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Tetraaquabis(4-carboxyphenoxyacetato)-magnesium(II)

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The title complex, $[Mg(C_9H_7O_5)_2(H_2O)_4]$, is a neutral mononuclear molecule consisting of an Mg^{II} ion, two 4-carboxyphenoxyacetate ligands and four coordinated water molecules. The Mg^{II} atom lies on an inversion center and is six-coordinate, with two O atoms of two *trans* 4-CPOAH$^-$ ligands and four water molecules. A supramolecular network structure is formed by intermolecular hydrogen bonds.

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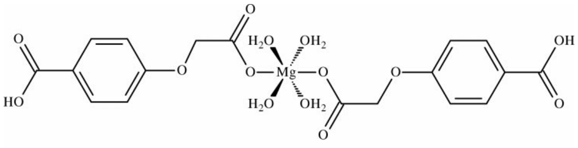
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.139
Data-to-parameter ratio = 13.4

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

Comment

4-Carboxyphenoxyacetic acid (4-CPOAH$_2$), widely used in biological activity studies, is a flexible multidentate ligand, with versatile binding modes. Structures of the complexes of 4-CPOAH$_2$ have been reported for sodium (Wai *et al.*, 1990), nickel, manganese and cobalt (Kennard *et al.*, 1984). Recently, we isolated a new Mg^{II} complex, *viz*. $Mg(4\text{-CPOAH})_2(H_2O)_4$, (I), from 4-CPOAH$_2$ and $Mg(ClO_4)_2\cdot6H_2O$. We report here the crystal structure of this complex.



(I)

As shown in Fig. 1, the title complex has a mononuclear structure, in which the 4-carboxyphenoxyacetate monoanions are bonded to the Mg^{II} atom in a monodentate fashion. The Mg^{II} atom is located on an inversion center and is coordinated by two O atoms of *trans* 4-CPOAH$^-$ ligands and four water molecules, forming an octahedral coordination geometry. The Mg—O(oxyacetate) bond distance is 2.086 (2) Å, and the average Mg—O(H_2O) distance is 2.072 (2) Å. The *cis* bond angles at the Mg^{II} atom are close to 90°. The coordinated oxyacetate group and benzene ring are almost coplanar, with a C3—O3—C2—C1 torsion angle of 178.2 (2)°. A supramolecular framework is formed through intermolecular hydrogen-bond interactions (Fig. 2). The uncoordinated carboxylic acid groups of adjacent molecules form O—H$\cdots$O hydrogen bonds with each other, resulting in a one-dimensional chain (Table 2). These chains are linked by other hydrogen bonds (Table 2).

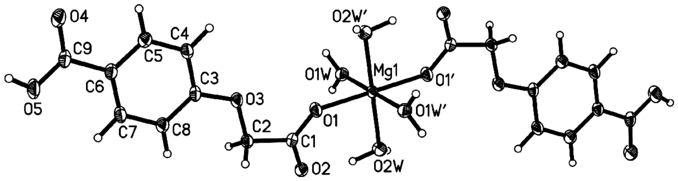


Figure 1
View of the title compound, with 30% probability displacement ellipsoids.

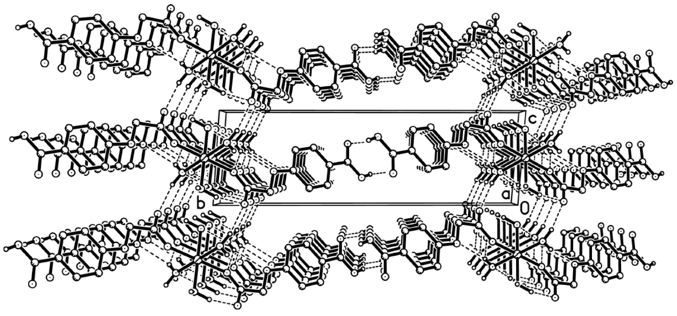


Figure 2
Hydrogen bonding in the crystal structure of (I).

Experimental

The title complex was prepared by the addition of a stoichiometric amount of $Mg(ClO_4)_2 \cdot 6H_2O$ (20 mmol) and NaOH (30 mmol) to a hot aqueous solution of 4-$CPOAH_2$ (20 mmol). The resulting solution was filtered, and colorless single crystals were obtained at room temperature over several days.

Crystal data

$[Mg(C_9H_7O_5)_2(H_2O)_4]$
$M_r = 486.67$
Triclinic, $P\bar{1}$
$a = 4.922$ (1) Å
$b = 5.755$ (1) Å
$c = 18.432$ (4) Å
$\alpha = 94.13$ (3)°
$\beta = 91.95$ (3)°
$\gamma = 96.13$ (3)°
$V = 517.3$ (2) Å^3

$Z = 1$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4564 reflections
$\theta = 3.3$–27.6°
$\mu = 0.16$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.30 × 0.28 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.953$, $T_{max} = 0.959$
4618 measured reflections

2244 independent reflections
1609 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.139$
$S = 1.04$
2244 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.1746P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mg1—O2*W*	2.042 (2)	Mg1—O1*W*	2.101 (2)
Mg1—O1	2.086 (2)		
O2*W*^{i}—Mg1—O1	89.31 (7)	O2*W*—Mg1—O1*W*	89.65 (8)
O2*W*—Mg1—O1	90.69 (7)	O1—Mg1—O1*W*	91.10 (7)
O2*W*—Mg1—O1*W*^{i}	90.35 (8)	C3—O3—C2	118.3 (2)
O1—Mg1—O1*W*^{i}	88.90 (7)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*WB*···O3^{ii}	0.812 (19)	2.26 (2)	3.001 (3)	151 (4)
O1*W*—H1*WB*···O1^{ii}	0.812 (19)	2.27 (3)	2.924 (3)	138 (4)
O1*W*—H1*WA*···O2^{iii}	0.828 (19)	1.94 (2)	2.748 (3)	166 (4)
O2*W*—H2*WB*···O2	0.829 (18)	1.90 (2)	2.704 (2)	164 (4)
O2*W*—H2*WA*···O1*W*^{iv}	0.817 (18)	2.17 (3)	2.888 (3)	147 (4)
O5—H12···O4^v	0.82	1.80	2.612 (2)	169

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

The H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, O—H = 0.82 Å and $U_{iso}(H) = 1.2U_{eq}$(parent atom), and refined as riding, except for the water molecules, for which the H atoms were located in difference Fourier maps and refined isotropically.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997; program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL*97.

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