Hexaaquamagnesium(II) benzene-1,4-dioxy-acetate

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The title complex, alternatively called hexaaquamagnesium(II) *p*-phenylenebis(oxyacetate), $[Mg(H_2O)_6]$-$(C_{10}H_8O_6)$, has been synthesized by the reaction of $Mg(NO_3)_2 \cdot 6H_2O$ and benzene-1,4-dioxyacetic acid in an aqueous solution. The Mg^{II} atom is coordinated by six water molecules to form an octahedron [Mg—O = 2.0433 (16)–2.1281 (18) Å]. The cations and anions, which lie on centres of symmetry, are linked by hydrogen bonds into a three-dimensional network structure.

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.122
Data-to-parameter ratio = 13.8

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

Comment

Benzene-1,4-dioxyacetic acid is known as a good candidate for the construction of supramolecular complexes; it can form regular hydrogen bonds by functioning as either hydrogen-bond donor or acceptor (Gao *et al.*, 2004). We have previously reported the structures of hexaaquacobalt(II) benzene-1,4-dioxyacetate (Liu, Huo *et al.*, 2004) and hexaaqua-manganese(II) benzene-1,4-dioxyacetate (Liu, Gao *et al.*, 2004). Recently, we found that benzene-1,4-dioxyacetic acid forms a hexaaquamagnesium(II) benzene-1,4-dioxyacetate complex, (I), under similar reaction conditions and that this is isomorphous with the Co^{II} and Mn^{II} analogues. Previous structural descriptions of the Co^{II} and Mn^{II} complexes apply to the present isostructural complex, (I) (Fig. 1).

(I)
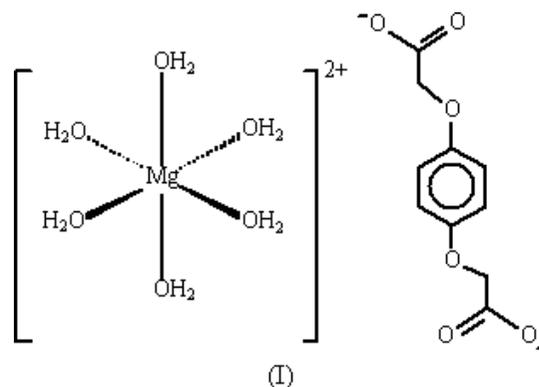
The Mg^{II} atom is six-coordinate in an octahedral environment. The anion is almost planar (r.m.s. deviation = 0.01 Å); the oxyacetate group and aromatic ring are essentially planar, with a torsion angle of −179.1 (15)° (C4—O3—C2—C1). The cation and anion both lie on inversion centres and are linked by extensive hydrogen bonds into a three-dimensional supramolecular network structure (Table 2).

metal-organic papers
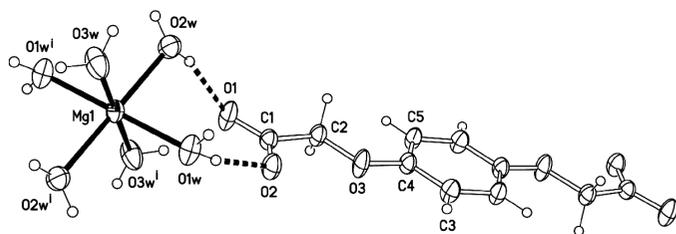
Figure 1
ORTEPII plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level and hydrogen bonds shown as dashed lines. Symmetry codes are as in Table 1.

Experimental

Benzene-1,4-dioxyacetic acid was prepared by the nucleophilic reaction of chloroacetate and hydroquinone under basic conditions, following the method described for the synthesis of benzene-1,2-dioxyacetic acid (Mirci, 1988). The title complex was prepared by the addition of $Mg(NO_3)_2 \cdot 6H_2O$ (5.13 g, 20 mmol) and KSCN (0.97 g, 10 mol) to an aqueous solution (25 ml) of benzene-1,4-dioxyacetic acid (4.52 g, 20 mmol). The resulting solution was stirred and the pH was adjusted to 7 with 0.1 M NaOH solution. Colourless crystals were separated from the filtered solution after several days. Analysis calculated for $C_{10}H_{20}MgO_{12}$: C 33.69, H 5.65%; found: C 33.80, H 5.61%.

Crystal data

$[Mg(H_2O)_6](C_{10}H_8O_6)$
$M_r = 356.57$
Triclinic, $P\bar{1}$
$a = 5.5677 (11)$ Å
$b = 6.3662 (13)$ Å
$c = 11.620 (2)$ Å
$\alpha = 102.11 (3)°$
$\beta = 95.59 (3)°$
$\gamma = 106.68 (3)°$
$V = 380.26 (16)$ Å^3

$Z = 1$
$D_x = 1.557$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3689 reflections
$\theta = 3.5–27.5°$
$\mu = 0.18$ mm^{-1}
$T = 296 (2)$ K
Prism, colourless
$0.37 \times 0.25 \times 0.18$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.947$, $T_{max} = 0.968$
3747 measured reflections

1710 independent reflections
1321 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$
$h = -7 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.122$
$S = 1.02$
1710 reflections
124 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.1773P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mg1—O1w	2.0433 (16)	O1—C1	1.237 (2)
Mg1—O2w	2.0677 (16)	O2—C1	1.265 (3)
Mg1—O3w	2.1281 (18)		
O1w—Mg1—O1w^i	180	O2w^i—Mg1—O2w	180
O1w—Mg1—O2w	92.50 (7)	O2w^i—Mg1—O3w	93.09 (7)
O1w—Mg1—O3w	92.03 (7)	O2w—Mg1—O3w	86.91 (7)
O1w^i—Mg1—O2w	87.50 (7)	O3w^i—Mg1—O3w	180
O1w^i—Mg1—O3w	87.97 (7)		

Symmetry code: (i) $1 - x, 1 - y, 1 - z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1w—H1w1$\cdots$O2^{ii}	0.85 (2)	2.03 (2)	2.823 (2)	155 (3)
O1w—H1w2$\cdots$O1^i	0.84 (2)	1.90 (2)	2.722 (2)	163 (3)
O2w—H2w1$\cdots$O3w^{ii}	0.86 (2)	2.16 (2)	2.993 (2)	164 (2)
O2w—H2w2$\cdots$O2	0.86 (2)	1.89 (2)	2.740 (2)	168 (3)
O3w—H3w1$\cdots$O1	0.84 (2)	2.06 (2)	2.869 (2)	161 (2)
O3w—H3w2$\cdots$O2^{iii}	0.85 (2)	1.87 (2)	2.707 (2)	170 (2)
O3w—H3w2$\cdots$O3^{iii}	0.85 (2)	2.58 (2)	3.094 (3)	120 (2)

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

Water H atoms were located in a difference map and refined with O—H distance restraints of 0.85 (1) Å and with $U_{iso}(H) = 1.5U_{eq}(O)$. The other H atoms were placed in calculated positions [C—H = 0.93 (aromatic) or 0.97 Å (aliphatic) and $U_{iso}(H) = 1.2U_{eq}(C)$] and were refined using the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 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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