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Diaquabis[2-(benzyloxy)acetato]-cobalt(II)

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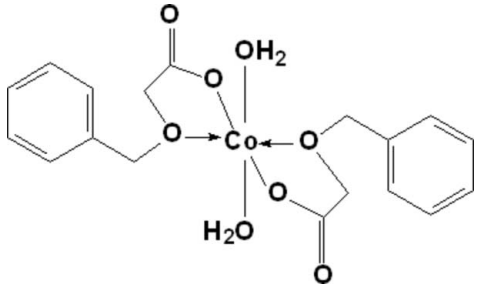
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.024; wR factor = 0.066; data-to-parameter ratio = 16.1.

In the mononuclear title complex, $[Co(C_9H_9O_3)_2(H_2O)_2]$, each Co^{II} atom is located on an inversion center and is hexacoordinated by four O atoms from two benzyloxyacetate ligands [Co—O bond lengths = 2.0487 (9) and 2.1090 (9) Å] and two water molecules [Co—O bond length = 2.0873 (9) Å] in a distorted octahedral geometry. In the crystal structure, intermolecular hydrogen bonds and π–π stacking interactions [centroid–centroid distance between phenyl rings = 3.692 (2) Å] link the molecules into a supramolecular structure.

Related literature

For the crystal structure of a similar Cu^{II} complex of benzyloxyacetate, see: Sun *et al.* (2008).



Experimental

Crystal data

$[Co(C_9H_9O_3)_2(H_2O)_2]$
M_r = 425.29
Monoclinic, $P2_1/c$
a = 11.4968 (1) Å
b = 7.1557 (1) Å
c = 12.0054 (1) Å
β = 109.708 (1)°
V = 929.80 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 296 (2) K
0.32 × 0.26 × 0.18 mm

Data collection

Bruker P4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.743, T_{max} = 0.835
7958 measured reflections
2126 independent reflections
1904 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.066
S = 1.07
2115 reflections
131 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2^{i}	0.84 (2)	1.94 (1)	2.768 (2)	169 (2)
O1W—H1W2···O2^{ii}	0.846 (9)	1.94 (1)	2.773 (1)	171 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: LX2056).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supporting information

Acta Cryst. (2008). E**64**, m890 [doi:10.1107/S1600536808016899]

Diaquabis[2-(benzyloxy)acetato]cobalt(II)

Chun-Liang Chen, Sheng-Li Sun, Chang-Sheng Gu, Weng-Dong Song and Xiao-Min Hao

S1. Comment

Recently, we have reported the crystal structure of the complex of benzyloxyacetate, $[Cu(C_9H_9O_3)_2.2(H_2O)]$, (Sun *et al.*, 2008). Here we report the crystal structure of the title mononuclear complex of benzyloxyacetate, $[Co(C_9H_9O_3)_2.2(H_2O)]$, (Fig. 1).

The structure of the title compound is similar to that of the Cu(II) complex (Sun *et al.*, 2008). The Co atom lies on an inversion center and displays an octahedral geometry defined by two carboxylate O atoms and two benzyloxy O atoms from two benzyloxyacetate ligands, and two water molecules, respectively. The Co—O and Co—Ow bond lengths are 2.0487 (9), 2.1090 (9) and 2.0873 (9) Å, respectively. The characteristic C—O(carboxylate) bond lengths suggest electron localization of the carboxylate groups of the anionic ligands. The molecular packing is stabilized by intermolecular O—H···O hydrogen bond interactions (Table 1). The crystal packing (Fig. 2) is further stabilized by aromatic π—π stacking interaction between the benzene ring from neighbouring molecules. The Cg···Cg^{ii} distance is 3.692 (2) Å (*Cg* is the centroids of the C4-C9 benzene ring, symmetry code as in Fig. 2).

S2. Experimental

The ligand, benzyloxyacetic acid was commercially available and used without further purification. The title complex was prepared by the addition of Cobalt diacetate trihydrate (2.38 g, 10 mmol) to a hot aqueous solution of benzyloxyacetic acid (1.66 g, 10 mmol); the pH was adjusted to 6 with 0.1*M* sodium hydroxide. The solution was allowed to evaporate at room temperature. Pink prismatic crystals separated from the filtered solution after several days. C&H analysis. Calc. for $C_{18}H_{22}CoO_8$: C 50.83, H 5.21%. Found: C 50.81, H 5.22%.

S3. Refinement

The H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and U_{iso}(H) = 1.2U_{eq}(C), and were refined in the riding-model approximation. The H atoms of the water molecule were was located in a difference Fourier map and refined with O—H = 0.85Å and U_{iso}(H) = 1.5U_{eq}(O).

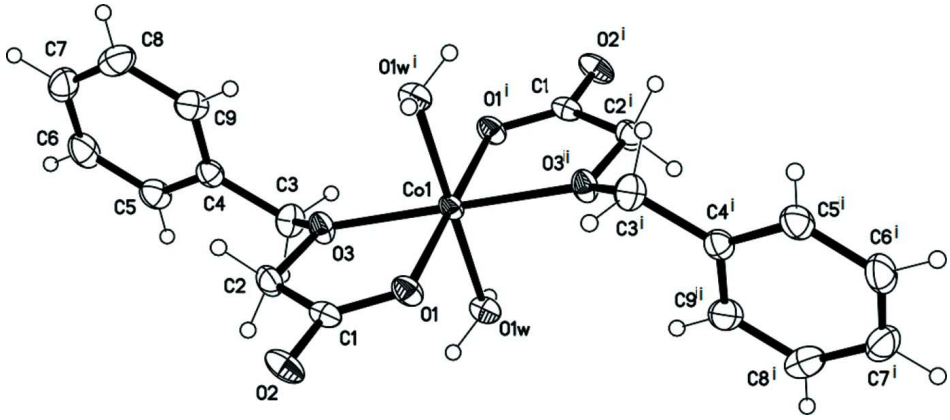

Figure 1

Molecular structure of (I) with 30% probability ellipsoids. [Symmetry code: (i) -x, -y+1, -z+1.]

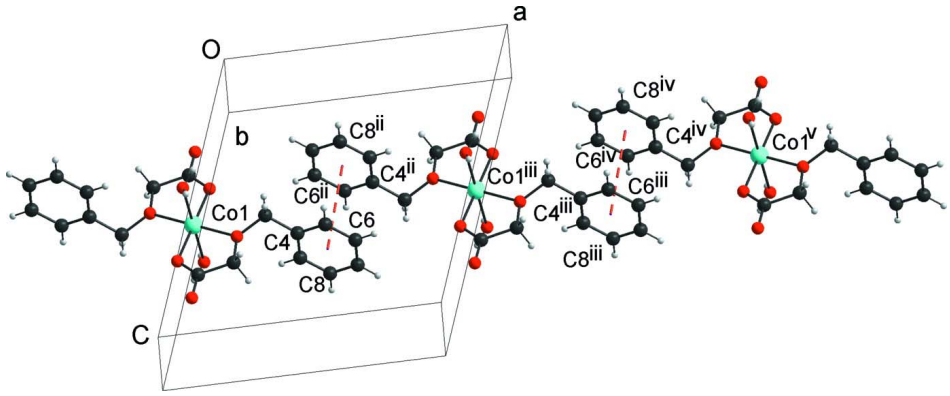

Figure 2

π—π interaction (dotted lines) in the title compound. *Cg* denotes the ring centroid. [Symmetry code: (ii) -x+1, -y+1, -z+1; (iii) x+1, y , z; (iv) -x+2, -y+1, -z+1; (v) x+2, y, z.]

Diaquabis[2-(benzyloxy)acetato]cobalt(II)

Crystal data

$[Co(C_9H_9O_3)_2(H_2O)_2]$
M_r = 425.29
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.4968 (1) Å
b = 7.1557 (1) Å
c = 12.0054 (1) Å
β = 109.708 (1)°
V = 929.80 (2) Å^3
Z = 2
$F(000)$ = 442
D_x = 1.519 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7958 reflections
θ = 1.9–27.5°
μ = 0.97 mm^{-1}
T = 296 K
Prism, pink
0.32 × 0.26 × 0.18 mm

Data collection

Bruker P4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.743, T_{max} = 0.835
7958 measured reflections

2126 independent reflections
1904 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -14 \rightarrow 14$
$k = -9 \rightarrow 8$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.066$
$S = 1.07$
2115 reflections
131 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 0.2056P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.042 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.0000	0.5000	0.5000	0.02597 (10)
O1W	−0.07843 (9)	0.62124 (13)	0.33323 (8)	0.0367 (2)
O1	−0.04160 (8)	0.73017 (12)	0.58087 (8)	0.0344 (2)
O2	0.02557 (13)	1.00099 (11)	0.66922 (10)	0.0431 (3)
O3	0.15775 (8)	0.66897 (13)	0.52873 (8)	0.0349 (2)
C1	0.03731 (12)	0.85740 (17)	0.61469 (10)	0.0309 (3)
C2	0.15726 (12)	0.83967 (19)	0.58941 (12)	0.0363 (3)
C3	0.24243 (12)	0.6638 (2)	0.46413 (12)	0.0395 (3)
C4	0.37510 (12)	0.66780 (18)	0.54400 (12)	0.0339 (3)
C5	0.46331 (15)	0.7544 (2)	0.50689 (15)	0.0433 (3)
C6	0.58642 (15)	0.7538 (2)	0.57881 (19)	0.0553 (4)
C7	0.62120 (15)	0.6693 (2)	0.68845 (17)	0.0549 (4)
C8	0.53398 (15)	0.5825 (3)	0.72509 (15)	0.0523 (4)
C9	0.41170 (14)	0.5813 (2)	0.65364 (13)	0.0433 (3)
H2A	0.1659	0.9441	0.5413	0.044*
H2B	0.2264	0.8420	0.6631	0.044*
H3A	0.2269	0.7701	0.4110	0.047*
H3B	0.2279	0.5512	0.4165	0.047*
H5	0.4400	0.8132	0.4335	0.052*
H6	0.6456	0.8105	0.5531	0.066*
H7	0.7035	0.6711	0.7373	0.066*
H8	0.5575	0.5241	0.7986	0.063*
H9	0.3533	0.5219	0.6792	0.052*
H1W1	−0.0549 (19)	0.573 (2)	0.2805 (15)	0.065*
H1W2	−0.0696 (19)	0.7387 (13)	0.3341 (17)	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02885 (15)	0.01952 (14)	0.03148 (15)	−0.00140 (8)	0.01273 (10)	−0.00332 (8)
O1W	0.0462 (5)	0.0281 (5)	0.0367 (5)	0.0011 (4)	0.0153 (4)	0.0015 (4)
O1	0.0407 (5)	0.0245 (4)	0.0436 (5)	−0.0009 (4)	0.0216 (4)	−0.0046 (4)
O2	0.0696 (7)	0.0230 (5)	0.0448 (6)	−0.0019 (4)	0.0299 (5)	−0.0070 (4)
O3	0.0326 (4)	0.0299 (5)	0.0470 (5)	−0.0057 (4)	0.0197 (4)	−0.0106 (4)
C1	0.0446 (7)	0.0220 (6)	0.0275 (5)	0.0022 (5)	0.0139 (5)	0.0011 (5)
C2	0.0383 (7)	0.0265 (6)	0.0434 (7)	−0.0058 (5)	0.0126 (6)	−0.0080 (5)
C3	0.0362 (7)	0.0477 (8)	0.0386 (7)	−0.0027 (6)	0.0178 (5)	−0.0039 (6)
C4	0.0347 (6)	0.0295 (6)	0.0409 (7)	−0.0001 (5)	0.0170 (5)	−0.0025 (5)
C5	0.0432 (7)	0.0376 (8)	0.0559 (9)	−0.0003 (6)	0.0258 (7)	0.0035 (6)
C6	0.0400 (8)	0.0425 (9)	0.0919 (13)	−0.0059 (7)	0.0333 (8)	−0.0052 (9)
C7	0.0360 (7)	0.0473 (9)	0.0726 (11)	0.0065 (7)	0.0068 (7)	−0.0131 (8)
C8	0.0505 (9)	0.0526 (10)	0.0488 (8)	0.0164 (8)	0.0101 (7)	0.0011 (7)
C9	0.0440 (8)	0.0403 (8)	0.0491 (8)	0.0040 (6)	0.0202 (6)	0.0056 (7)

Geometric parameters (Å, º)

Co1—O1	2.0487 (9)	C3—C4	1.503 (2)
Co1—O3	2.1090 (9)	C3—H3A	0.9700
Co1—O1W	2.0873 (9)	C3—H3B	0.9700
O1—C1	1.252 (2)	C4—C5	1.384 (2)
O2—C1	1.250 (2)	C4—C9	1.385 (2)
Co1—O1^{i}	2.0487 (9)	C5—C6	1.387 (2)
Co1—O3^{i}	2.1090 (9)	C5—H5	0.9300
Co1—O1W^{i}	2.0873 (9)	C6—C7	1.380 (3)
O3—C2	1.423 (2)	C6—H6	0.9300
O3—C3	1.435 (2)	C7—C8	1.372 (3)
O1W—H1W1	0.84 (2)	C7—H7	0.9300
O1W—H1W2	0.846 (9)	C8—C9	1.378 (2)
C1—C2	1.514 (2)	C8—H8	0.9300
C2—H2A	0.9700	C9—H9	0.9300
C2—H2B	0.9700		
O1—Co1—O1^{i}	180.0	C1—C2—H2B	109.7
O1—Co1—O3	77.70 (3)	C2—O3—C3	114.77 (10)
O1—Co1—O3^{i}	102.30 (3)	C2—O3—Co1	115.10 (7)
O1—Co1—O1W	91.49 (4)	C3—O3—Co1	126.84 (8)
O1—Co1—O1W^{i}	88.51 (4)	C4—C3—H3A	109.1
O3^{i}—Co1—O3	180.00 (7)	C4—C3—H3B	109.1
O1W—Co1—O3^{i}	90.68 (4)	C4—C5—C6	120.18 (15)
O1W—Co1—O3	89.32 (4)	C4—C5—H5	119.9
O1W^{i}—Co1—O1W	180.0	C4—C9—H9	119.7
Co1—O1W—H1W1	114.1 (14)	C5—C4—C9	119.03 (13)
Co1—O1W—H1W2	112.9 (13)	C5—C4—C3	119.94 (13)
O1^{i}—Co1—O3	102.30 (3)	C5—C6—H6	119.9

O1^{i}—Co1—O3^{i}	77.70 (3)	C6—C5—H5	119.9
O1^{i}—Co1—O1W^{i}	91.49 (4)	C6—C7—H7	120.1
O1^{i}—Co1—O1W	88.51 (4)	C7—C8—C9	120.38 (16)
O1W^{i}—Co1—O3^{i}	89.32 (4)	C7—C8—H8	119.8
O1W^{i}—Co1—O3	90.68 (4)	C7—C6—C5	120.12 (15)
O1—C1—C2	118.90 (11)	C7—C6—H6	119.9
O2—C1—O1	124.96 (13)	C8—C7—C6	119.76 (15)
O2—C1—C2	116.14 (12)	C8—C7—H7	120.1
O3—C2—C1	109.61 (10)	C8—C9—C4	120.52 (15)
O3—C2—H2A	109.7	C8—C9—H9	119.7
O3—C2—H2B	109.7	C9—C4—C3	121.01 (12)
O3—C3—C4	112.47 (11)	C9—C8—H8	119.8
O3—C3—H3A	109.1	H1W1—O1W—H1W2	110.4 (14)
O3—C3—H3B	109.1	H2A—C2—H2B	108.2
C1—O1—Co1	118.60 (8)	H3A—C3—H3B	107.8
C1—C2—H2A	109.7		

O1W^{i}—Co1—O1—C1	88.19 (9)	Co1—O3—C2—C1	−1.77 (13)
O1W—Co1—O1—C1	−91.81 (9)	O2—C1—C2—O3	179.19 (11)
O3^{i}—Co1—O1—C1	177.16 (9)	O1—C1—C2—O3	−0.56 (17)
O3—Co1—O1—C1	−2.84 (9)	C2—O3—C3—C4	67.25 (15)
O1—Co1—O3—C2	2.39 (9)	C1—O3—C3—C4	90.21 (17)
O1^{i}—C1—O3—C2	−177.45 (11)	O3—C3—C4—C5	−147.57 (13)
O1W^{i}—Co1—O3—C2	−85.93 (9)	O3—C3—C4—C9	34.23 (19)
O1W—Co1—O3—C2	94.07 (9)	C9—C4—C5—C6	0.1 (2)
O1—Co1—O3—C3	−155.88 (11)	C3—C4—C5—C6	−178.14 (14)
O1^{i}—Co1—O3—C3	24.12 (11)	C4—C5—C6—C7	−1.0 (2)
O1W^{i}—Co1—O3—C3	115.79 (11)	C5—C6—C7—C8	1.3 (3)
O1W—Co1—O3—C3	−64.21 (11)	C6—C7—C8—C9	−0.8 (3)
Co1—O1—C1—O2	−176.97 (10)	C7—C8—C9—C4	−0.1 (3)
Co1—O1—C1—C2	2.76 (15)	C5—C4—C9—C8	0.4 (2)
C3—O3—C2—C1	159.19 (11)	C3—C4—C9—C8	178.66 (14)

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{ii}	0.84 (2)	1.94 (1)	2.768 (2)	169 (2)
O1*W*—H1*W*2···O2^{iii}	0.85 (1)	1.94 (1)	2.773 (1)	171 (2)

Symmetry codes: (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*, −*y*+2, −*z*+1.