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Poly[[dimethanolmagnesium(II)]-μ-*p*-phenylenedioxydiacetato]: a three-dimensional magnesium(II) coordination polymer

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Key indicators

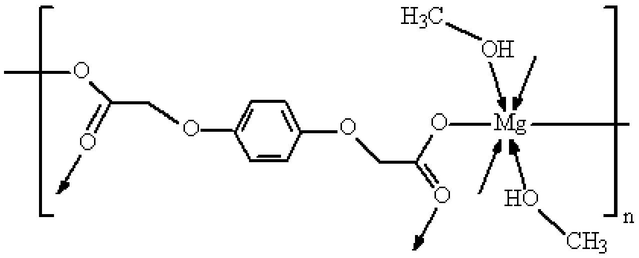
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.063
wR factor = 0.166
Data-to-parameter ratio = 13.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The Mg^{II} ion and the 1,4-BDOA^{2-} ligand in the title coordination polymer, [Mg(1,4-BDOA)(CH$_3$OH)$_2$]$_n$ (where 1,4-BDOA^{2-} is the *p*-phenylenedioxydiacetate dianion, $C_{10}H_8O_6^{2-}$), lie on inversion centers. The Mg^{II} center has an octahedral coordination geometry defined by four carboxyl O atoms from four different 1,4-BDOA^{2-} ligands and two hydroxy O atoms from two methanol molecules. The Mg^{II} atoms are bridged by 1,4-BDOA^{2-} ligands, leading to a three-dimensional infinite network structure.

Comment

The coordination chemistry of the alkaline earth metals has, until recently, remained a largely underdeveloped area (Sen *et al.*, 2003). Although transition metal carboxylates have been widely investigated (Reyes *et al.*, 2003), reports on magnesium coordination polymers with carboxylate ligands are very rare (Wang *et al.*, 1994). The flexible benzene-1,4-dioxydiacetic acid (1,4-BDOAH$_2$) exhibits high symmetry and versatile binding modes, and hence it could generate various supramolecular architectures. Previously, our group has reported some one- and two-dimensional transition metal coordination polymers incorporating this ligand, in which the 1,4-BDOA^{2-} group shows the capability of acting as a bridging ligand in various coordination modes, including bidentate (Gao *et al.*, 2004*a*), tridentate (Gao *et al.*, 2004*b*), tetradentate (Gao, Liu, Huo, Xu & Zhao, 2005) and hexadentate (Gao, Liu, Huo, Zhao & Zhao, 2005). As part of our continuing investigations into the coordination behavior of this ligand, we report here the crystal structure of a new three-dimensional coordination polymer, [Mg(1,4-BDOA)(CH$_3$OH)$_2$]$_n$, (I).



(I)

As shown in Fig. 1, the Mg^{II} atom and 1,4-BDOA^{2-} ligand lie on inversion centers, and the fully deprotonated carboxylate groups are bonded to the Mg^{II} ions in a monodentate fashion. Each Mg^{II} atom is covalently bonded to four carboxyl O atoms from four different 1,4-BDOA^{2-} ligands and two hydroxy O atoms from two coordinated methanol molecules, displaying an approximate octahedral coordination

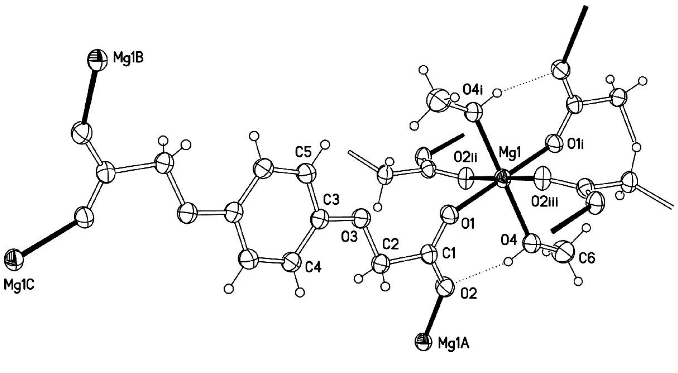


Figure 1
ORTEPII plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are indicated by dotted lines. [Symmetry codes: (i) $1-x, 1-y, -z$; (ii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (*A*) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (*B*) $1+x, \frac{3}{2}-y, \frac{1}{2}+z$; (*C*) $-x, 1-y, 1-z$.]

configuration. Methanol atom O4 not only engages in coordination but also forms an intramolecular hydrogen bond with the coordinated carboxyl atom O2, consolidating the structure (Table 2).

Two adjacent Mg^{II} atoms are linked through one bis(monodentate) carboxyl group, with an Mg1···Mg1*A* distance of 5.320 (3) Å [symmetry code: (*A*) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$]. Pairs of Mg^{II} atoms are further connected *via* four carboxyl O atoms of one 1,4-BDOA^{2-} ligand, with Mg1···Mg1*B* [symmetry code: (*B*) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$] and Mg1···Mg1*C* [symmetry code: (*C*) $x-1, y, z+1$] distances of 13.273 (3) and 14.278 (3) Å, respectively. It can be seen from a perspective view of the title complex along the *c* axis (Fig. 2) that each 1,4-BDOA^{2-} group acts as a tetrakis(monodentate) ligand to link four Mg^{II} ions, resulting in the formation of a regular three-dimensional open framework with a triangular channel, which holds the coordinated methanol.

Experimental

The 1,4-BDOAH$_2$ ligand was prepared by the reaction of chloroacetic acid with hydroquinol (Mirci, 1990). The title complex was prepared by the addition of magnesium perchlorate hexahydrate (5.13 g, 20 mmol) to a methanol solution (20 ml) containing 1,4-BDOAH$_2$ (4.52 g, 20 mmol), and the pH value was adjusted to 7 with 0.1 *M* NaOH solution. The resulting solution was stirred for 30 min at room temperature and then filtered. Colorless prismatic single crystals were isolated from the solution at room temperature over a period of several days. Analysis calculated for $C_{12}H_{16}O_8Mg$: C 46.11, H 5.16%; found: C 46.13, H 5.12%.

Crystal data

$[Mg(C_{11}H_{14}O_6)(CH_4O)_2]$
$M_r = 312.56$
Monoclinic, $P2_1/c$
$a = 12.070$ (2) Å
$b = 7.7088$ (15) Å
$c = 7.3332$ (15) Å
$\beta = 91.42$ (3)°
$V = 682.1$ (2) Å^3
$Z = 2$
$D_x = 1.522$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 4419 reflections
$\theta = 3.1$–25.9°
$\mu = 0.17$ mm^{-1}
$T = 295$ (2) K
Prism, colorless
0.23 × 0.18 × 0.08 mm

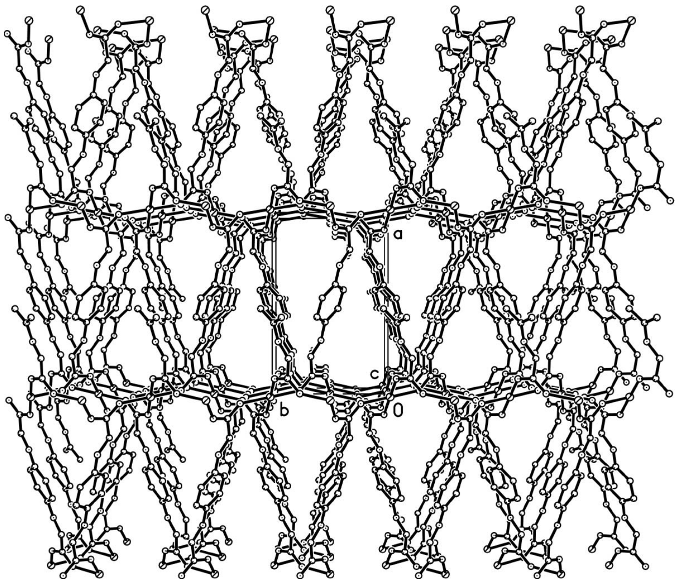


Figure 2
Packing diagram of the title complex, viewed along the *c* axis. The coordinated methanol molecules have been omitted for clarity; they occupy the apparent triangular channels.

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.962$, $T_{max} = 0.987$
4471 measured reflections

1328 independent reflections
1082 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 26.0°$
$h = -14 \rightarrow 14$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.166$
$S = 1.08$
1328 reflections
102 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.104P)^2 + 0.0721P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mg1—O1	2.033 (2)	O1—C1	1.246 (4)
Mg1—O2^{i}	2.111 (2)	O2—C1	1.259 (4)
Mg1—O4	2.080 (3)		
O1^{ii}—Mg1—O1	180	O2^{i}—Mg1—O2^{iii}	180
O1—Mg1—O4	88.22 (10)	O4—Mg1—O2^{i}	90.92 (11)
O1^{ii}—Mg1—O4	91.78 (10)	O4^{ii}—Mg1—O2^{i}	89.08 (11)
O1^{ii}—Mg1—O2^{i}	93.03 (10)	O4—Mg1—O4^{ii}	180
O1—Mg1—O2^{i}	86.97 (10)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H7···O2	0.84 (3)	2.02 (2)	2.798 (3)	153 (4)

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C-bound H atoms were placed in calculated positions, with C—H = 0.93 (aromatic), 0.96 (CH_3) or 0.97 Å (CH_2) and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl})$, and were refined in the riding-model approximation. The hydroxy H atom of the methanol molecule was located in a difference Fourier map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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