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Hexaaquacobalt(II) benzene-1,4-dioxydiacetate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.127
Data-to-parameter ratio = 13.9

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

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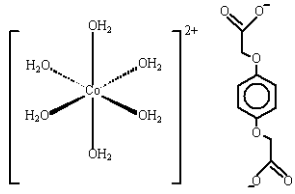
The cation and anion of the title compound, $[Co(H_2O)_6](C_{10}H_8O_6)$, lie on different inversion sites. The Co^{II} atom shows octahedral coordination. The cations and anions are linked by hydrogen bonds into a three-dimensional network structure.

Comment

A number of metal derivatives of benzene-1,2-dioxyacetic acid have been structurally characterized (McCann *et al.*, 1994; Smith *et al.*, 1987; Smith *et al.*, 1991), but complexes of the related benzene-1,4-dioxyacetic acid are less well documented. The present study of the title hexaaquacobalt(II) complex, (I) (Fig. 1), follows a recent study of a bis(phenanthroline)-chelated manganese(II) salt, whose benzene-1,4-dioxyacetate anion interacts indirectly, through the uncoordinated and coordinated water molecules, with the metal center (Gao *et al.*, 2004).



(I)

The Co^{II} atom is six-coordinate in an octahedral environment. The anion is almost planar (r.m.s. deviation = 0.008 Å); the planarity forces the ether linkage (C2—O3—C3) to open to 117.3 (2)° (idealized angle = 109.5°). The cation and anion both lie on inversion sites, and they are linked by hydrogen bonds into a three-dimensional network structure (Table 2 and Fig. 2).

Experimental

Benzene-1,4-dioxyacetic acid was prepared by the nucleophilic reaction of chloroacetic acid and hydroquinone under basic conditions, following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). Cobalt diacetate trihydrate

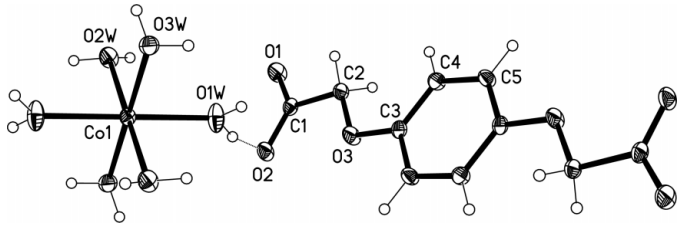


Figure 1
A view of $[Co(H_2O)_6](C_{10}H_8O_6)$, with displacement ellipsoids drawn at the 30% probability level.

(4.76 g, 20 mmol) and benzene-1,4-dioxyacetic acid (9.04 g, 40 mmol) were dissolved in water and the pH was adjusted to 6 with 0.1*M* sodium hydroxide. Pink crystals separated from the filtered solution after several days. Analysis calculated for $C_{10}H_{20}CoO_{12}$: C 30.70, H 5.15%; found: C 30.48, H 5.28%.

Crystal data

$[Co(H_2O)_6](C_{10}H_8O_6)$	$Z = 1$
$M_r = 391.19$	$D_x = 1.709$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 5.568$ (2) Å	Cell parameters from 1613 reflections
$b = 6.366$ (2) Å	$\theta = 3.6$–$27.4°$
$c = 11.620$ (3) Å	$\mu = 1.19$ mm^{-1}
$\alpha = 102.21$ (2)°	$T = 293$ (2) K
$\beta = 95.59$ (2)°	Prism, pink
$\gamma = 106.68$ (1)°	0.36 × 0.28 × 0.18 mm
$V = 380.1$ (2) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	1722 independent reflections
	1625 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.018$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$\theta_{max} = 27.5°$
	$h = -7 \rightarrow 7$
$T_{min} = 0.674$, $T_{max} = 0.814$	$k = -7 \rightarrow 8$
3456 measured reflections	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0883P)^2 + 0.2735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.08$	$\Delta\rho_{max} = 1.28$ e Å^{-3}
1722 reflections	$\Delta\rho_{min} = -0.39$ e Å^{-3}
124 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Co1—O1*W*	2.067 (2)	Co1—O3*W*	2.149 (2)
Co1—O2*W*	2.090 (2)		
O1*W*—Co1—O1*W*^{i}	180	O2*W*—Co1—O2*W*^{i}	180
O1*W*—Co1—O2*W*	92.2 (1)	O2*W*—Co1—O3*W*	93.1 (1)
O1*W*—Co1—O2*W*^{i}	87.8 (1)	O2*W*—Co1—O3*W*^{i}	86.9 (1)
O1*W*—Co1—O3*W*	87.7 (1)	O3*W*—Co1—O3*W*^{i}	180
O1*W*—Co1—O3*W*^{i}	92.3 (1)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2	0.85 (3)	2.00 (3)	2.814 (3)	159 (4)
O1*W*—H1*W*2···O1^{ii}	0.84 (3)	1.88 (3)	2.700 (3)	163 (3)
O2*W*—H2*W*1···O3*W*^{iii}	0.85 (3)	2.12 (3)	2.957 (3)	168 (3)
O2*W*—H2*W*2···O2^{iv}	0.85 (3)	1.91 (3)	2.740 (3)	165 (3)
O3*W*—H3*W*1···O2^{v}	0.84 (3)	1.88 (3)	2.724 (3)	172 (3)
O3*W*—H3*W*2···O1^{ii}	0.84 (3)	2.05 (3)	2.863 (3)	163 (3)

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

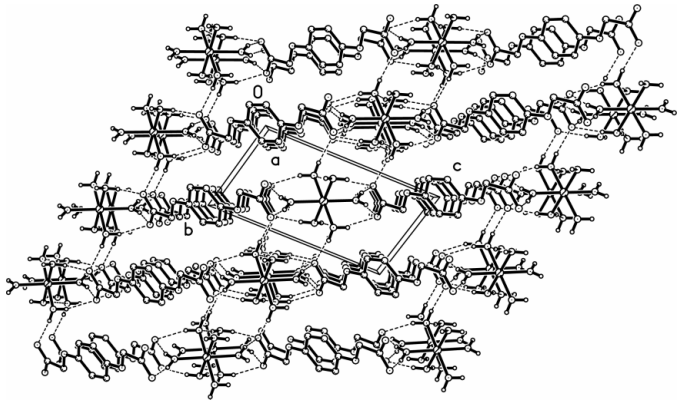


Figure 2
A packing diagram of $[Co(H_2O)_6](C_{10}H_8O_6)$. Hydrogen bonds are indicated by dashed lines.

C-bound H atoms were placed in calculated positions [C—H = 0.93 Å (aromatic) and 0.97 Å (aliphatic), and $U(H) = 1.2U_{eq}(C)$] in the riding-model approximation. The H atoms of water molecules were refined with O—H and H···H distance restraints [0.85 (1) and 1.39 (1) Å, respectively] and $U(H) = 1.5U_{eq}(O)$. The largest peak in the final difference Fourier map is 1.12 Å from atom Co1.

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: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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