. However, each Mg^{2+} is coordinated by six O atoms, five of which are from three oxalate ions and the other from one H_2O molecule. The MgO_6 octahedron is strongly distorted, with the 180° octahedral angles being $162.33(4)$ – $171.66(3)^\circ$, and the 90° octahedral angles in the range $78.40(3)$ – $99.05(4)^\circ$, the smallest angle being associated with the constrained $Mg1-O4^i-C2^i-C3^i-O5^i$ five-membered ring [Symmetry codes: (i) $-1 + x, y, z$]. The Mg—O distances of 2.0436 (9)–2.1429 (9) Å (average

supplementary materials

2.078 Å) are very reasonable when compared with the ranges 2.057 (9)–2.080 (9) Å (average 2.065 Å) in $\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, where octahedrally coordinated Mg^{2+} is also found (Schefer & Grube, 1995). The calculated BVS value for Mg is also reasonable, at 2.12. Of the two unique oxalate ions, the C1-based oxalate sits on an inversion center and the C2/C3-based one on a general position. Both oxalate ions are nearly planar, with a mean deviation of 0.0004 and 0.1418 Å, respectively, and the bond geometries of $[\text{C}_2\text{O}_4]^{2-}$ are in accord with those observed in other oxalate compounds (Lethbridge *et al.*, 2003).

Experimental

The title compound was synthesized by a two-step process. First, for the preparation of the precursor, $\text{Na}_3\text{MgB}_5\text{O}_{10}$, a stoichiometric mixture of Na_2CO_3 , MgO , and H_3BO_3 was heated at 873 K for two weeks with several intermediate re-mixings and the resulting product was identified to be the pure phase of $\text{Na}_3\text{MgB}_5\text{O}_{10}$ based on the powder XRD analysis. Then, a 0.300 g (0.976 mmol) sample of $\text{Na}_3\text{MgB}_5\text{O}_{10}$, 0.300 g (2.380 mmol) $\text{H}_2(\text{C}_2\text{O}_4) \cdot 2\text{H}_2\text{O}$, and 3 ml H_2O were sealed in an 15-ml Teflon-lined autoclave and subsequently heated at 453 K for one week, then cooled slowly to room temperature. The product consisted of colorless, prismatic crystals with the largest having dimensions of $0.6 \times 0.6 \times 1.2 \text{ mm}^3$ in colorless mother liquor. The final pH of the reaction system was about 2.0. The crystals were isolated in about 70% yield (based on Mg) by washing the reaction product with deionized water and anhydrous ethanol followed by drying with anhydrous acetone. The powder XRD pattern of the ground crystals is in good agreement with that calculated from the single-crystal data, confirming that the pure phase of the title compound has been obtained. Although boron was not incorporated into the final structure, borate anions may serve as mineralizers to enhance the crystal growth.

Refinement

H-atom positions were located in a difference Fourier map and all associated parameters were refined freely.

Figures

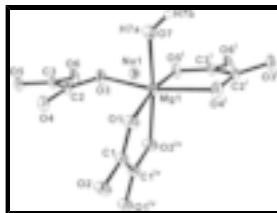


Fig. 1. The connectivity in $\text{Na}_2\text{Mg}_2(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$, shown with displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) $-1 + x, y, z$; (iv) $1 - x, 1 - y, 1 - z$]

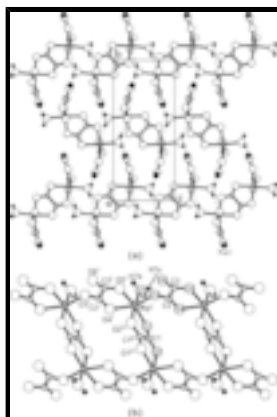


Fig. 2. The crystal structure of $\text{Na}_2\text{Mg}_2(\text{C}_2\text{O}_4)_3 \cdot 2\text{H}_2\text{O}$ projected along the $[100]$ direction (a) as well as the single chain of $[\text{Mg}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]_n^{2n-}$ (b). $\text{H} \cdots \text{O}$ hydrogen bond contacts are shown as dashed lines; symmetry codes are the same as those in Figure 1.

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Crystal data

$\text{Na}_2[\text{Mg}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2]$	$F(000) = 396$
$M_r = 394.70$	$D_x = 2.070 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
$a = 5.8460 (12) \text{ \AA}$	$\theta = 21.9\text{--}22.5^\circ$
$b = 15.726 (3) \text{ \AA}$	$\mu = 0.34 \text{ mm}^{-1}$
$c = 7.0190 (14) \text{ \AA}$	$T = 290 \text{ K}$
$\beta = 101.11 (3)^\circ$	Prism, colorless
$V = 633.2 (2) \text{ \AA}^3$	$0.4 \times 0.2 \times 0.2 \text{ mm}$
$Z = 2$	

Data collection

Rigaku AFC-7R diffractometer	2027 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube graphite	$R_{\text{int}} = 0.029$
2θ - ω scans	$\theta_{\text{max}} = 32.5^\circ$, $\theta_{\text{min}} = 2.6^\circ$
Absorption correction: ψ scan (Kopfmann & Huber, 1968)	$h = 0 \rightarrow 8$
$T_{\text{min}} = 0.912$, $T_{\text{max}} = 0.943$	$k = 0 \rightarrow 23$
2457 measured reflections	$l = -10 \rightarrow 10$
2280 independent reflections	3 standard reflections every 150 reflections
	intensity decay: 1.2%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	All H-atom parameters refined
$wR(F^2) = 0.095$	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.0731P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
2280 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
118 parameters	$\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.56 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.310 (14)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.46789 (7)	0.81852 (3)	0.30526 (7)	0.01952 (13)
Mg1	0.27308 (6)	0.60144 (2)	0.21580 (5)	0.01297 (12)
C1	0.49584 (17)	0.46394 (6)	0.42523 (14)	0.01492 (18)
O1	0.38596 (15)	0.47765 (5)	0.25634 (11)	0.01885 (17)
O2	0.60143 (15)	0.39673 (5)	0.48571 (11)	0.02059 (18)
C2	0.79984 (15)	0.64930 (6)	0.21459 (13)	0.01346 (18)
O3	0.58217 (13)	0.65770 (5)	0.17720 (13)	0.02067 (17)
O4	0.91349 (13)	0.58130 (5)	0.22737 (12)	0.01867 (17)
C3	0.94672 (16)	0.73184 (6)	0.24642 (14)	0.01425 (18)
O5	1.15751 (12)	0.72335 (5)	0.23254 (12)	0.01735 (17)
O6	0.85117 (14)	0.79871 (5)	0.28409 (15)	0.0255 (2)
O7	0.18307 (14)	0.58554 (5)	-0.08136 (12)	0.01742 (16)
H7A	0.174 (4)	0.5388 (16)	-0.124 (4)	0.058 (7)*
H7B	0.065 (5)	0.6120 (18)	-0.141 (4)	0.077 (9)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0152 (2)	0.0208 (2)	0.0230 (2)	-0.00005 (15)	0.00461 (16)	0.00233 (16)
Mg1	0.01111 (17)	0.01020 (17)	0.01744 (18)	0.00096 (10)	0.00233 (12)	0.00035 (10)
C1	0.0171 (4)	0.0111 (4)	0.0166 (4)	0.0015 (3)	0.0031 (3)	-0.0012 (3)
O1	0.0258 (4)	0.0130 (3)	0.0161 (3)	0.0031 (3)	-0.0001 (3)	-0.0011 (2)
O2	0.0289 (4)	0.0134 (3)	0.0179 (3)	0.0080 (3)	0.0005 (3)	-0.0014 (2)
C2	0.0104 (4)	0.0140 (4)	0.0165 (4)	-0.0015 (3)	0.0039 (3)	-0.0008 (3)
O3	0.0100 (3)	0.0223 (4)	0.0300 (4)	-0.0018 (3)	0.0045 (3)	0.0009 (3)
O4	0.0147 (3)	0.0120 (3)	0.0297 (4)	-0.0007 (2)	0.0054 (3)	-0.0008 (3)
C3	0.0105 (4)	0.0120 (4)	0.0200 (4)	0.0002 (3)	0.0022 (3)	-0.0009 (3)
O5	0.0102 (3)	0.0113 (3)	0.0310 (4)	0.0000 (2)	0.0051 (3)	-0.0008 (3)
O6	0.0150 (3)	0.0144 (3)	0.0470 (5)	0.0026 (3)	0.0062 (3)	-0.0083 (3)
O7	0.0176 (3)	0.0148 (3)	0.0191 (3)	0.0019 (3)	0.0017 (3)	-0.0011 (2)

Geometric parameters (Å, °)

Na1—O6	2.2952 (10)	Mg1—O4 ⁱ	2.1429 (9)
Na1—O5 ⁱ	2.3315 (9)	C1—O1	1.2533 (12)
Na1—O2 ⁱⁱ	2.3514 (10)	C1—O2	1.2559 (11)
Na1—O7 ⁱⁱⁱ	2.4886 (10)	C1—C1 ^{iv}	1.5399 (19)
Na1—O3 ⁱⁱⁱ	2.5941 (12)	C2—O4	1.2531 (12)
Na1—O1 ⁱⁱ	2.7059 (10)	C2—O3	1.2557 (11)
Na1—O3	2.8074 (10)	C2—C3	1.5485 (13)
Mg1—O5 ⁱ	2.0436 (9)	C3—O6	1.2428 (12)
Mg1—O1	2.058 (1)	C3—O5	1.2618 (11)
Mg1—O7	2.0656 (10)	O7—H7A	0.79 (3)
Mg1—O3	2.0761 (9)	O7—H7B	0.85 (3)
Mg1—O2 ^{iv}	2.0823 (10)		
O6—Na1—O5 ⁱ	128.83 (4)	O5 ⁱ —Mg1—O2 ^{iv}	89.17 (3)
O6—Na1—O2 ⁱⁱ	91.25 (4)	O1—Mg1—O2 ^{iv}	80.36 (3)
O5 ⁱ —Na1—O2 ⁱⁱ	98.57 (4)	O7—Mg1—O2 ^{iv}	171.66 (3)
O6—Na1—O7 ⁱⁱⁱ	145.56 (3)	O3—Mg1—O2 ^{iv}	88.78 (5)
O5 ⁱ —Na1—O7 ⁱⁱⁱ	85.34 (3)	O5 ⁱ —Mg1—O4 ⁱ	78.40 (3)
O2 ⁱⁱ —Na1—O7 ⁱⁱⁱ	86.94 (4)	O1—Mg1—O4 ⁱ	98.38 (4)
O6—Na1—O3 ⁱⁱⁱ	91.11 (4)	O7—Mg1—O4 ⁱ	87.68 (5)
O5 ⁱ —Na1—O3 ⁱⁱⁱ	110.58 (4)	O3—Mg1—O4 ⁱ	162.33 (4)
O2 ⁱⁱ —Na1—O3 ⁱⁱⁱ	140.04 (3)	O2 ^{iv} —Mg1—O4 ⁱ	97.00 (5)
O7 ⁱⁱⁱ —Na1—O3 ⁱⁱⁱ	69.46 (3)	O1—C1—O2	126.40 (9)
O6—Na1—O1 ⁱⁱ	76.88 (3)	O1—C1—C1 ^{iv}	117.46 (10)
O5 ⁱ —Na1—O1 ⁱⁱ	144.59 (3)	O2—C1—C1 ^{iv}	116.14 (11)
O2 ⁱⁱ —Na1—O1 ⁱⁱ	52.00 (3)	C1—O1—Mg1	112.70 (6)
O7 ⁱⁱⁱ —Na1—O1 ⁱⁱ	75.03 (3)	C1—O2—Mg1 ^{iv}	112.55 (6)
O3 ⁱⁱⁱ —Na1—O1 ⁱⁱ	89.97 (3)	O4—C2—O3	127.35 (9)
O6—Na1—O3	63.99 (3)	O4—C2—C3	115.69 (8)
O5 ⁱ —Na1—O3	64.84 (3)	O3—C2—C3	116.96 (8)
O2 ⁱⁱ —Na1—O3	101.83 (3)	C2—O3—Mg1	143.16 (7)
O7 ⁱⁱⁱ —Na1—O3	149.74 (3)	C2—O4—Mg1 ^v	112.43 (6)
O3 ⁱⁱⁱ —Na1—O3	114.90 (3)	O6—C3—O5	126.27 (9)
O1 ⁱⁱ —Na1—O3	132.84 (3)	O6—C3—C2	118.71 (8)
O5 ⁱ —Mg1—O1	168.63 (4)	O5—C3—C2	115.01 (8)
O5 ⁱ —Mg1—O7	98.56 (4)	C3—O5—Mg1 ^v	116.25 (6)
O1—Mg1—O7	92.16 (3)	Mg1—O7—H7A	118.6 (19)
O5 ⁱ —Mg1—O3	85.03 (3)	Mg1—O7—H7B	117.6 (19)
O1—Mg1—O3	99.05 (4)	H7A—O7—H7B	106 (2)
O7—Mg1—O3	88.77 (4)		

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, y+1/2, -z+1/2$; (iii) $x, -y+3/2, z+1/2$; (iv) $-x+1, -y+1, -z+1$; (v) $x+1, y, z$.

supplementary materials

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O7-H7a\cdots O4^{vi}$	0.78 (3)	2.06 (3)	2.8335 (13)	170 (2)
$O7-H7b\cdots O6^{vii}$	0.84 (3)	1.89 (3)	2.6952 (13)	162 (3)

Symmetry codes: (vi) $-x+1, -y+1, -z$; (vii) $x-1, -y+3/2, z-1/2$.

Fig. 1

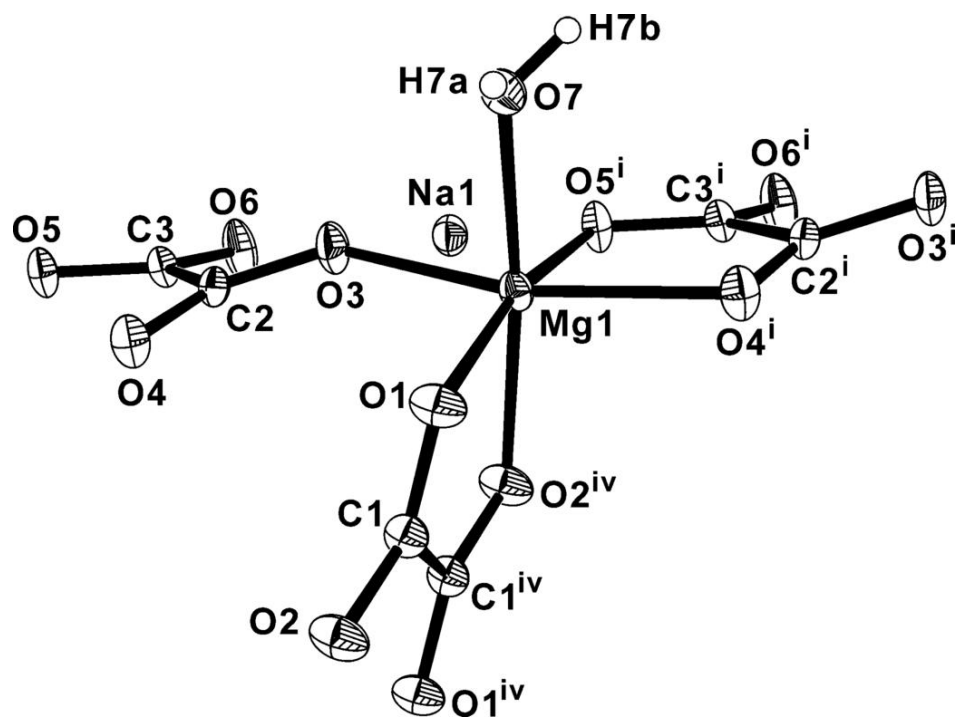


Fig. 2

