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Tetraaquabis[3-(4-carboxyphenoxy)-propionato-κO]copper(II) dihydrate

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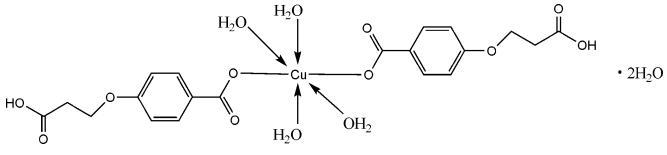
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.144; data-to-parameter ratio = 14.2.

The title compound, $[Cu(C_{10}H_9O_5)_2(H_2O)_4]\cdot 2H_2O$, is a neutral mononuclear complex. The Cu^{II} ion, which lies on an inversion center, displays an octahedral coordination geometry defined by two carboxylate O atoms of two different 3-(4-carboxyphenoxy)propionate ligands and four water molecules. The crystal structure is stabilized through strong O—H···O hydrogen bonds involving uncoordinated carboxylic acid groups, and coordinated and solvent water molecules, leading to a three-dimensional network. The O···O separations range from 2.623 (3) to 2.909 (3) Å and O—H···O angles range from 163 (4) to 179 (4)°.

Related literature

The structure of 3-(4-carboxyphenoxy)propionic acid, 3-(*p*-CPOPH$_2$), has been reported previously (Gao & Ng, 2006). In our previous work, a Co^{II} complex of 3-(*p*-CPOP) has been characterized by X-ray crystallography (Xiao *et al.*, 2006).



Experimental

Crystal data

$[Cu(C_{10}H_9O_5)_2(H_2O)_4]\cdot 2H_2O$
M_r = 589.98
Monoclinic, $P2_1/c$
a = 22.481 (5) Å
b = 10.489 (2) Å
c = 5.0315 (10) Å
β = 92.01 (3)°
V = 1185.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 295 (2) K
0.34 × 0.24 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.727, T_{max} = 0.856
18487 measured reflections
2700 independent reflections
1952 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.144
S = 1.11
2700 reflections
190 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H10···O4^{i}	0.85 (4)	1.79 (4)	2.632 (4)	176 (6)
O1W—H1W1···O2^{ii}	0.841 (17)	1.805 (13)	2.623 (3)	164 (4)
O1W—H1W2···O2W^{iii}	0.85 (4)	2.072 (11)	2.909 (3)	170 (3)
O2W—H2W1···O3W	0.85 (4)	1.95 (3)	2.798 (4)	179 (4)
O2W—H2W2···O1^{iv}	0.85 (4)	1.92 (3)	2.756 (3)	173 (3)
O3W—H3W1···O3^{ii}	0.85 (4)	2.01 (4)	2.838 (4)	163 (4)
O3W—H3W2···O3W^{v}	0.85 (4)	1.985 (15)	2.811 (2)	166 (4)

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 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: *CrystalStructure*; 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: BH2101).

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supplementary materials

Acta Cryst. (2007). E**63**, m1750 [**doi:10.1107/S1600536807023744**]

Tetraaquabis[3-(4-carboxyphenoxy)propionato-*κO*]copper(II) dihydrate

Y.-H. Xiao, L.-L. Kong and S. Gao

Comment

3-(4-Carboxyphenoxy)propionic acid acid [3-(*p*-CPOPH$_2$)] is a dicarboxylic acid with both rigid and flexible parts, and is an excellent candidate for the construction of supramolecular architectures (Gao & Ng, 2006). Recently, we have reported a dinuclear Co^{II} complex based on the 3-(4-carboxylatophenoxy)propionate ligand, 3-(*p*-CPOP), namely [Co$_2$(C$_{10}$H$_8$O$_5$)$_2$(H$_2$O)$_8$]·4H$_2$O (Xiao *et al.*, 2006).

As illustrated in Fig. 1, the title complex has a mononuclear structure, in which the 3-(4-carboxyphenoxy)propionate ligands are coordinated to the Cu atom through the carboxylate O atoms in a monodentate fashion. The Cu atom is located on an inversion center and is coordinated by two O atoms of [3-(*p*-CPOPH)]$^-$ groups and four water molecules. The Cu—O$_{carboxyl}$ bond length is 2.072 (2) Å, and the Cu—O1w and Cu—O2w bond lengths are 2.055 (2) and 2.091 (2) Å. The oxypropionate group is twisted out of the benzene plane and the C4—O3—C3—C2 torsion angle is 175.1 (3)°. A three-dimensional supramolecular network structure is formed through the extended hydrogen-bonding interactions between water molecules and 3-(4-carboxyphenoxy)propionate ligands.

Experimental

Copper(II) diacetate monohydrate (2 g, 10 mmol) was added to a hot aqueous solution of 3-(4-carboxyphenoxy)propionic acid (2.10 g, 10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 6. Blue single crystals separated from the filtered solution after several days. C, H analysis: calc. for C$_{20}$H$_{30}$O$_{16}$Cu: C 40.72, H 5.13%. Found: C 40.75, H 5.11%.

Refinement

All C-bonded H atoms were placed in calculated positions with C—H = 0.93 (aromatic CH) or 0.97 Å (methylene CH$_2$) and U_{iso}(H) = 1.2U_{eq} (carrier C). They were included in the refinement in the riding model approximation. H atoms of water molecules and carboxylic acid group were located in a difference map and refined with O—H and H···H distances restrained to 0.85 (1) and 1.39 (1) Å, respectively, and with U_{iso}(H) = 1.5U_{eq}(carrier O).

Figures

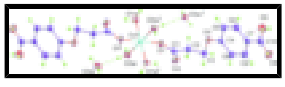


Fig. 1. Molecular structure of the title compound with displacement ellipsoids at the 30% probability level for non-H atoms. Dashed lines indicate O—H···O hydrogen bonds. Symmetry code: (i) -*x* + 1, -*y* + 1, -*z* + 1.

Tetraaquabis[3-(4-carboxyphenoxy)propionato-κ*O*]copper(II) dihydrate

Crystal data

$[Cu(C_{10}H_9O_5)_2(H_2O)_4]\cdot 2H_2O$	$F_{000} = 614$
$M_r = 589.98$	$D_x = 1.652$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 12020 reflections
$a = 22.481$ (5) Å	$\theta = 3.3$–27.5º
$b = 10.489$ (2) Å	$\mu = 1.00$ mm^{-1}
$c = 5.0315$ (10) Å	$T = 295$ (2) K
$\beta = 92.01$ (3)º	Block, blue
$V = 1185.7$ (4) Å^3	0.34 × 0.24 × 0.16 mm
$Z = 2$	

Data collection

Rigaku R-AXIS RAPID diffractometer	2700 independent reflections
Radiation source: fine-focus sealed tube	1952 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.058$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295$(2) K	$\theta_{min} = 3.3$º
ω scan	$h = -27\rightarrow28$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13\rightarrow13$
$T_{min} = 0.727$, $T_{max} = 0.856$	$l = -6\rightarrow5$
18487 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.144$	$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 1.427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
2700 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}
10 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.5000	0.5000	0.02591 (19)
O1W	0.48049 (10)	0.6638 (2)	0.2903 (5)	0.0271 (5)
H1W1	0.4445 (6)	0.670 (3)	0.329 (8)	0.041*
H1W2	0.4980 (12)	0.7350 (19)	0.306 (8)	0.041*
O2W	0.45059 (10)	0.3984 (2)	0.2108 (4)	0.0285 (5)
H2W1	0.4174 (9)	0.372 (4)	0.263 (7)	0.043*
H2W2	0.4461 (15)	0.436 (4)	0.063 (5)	0.043*
O3W	0.34049 (12)	0.3097 (3)	0.3764 (5)	0.0391 (6)
H3W1	0.3159 (17)	0.371 (3)	0.388 (7)	0.059*
H3W2	0.3470 (19)	0.276 (4)	0.527 (4)	0.059*
O1	0.57442 (10)	0.4844 (2)	0.2707 (4)	0.0267 (5)
O2	0.62831 (10)	0.3584 (3)	0.5433 (5)	0.0349 (6)
O3	0.74732 (10)	0.5110 (2)	0.4805 (5)	0.0316 (5)
O4	0.97158 (12)	0.4020 (3)	1.2501 (6)	0.0496 (7)
O5	0.94757 (13)	0.6015 (3)	1.3586 (6)	0.0532 (8)
H10	0.9724 (19)	0.601 (6)	1.489 (7)	0.080*
C1	0.62233 (14)	0.4256 (3)	0.3416 (6)	0.0248 (7)
C2	0.67492 (14)	0.4399 (3)	0.1609 (6)	0.0280 (7)
H7	0.6690	0.3842	0.0084	0.034*
H2	0.6762	0.5269	0.0961	0.034*
C3	0.73369 (14)	0.4085 (3)	0.2980 (6)	0.0281 (7)
H4	0.7310	0.3284	0.3933	0.034*
H3	0.7645	0.4009	0.1689	0.034*
C4	0.79649 (14)	0.5024 (3)	0.6474 (7)	0.0263 (7)
C5	0.83516 (15)	0.3997 (3)	0.6581 (7)	0.0311 (7)
H5	0.8293	0.3309	0.5435	0.037*
C6	0.88292 (15)	0.4003 (4)	0.8421 (7)	0.0322 (8)
H6	0.9091	0.3315	0.8497	0.039*
C7	0.89182 (15)	0.5021 (3)	1.0134 (7)	0.0303 (7)
C8	0.85372 (17)	0.6061 (4)	0.9960 (8)	0.0370 (8)
H8	0.8603	0.6760	1.1070	0.044*
C9	0.80624 (15)	0.6065 (3)	0.8157 (7)	0.0342 (8)
H9	0.7807	0.6762	0.8061	0.041*
C10	0.94073 (16)	0.5011 (4)	1.2192 (7)	0.0330 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0282 (3)	0.0251 (3)	0.0243 (3)	0.0013 (2)	−0.0005 (2)	0.0011 (2)
O1W	0.0294 (12)	0.0222 (12)	0.0296 (12)	0.0005 (9)	0.0010 (10)	0.0045 (9)
O2W	0.0295 (12)	0.0306 (13)	0.0252 (12)	−0.0029 (10)	−0.0003 (10)	0.0017 (9)
O3W	0.0416 (15)	0.0366 (15)	0.0389 (15)	0.0026 (12)	−0.0002 (12)	−0.0001 (12)
O1	0.0229 (11)	0.0348 (13)	0.0224 (11)	0.0045 (9)	−0.0006 (9)	0.0040 (9)
O2	0.0312 (13)	0.0435 (15)	0.0298 (13)	0.0054 (11)	0.0004 (10)	0.0134 (11)

O3	0.0292 (12)	0.0308 (13)	0.0341 (13)	0.0044 (10)	−0.0098 (10)	−0.0068 (10)
O4	0.0429 (15)	0.0512 (18)	0.0534 (18)	0.0084 (13)	−0.0180 (13)	−0.0014 (14)
O5	0.0532 (17)	0.0535 (19)	0.0510 (19)	−0.0015 (14)	−0.0258 (14)	−0.0071 (14)
C1	0.0278 (16)	0.0251 (16)	0.0213 (15)	−0.0016 (13)	−0.0031 (12)	−0.0041 (12)
C2	0.0270 (16)	0.0305 (18)	0.0263 (16)	0.0008 (13)	−0.0012 (13)	−0.0015 (13)
C3	0.0263 (16)	0.0302 (18)	0.0276 (17)	0.0004 (13)	−0.0015 (13)	−0.0045 (13)
C4	0.0205 (14)	0.0312 (17)	0.0267 (16)	−0.0018 (13)	−0.0042 (12)	0.0029 (13)
C5	0.0309 (17)	0.0303 (18)	0.0319 (18)	0.0007 (14)	−0.0019 (14)	−0.0031 (14)
C6	0.0274 (17)	0.0344 (19)	0.0346 (19)	0.0039 (14)	−0.0031 (14)	0.0032 (14)
C7	0.0238 (16)	0.0368 (19)	0.0300 (17)	−0.0018 (14)	−0.0029 (13)	0.0025 (14)
C8	0.0379 (19)	0.034 (2)	0.038 (2)	−0.0003 (15)	−0.0066 (15)	−0.0069 (15)
C9	0.0314 (18)	0.0292 (19)	0.041 (2)	0.0030 (14)	−0.0077 (15)	−0.0016 (15)
C10	0.0301 (17)	0.040 (2)	0.0288 (17)	−0.0027 (15)	−0.0050 (14)	0.0022 (15)

Geometric parameters (Å, °)

Cu1—O1W	2.055 (2)	O5—H10	0.85 (4)
Cu1—O1W^{i}	2.055 (2)	C1—C2	1.524 (5)
Cu1—O1^{i}	2.072 (2)	C2—C3	1.505 (4)
Cu1—O1	2.072 (2)	C2—H7	0.9700
Cu1—O2W	2.091 (2)	C2—H2	0.9700
Cu1—O2W^{i}	2.091 (2)	C3—H4	0.9700
O1W—H1W1	0.841 (10)	C3—H3	0.9700
O1W—H1W2	0.846 (10)	C4—C5	1.384 (5)
O2W—H2W1	0.85 (3)	C4—C9	1.394 (5)
O2W—H2W2	0.85 (3)	C5—C6	1.393 (5)
O3W—H3W1	0.85 (3)	C5—H5	0.9300
O3W—H3W2	0.85 (3)	C6—C7	1.382 (5)
O1—C1	1.281 (4)	C6—H6	0.9300
O2—C1	1.240 (4)	C7—C8	1.388 (5)
O3—C4	1.368 (4)	C7—C10	1.484 (5)
O3—C3	1.440 (4)	C8—C9	1.376 (5)
O4—C10	1.256 (5)	C8—H8	0.9300
O5—C10	1.272 (5)	C9—H9	0.9300
O1W—Cu1—O1W^{i}	180.0	C3—C2—H2	109.0
O1W—Cu1—O1^{i}	93.34 (9)	C1—C2—H2	109.0
O1W^{i}—Cu1—O1^{i}	86.66 (9)	H7—C2—H2	107.8
O1W—Cu1—O1	86.66 (9)	O3—C3—C2	107.0 (3)
O1W^{i}—Cu1—O1	93.34 (9)	O3—C3—H4	110.3
O1^{i}—Cu1—O1	180.0	C2—C3—H4	110.3
O1W—Cu1—O2W	88.27 (9)	O3—C3—H3	110.3
O1W^{i}—Cu1—O2W	91.73 (9)	C2—C3—H3	110.3
O1^{i}—Cu1—O2W	90.46 (9)	H4—C3—H3	108.6
O1—Cu1—O2W	89.54 (9)	O3—C4—C5	124.6 (3)
O1W—Cu1—O2W^{i}	91.73 (9)	O3—C4—C9	115.4 (3)
O1W^{i}—Cu1—O2W^{i}	88.27 (9)	C5—C4—C9	120.0 (3)

O1^{i}—Cu1—O2W^{i}	89.54 (9)	C4—C5—C6	119.4 (3)
O1—Cu1—O2W^{i}	90.46 (9)	C4—C5—H5	120.3
O2W—Cu1—O2W^{i}	180.0	C6—C5—H5	120.3
Cu1—O1W—H1W1	98 (3)	C7—C6—C5	120.6 (3)
Cu1—O1W—H1W2	127 (3)	C7—C6—H6	119.7
H1W1—O1W—H1W2	110.8 (17)	C5—C6—H6	119.7
Cu1—O2W—H2W1	114 (3)	C6—C7—C8	119.5 (3)
Cu1—O2W—H2W2	115 (3)	C6—C7—C10	121.1 (3)
H2W1—O2W—H2W2	110.3 (17)	C8—C7—C10	119.3 (3)
H3W1—O3W—H3W2	110 (4)	C9—C8—C7	120.4 (3)
C1—O1—Cu1	124.8 (2)	C9—C8—H8	119.8
C4—O3—C3	119.5 (2)	C7—C8—H8	119.8
C10—O5—H10	119 (4)	C8—C9—C4	120.0 (3)
O2—C1—O1	124.6 (3)	C8—C9—H9	120.0
O2—C1—C2	118.7 (3)	C4—C9—H9	120.0
O1—C1—C2	116.7 (3)	O4—C10—O5	124.1 (3)
C3—C2—C1	113.1 (3)	O4—C10—C7	119.0 (3)
C3—C2—H7	109.0	O5—C10—C7	116.8 (3)
C1—C2—H7	109.0		
O1W—Cu1—O1—C1	154.6 (3)	C9—C4—C5—C6	1.4 (5)
O1W^{i}—Cu1—O1—C1	−25.4 (3)	C4—C5—C6—C7	0.1 (5)
O2W—Cu1—O1—C1	−117.1 (3)	C5—C6—C7—C8	−1.9 (5)
O2W^{i}—Cu1—O1—C1	62.9 (3)	C5—C6—C7—C10	176.9 (3)
Cu1—O1—C1—O2	8.4 (5)	C6—C7—C8—C9	2.1 (6)
Cu1—O1—C1—C2	−172.1 (2)	C10—C7—C8—C9	−176.7 (3)
O2—C1—C2—C3	−20.4 (4)	C7—C8—C9—C4	−0.5 (6)
O1—C1—C2—C3	160.1 (3)	O3—C4—C9—C8	178.4 (3)
C4—O3—C3—C2	175.1 (3)	C5—C4—C9—C8	−1.2 (5)
C1—C2—C3—O3	−72.2 (3)	C6—C7—C10—O4	−5.3 (5)
C3—O3—C4—C5	−0.7 (5)	C8—C7—C10—O4	173.5 (4)
C3—O3—C4—C9	179.7 (3)	C6—C7—C10—O5	176.4 (3)
O3—C4—C5—C6	−178.2 (3)	C8—C7—C10—O5	−4.9 (5)

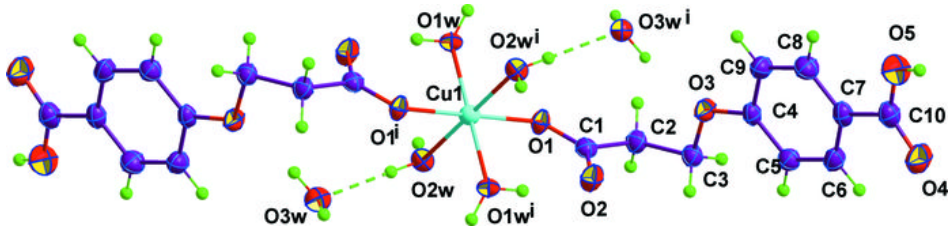
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H10···O4^{ii}	0.85 (4)	1.79 (4)	2.632 (4)	176 (6)
O1W—H1W1···O2^{i}	0.841 (17)	1.805 (13)	2.623 (3)	164 (4)
O1W—H1W2···O2W^{iii}	0.85 (4)	2.072 (11)	2.909 (3)	170 (3)
O2W—H2W1···O3W	0.85 (4)	1.95 (3)	2.798 (4)	179 (4)
O2W—H2W2···O1^{iv}	0.85 (4)	1.92 (3)	2.756 (3)	173 (3)
O3W—H3W1···O3^{i}	0.85 (4)	2.01 (4)	2.838 (4)	163 (4)
O3W—H3W2···O3W^{v}	0.85 (4)	1.985 (15)	2.811 (2)	166 (4)

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

Fig. 1


O1w
O2w^{i}
O3w^{i}
Cu1
O1^{i}
O1
C1
C2
O3
C8
C9
C4
C7
O5
C10
C5
C6
O4
C3
O2
O2w
O3w
O1w^{i}