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Diaquabis(benzyloxyacetato)copper(II)

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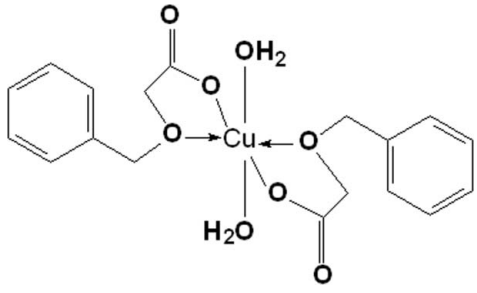
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.083; data-to-parameter ratio = 16.5.

In the title mononuclear complex, $[Cu(C_9H_9O_3)_2(H_2O)_2]$, the Cu^{II} ion, located on an inversion center, is hexacoordinated by four O atoms from two benzyloxyacetate ligands [Cu—O = 1.9420 (14) and 2.2922 (14) Å] and two water molecules [Cu—O = 2.0157 (15) Å] in a distorted octahedral geometry. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into layers parallel to the bc plane.

Related literature

For general background, see: Eddaoudi *et al.* (2005).



Experimental

Crystal data

$[Cu(C_9H_9O_3)_2(H_2O)_2]$
M_r = 429.91
Monoclinic, $P2_1/c$
a = 11.8847 (4) Å
b = 7.1509 (2) Å
c = 11.6564 (5) Å
β = 110.283 (3)°
V = 929.21 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 296 (2) K
0.32 × 0.24 × 0.18 mm

Data collection

Bruker P4/APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.711, T_{max} = 0.803
7991 measured reflections
2144 independent reflections
1606 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
S = 1.03
2144 reflections
130 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 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}	0.839 (9)	1.978 (12)	2.796 (2)	165 (2)
O1W—H1W2···O2^{ii}	0.83 (2)	1.964 (10)	2.788 (2)	173 (2)

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

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: CV2398).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m691 [doi:10.1107/S1600536808010593]

Diaquabis(benzyloxyacetato)copper(II)

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

S1. Comment

Current interests in supramolecular chemistry are rapidly expanding for their intriguing architectures and potential applications (Eddaoudi *et al.*, 2005). The organic aromatic carboxylate ligand, benzyloxyacetate, has various coordination modes and can link metal centres through carboxylate groups or/and benzyloxy group into different extended architectures. Therefore, benzyloxyacetate can be considered as a good candidate to construct various metal-organic complexes. Herein we report the crystal structure of the title mononuclear complex of benzyloxyacetate, $[Cu(C_9H_9O_3)_2(H_2O)_2]$, (I).

As illustrated in Fig. 1, the Cu^{II} ion lies on an inversion center and displays an octahedral geometry defined by four carboxylate O atoms from two different benzyloxyacetate ligands and two water molecules. The Cu—O and Cu—Ow bond lengths are 1.942 (1), 2.292 (1) and 2.016 (2) Å, respectively. The characteristic *C*—*O*(carboxylate) bond lengths suggest electron localization of the carboxylate groups of the anionic ligands. In the crystal structure, intermolecular hydrogen bonds (Table 1) give rise to a supramolecular structure.

S2. Experimental

The ligand, benzyloxyacetic acid was commercially available and used without further purification. The title complex was prepared by the addition of $Cu(Ac)_2.H_2O$ (4.00 g, 20 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. Blue prismatic crystals were separated from the filtered solution after several days. C&H analysis. Calc. for $C_{18}H_{22}CuO_8$: C 50.28, H 5.16%. Found: C 50.26, H 5.17%.

S3. Refinement

The C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and were refined in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The H atoms of the water molecule were located in a difference Fourier map and refined with bond restrint O—H = 0.84 (2) Å in the riding-model approximation, with U_{iso}(H) = 1.5U_{eq}(O).

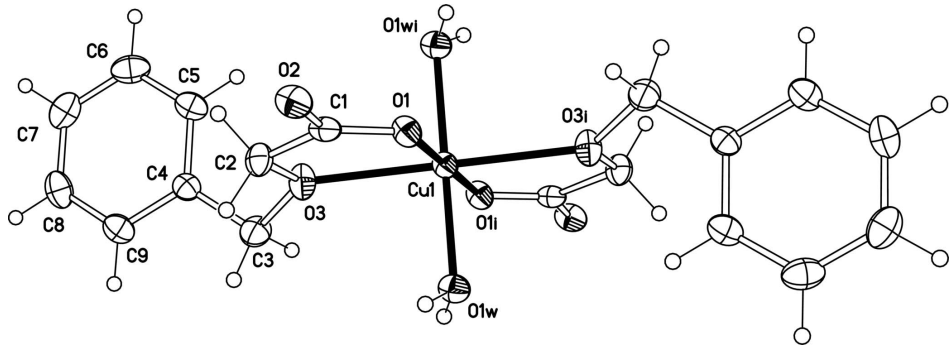

Figure 1

The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids [symmetry code: (i) -x+1, -y, -z+1].

Diaquabis(benzyloxyacetato)copper(II)

Crystal data

$[Cu(C_9H_9O_3)_2(H_2O)_2]$
M_r = 429.91
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.8847 (4) Å
b = 7.1509 (2) Å
c = 11.6564 (5) Å
β = 110.283 (3)°
V = 929.21 (6) Å^3
Z = 2
$F(000)$ = 446
D_x = 1.536 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7991 reflections
θ = 1.8–27.6°
μ = 1.22 mm^{-1}
T = 296 K
Prism, blue
0.32 × 0.24 × 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, 1996)
T_{min} = 0.711, T_{max} = 0.803
7991 measured reflections
2144 independent reflections
1606 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.6°, θ_{min} = 1.8°
h = −15→15
k = −9→8
l = −15→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
S = 1.03
2144 reflections
130 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
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.0000	0.5000	0.02860 (13)
O1	0.47417 (14)	0.2249 (2)	0.58090 (13)	0.0345 (4)
O2	0.53762 (17)	0.4957 (2)	0.67150 (14)	0.0417 (4)
O3	0.66880 (13)	0.1742 (2)	0.52517 (14)	0.0407 (4)
O1W	0.42562 (15)	0.1187 (2)	0.33393 (14)	0.0374 (4)
C1	0.5503 (2)	0.3554 (3)	0.61482 (17)	0.0325 (5)
C2	0.6644 (2)	0.3444 (3)	0.5852 (2)	0.0376 (5)
C3	0.7506 (2)	0.1723 (4)	0.4603 (2)	0.0442 (6)
C4	0.8798 (2)	0.1745 (3)	0.54208 (19)	0.0341 (5)
C5	0.9166 (2)	0.0908 (4)	0.6556 (2)	0.0427 (6)
C6	1.0355 (3)	0.0908 (4)	0.7283 (2)	0.0510 (7)
C7	1.1196 (2)	0.1751 (4)	0.6891 (2)	0.0513 (7)
C8	1.0844 (2)	0.2568 (4)	0.5758 (3)	0.0507 (7)
C9	0.9650 (2)	0.2583 (4)	0.5025 (2)	0.0430 (6)
H1W1	0.425 (2)	0.2360 (13)	0.335 (2)	0.056*
H1W2	0.457 (2)	0.075 (3)	0.286 (2)	0.056*
H2A	0.6675	0.4486	0.5331	0.045*
H2B	0.7333	0.3530	0.6601	0.045*
H3A	0.7352	0.2803	0.4067	0.053*
H3B	0.7361	0.0612	0.4094	0.053*
H5A	0.8604	0.0339	0.6833	0.051*
H6A	1.0593	0.0333	0.8045	0.061*
H7A	1.1998	0.1768	0.7392	0.062*
H8A	1.1414	0.3115	0.5482	0.061*
H9A	0.9416	0.3157	0.4262	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0348 (2)	0.0229 (2)	0.03073 (19)	−0.00185 (16)	0.01464 (16)	−0.00319 (15)
O1	0.0435 (9)	0.0261 (8)	0.0393 (8)	−0.0028 (7)	0.0212 (7)	−0.0052 (7)
O2	0.0643 (11)	0.0267 (9)	0.0400 (8)	−0.0002 (8)	0.0254 (8)	−0.0066 (7)
O1W	0.0465 (10)	0.0316 (9)	0.0357 (8)	0.0020 (8)	0.0160 (7)	0.0004 (7)
C1	0.0444 (13)	0.0287 (12)	0.0245 (9)	0.0028 (10)	0.0122 (10)	0.0021 (9)
C2	0.0400 (13)	0.0300 (13)	0.0423 (12)	−0.0057 (10)	0.0136 (11)	−0.0086 (10)
O3	0.0369 (9)	0.0375 (9)	0.0537 (9)	−0.0061 (7)	0.0234 (8)	−0.0147 (8)
C3	0.0414 (14)	0.0559 (17)	0.0389 (12)	−0.0013 (12)	0.0188 (11)	−0.0086 (11)
C4	0.0382 (12)	0.0335 (12)	0.0347 (11)	0.0017 (10)	0.0178 (10)	−0.0028 (9)
C5	0.0493 (16)	0.0419 (14)	0.0427 (12)	0.0061 (12)	0.0233 (12)	0.0054 (11)
C6	0.0590 (18)	0.0537 (17)	0.0393 (13)	0.0205 (14)	0.0158 (13)	0.0053 (12)
C7	0.0400 (14)	0.0482 (17)	0.0584 (15)	0.0070 (13)	0.0077 (13)	−0.0118 (13)
C8	0.0413 (15)	0.0456 (16)	0.0726 (18)	−0.0036 (12)	0.0289 (14)	−0.0005 (14)
C9	0.0453 (14)	0.0432 (15)	0.0459 (13)	0.0038 (11)	0.0225 (12)	0.0055 (11)

Geometric parameters (Å, º)

Cu1—O1	1.9420 (14)	C3—C4	1.500 (3)
Cu1—O3	2.2922 (14)	C3—H3A	0.9700
Cu1—O1W	2.0157 (15)	C3—H3B	0.9700
O1—C1	1.264 (3)	C4—C5	1.379 (3)
O2—C1	1.239 (2)	C4—C9	1.386 (3)
Cu1—O1^{i}	1.9420 (14)	C5—C6	1.372 (4)
Cu1—O3^{i}	2.2922 (14)	C5—H5A	0.9300
Cu1—O1W^{i}	2.0157 (15)	C6—C7	1.374 (4)
O3—C3	1.424 (2)	C6—H6A	0.9300
O1W—H1W1	0.839 (9)	C7—C8	1.370 (4)
O1W—H1W2	0.83 (2)	C7—H7A	0.9300
C1—C2	1.512 (3)	C8—C9	1.380 (4)
C2—O3	1.414 (2)	C8—H8A	0.9300
C2—H2A	0.9700	C9—H9A	0.9300
C2—H2B	0.9700		
O1^{i}—Cu1—O1	180.00 (7)	C1—C2—H2B	109.6
O1^{i}—Cu1—O3	103.51 (6)	C2—O3—C3	114.88 (17)
O1—Cu1—O3	76.49 (6)	C2—O3—Cu1	110.48 (12)
O1^{i}—Cu1—O1W	88.45 (6)	C3—O3—Cu1	130.94 (13)
O1—Cu1—O1W	91.55 (6)	C4—C3—H3A	108.9
O3—Cu1—O3^{i}	180.0	C4—C3—H3B	108.9
O1W—Cu1—O3	88.11 (6)	C4—C5—H5A	119.7
O1W^{i}—Cu1—O3	91.89 (6)	C4—C9—H9A	119.9
O1W—Cu1—O1W^{i}	180.0	C5—C4—C9	118.8 (2)
Cu1—O1W—H1W1	114.0 (18)	C5—C4—C3	121.3 (2)
Cu1—O1W—H1W2	109.5 (18)	C5—C6—C7	120.4 (2)
O1^{i}—Cu1—O3^{i}	76.49 (6)	C5—C6—H6A	119.8
O1—Cu1—O3^{i}	103.51 (6)	C6—C5—C4	120.6 (2)
O1^{i}—Cu1—O1W^{i}	91.55 (6)	C6—C5—H5A	119.7
O1—Cu1—O1W^{i}	88.45 (6)	C6—C7—H7A	120.2
O1—C1—C2	119.44 (18)	C7—C6—H6A	119.8
O2—C1—O1	123.9 (2)	C7—C8—C9	120.3 (2)
O2—C1—C2	116.6 (2)	C7—C8—H8A	119.9
O3—C2—C1	110.35 (18)	C8—C7—C6	119.6 (2)
O3—C2—H2A	109.6	C8—C7—H7A	120.2
O3—C2—H2B	109.6	C8—C9—C4	120.3 (2)
O3—C3—C4	113.51 (18)	C8—C9—H9A	119.9
O3—C3—H3A	108.9	C9—C8—H8A	119.9
O3—C3—H3B	108.9	C9—C4—C3	119.9 (2)
O1W—Cu1—O3^{i}	91.89 (6)	H1W1—O1W—H1W2	113.6 (15)
O1W^{i}—Cu1—O3^{i}	88.11 (6)	H2A—C2—H2B	108.1
C1—O1—Cu1	123.14 (13)	H3A—C3—H3B	107.7
C1—C2—H2A	109.6		
Cu1—O1—C1—O2	−176.53 (15)	O1W—Cu1—O3—C2	92.76 (14)

Cu1—O1—C1—C2	3.9 (3)	O1W^{i}—Cu1—O3—C2	−87.24 (14)
Cu1—O3—C3—C4	−134.22 (17)	O1W—Cu1—O3—C3	−63.95 (19)
O1^{i}—Cu1—O3—C2	−179.29 (13)	O1W^{i}—Cu1—O3—C3	116.05 (19)
O1—Cu1—O3—C2	0.71 (13)	C1—C2—O3—C3	161.48 (18)
O1^{i}—Cu1—O3—C3	24.0 (2)	C1—C2—O3—Cu1	0.7 (2)
O1—Cu1—O3—C3	−156.0 (2)	C2—O3—C3—C4	69.9 (3)
O1—C1—C2—O3	−2.8 (3)	C3—C4—C5—C6	178.6 (2)
O2—C1—C2—O3	177.60 (17)	C3—C4—C9—C8	−178.3 (2)
O3—Cu1—O1—C1	−2.51 (15)	C4—C5—C6—C7	0.3 (4)
O3^{i}—Cu1—O1—C1	177.49 (15)	C5—C4—C9—C8	0.2 (3)
O3—C3—C4—C5	31.9 (3)	C5—C6—C7—C8	−1.2 (4)
O3—C3—C4—C9	−149.7 (2)	C6—C7—C8—C9	1.5 (4)
O1W—Cu1—O1—C1	−90.19 (16)	C7—C8—C9—C4	−1.0 (4)
O1W^{i}—Cu1—O1—C1	89.81 (16)	C9—C4—C5—C6	0.1 (3)

Symmetry code: (i) −*x*+1, −*y*, −*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 (1)	1.98 (1)	2.796 (2)	165 (2)
O1*W*—H1*W*2···O2^{iii}	0.83 (2)	1.96 (1)	2.788 (2)	173 (2)

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