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Poly[tetraaqua(μ_6-benzene-1,2,4,5-tetracarboxylato)dicopper(II)]

Zhang Ling

Department of Chemistry, Lishui College, 323000 Lishui, ZheJiang, People's Republic of China
Correspondence e-mail: zjlswgl@126.com

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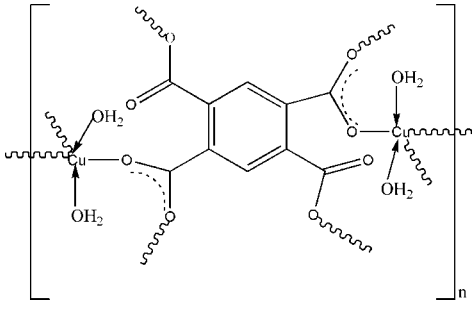
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.112; data-to-parameter ratio = 9.9.

The title compound, $[Cu_2(C_{10}H_2O_8)(H_2O)_4]_n$, is isostructural with the analogous Zn polymeric compound [Wang, Lu, Yang, Zhao & Ng (2007). *Acta Cryst.* E**63**, m2986]. Each Cu^{II} ion is coordinated by five O atoms [Cu—O = 1.968 (2)–2.268 (3) Å] in a trigonal–bipyramidal geometry. The coordinating water molecules are involved in intermolecular O—H···O hydrogen bonds [O···O = 2.726 (3)–2.767 (3) Å], which consolidate the packing.

Related literature

The crystal structure of the analogous Zn compound has been reported by Wang *et al.* (2007).



Experimental

Crystal data

$[Cu_2(C_{10}H_2O_8)(H_2O)_4]$
M_r = 224.63
Monoclinic, $P2_1/n$
a = 5.2594 (10) Å
b = 16.342 (3) Å
c = 8.1426 (15) Å
β = 97.939 (2)°
V = 693.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.14 mm^{-1}
T = 298 (2) K
0.28 × 0.19 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.474, T_{max} = 0.651
3586 measured reflections
1261 independent reflections
1181 reflections with $I > 2\sigma(I)$
R_{int} = 0.107

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.112
S = 1.05
1261 reflections
127 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.63 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3WA···O6^{i}	0.86 (3)	1.933 (17)	2.767 (3)	163 (5)
O3—H3WB···O1^{ii}	0.86 (4)	2.38 (4)	3.112 (3)	143 (5)
O3—H3WB···O2^{iii}	0.86 (4)	2.01 (4)	2.748 (3)	143 (5)
O4—H4WA···O6^{i}	0.86 (3)	1.87 (3)	2.726 (3)	173 (4)
O4—H4WB···O3^{iv}	0.86 (3)	1.89 (3)	2.744 (3)	171 (5)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2358).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m3190 [**doi:10.1107/S1600536807062198**]

Poly[tetraaqua(μ_6-benzene-1,2,4,5-tetracarboxylato)dicopper(II)]

Z. Ling

Comment

A zinc compound with 1,2,4,5-benzenetetracarboxylate was reported recently (Wang *et al.*, 2007). A slight variation of the synthesis has yielded the title compound, which features trigonal-bipyramidal copper coordination environment.

Experimental

Benzenetetracarboxylic acid (0.023 g, 0.015 mmol), CuCl2 (0.018 g, 0.013 mmol) and NaOH(0.048 mmol,0.12 mmol), were added in a mixed solvent of ethanol, the mixture was heated for ten hours under reflux, applying stirring and influx. The resultant was then filtered to give a pure solution which was infiltrated by diethyl ether freely in a closed vessel. Two weeks later several single crystals of the size suitable for X-Ray diffraction analysis were obtained.

Refinement

C-bound H atoms were placed in calculated positions [Csp^2—H = 0.93 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The water' H atoms were found in a difference map and isotropically refined using bond restraint O—H = 0.86 (3) Å.

Poly[tetraaqua(μ$_6$-benzene-1,2,4,5-tetracarboxylato)dicopper(II)]

Crystal data

$[Cu_2(C_{10}H_2O_8)(H_2O)_4]$	F_{000} = 448
M_r = 224.63	D_x = 2.153 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1261 reflections
a = 5.2594 (10) Å	θ = 2.5–25.3°
b = 16.342 (3) Å	μ = 3.14 mm^{-1}
c = 8.1426 (15) Å	T = 298 (2) K
β = 97.939 (2)°	Block, blue
V = 693.1 (2) Å^3	0.28 × 0.19 × 0.15 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	1261 independent reflections

Radiation source: fine-focus sealed tube	1181 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.107$
$T = 298(2)$ K	$\theta_{max} = 25.3°$
φ and ω scan	$\theta_{min} = 2.5°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -6\rightarrow5$
$T_{min} = 0.474$, $T_{max} = 0.651$	$k = -19\rightarrow16$
3586 measured reflections	$l = -9\rightarrow9$

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
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0794P)^2 + 0.002P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
1261 reflections	$\Delta\rho_{max} = 0.77$ e Å^{-3}
127 parameters	$\Delta\rho_{min} = -1.62$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6295 (4)	0.78499 (13)	1.0770 (3)	0.0251 (5)
O5	0.9211 (4)	0.87035 (13)	0.7881 (3)	0.0234 (5)
C4	0.8535 (5)	0.94425 (18)	0.7784 (4)	0.0185 (7)
Cu1	0.14625 (6)	0.83280 (2)	0.62933 (4)	0.0155 (3)
O2	0.4254 (4)	0.79262 (13)	0.8192 (2)	0.0224 (5)
O6	0.9316 (4)	0.99467 (13)	0.6821 (3)	0.0263 (6)
O3	−0.1623 (5)	0.86478 (15)	0.4160 (3)	0.0262 (6)
C1	0.5292 (6)	0.82451 (18)	0.9505 (4)	0.0181 (7)

O4	0.3800 (4)	0.90417 (15)	0.5221 (3)	0.0307 (6)
C5	0.6389 (6)	1.05457 (18)	0.9193 (4)	0.0192 (7)
H13	0.7321	1.0916	0.8645	0.023*
C2	0.5243 (6)	0.91568 (18)	0.9736 (3)	0.0164 (6)
C3	0.6668 (5)	0.97141 (18)	0.8918 (3)	0.0174 (6)
H3WA	−0.120 (9)	0.9099 (15)	0.372 (5)	0.061 (16)*
H4WA	0.293 (6)	0.938 (2)	0.455 (4)	0.041 (12)*
H4WB	0.515 (6)	0.888 (3)	0.482 (5)	0.062 (15)*
H3WB	−0.175 (12)	0.825 (2)	0.346 (5)	0.09 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0368 (14)	0.0178 (11)	0.0196 (11)	−0.0001 (9)	0.0002 (9)	0.0012 (9)
O5	0.0260 (12)	0.0217 (12)	0.0254 (11)	0.0056 (9)	0.0136 (9)	0.0008 (9)
C4	0.0162 (15)	0.0232 (17)	0.0174 (15)	−0.0011 (12)	0.0071 (12)	−0.0013 (12)
Cu1	0.0164 (3)	0.0160 (4)	0.0162 (4)	0.00117 (12)	0.0090 (2)	−0.00035 (12)
O2	0.0250 (12)	0.0207 (12)	0.0210 (11)	0.0012 (9)	0.0017 (9)	−0.0021 (9)
O6	0.0290 (12)	0.0264 (11)	0.0275 (13)	0.0011 (9)	0.0182 (10)	0.0047 (10)
O3	0.0278 (13)	0.0260 (13)	0.0268 (12)	−0.0019 (11)	0.0111 (9)	−0.0018 (11)
C1	0.0154 (16)	0.0213 (16)	0.0193 (18)	0.0006 (11)	0.0088 (13)	0.0004 (12)
O4	0.0217 (13)	0.0379 (14)	0.0352 (14)	0.0044 (10)	0.0134 (11)	0.0143 (11)
C5	0.0200 (15)	0.0222 (16)	0.0168 (15)	−0.0022 (12)	0.0078 (11)	0.0018 (12)
C2	0.0164 (15)	0.0190 (14)	0.0142 (14)	0.0018 (11)	0.0032 (11)	−0.0003 (12)
C3	0.0192 (15)	0.0206 (15)	0.0136 (15)	0.0020 (12)	0.0060 (11)	−0.0002 (12)

Geometric parameters (Å, °)

O1—C1	1.267 (4)	O2—C1	1.246 (4)
O1—Cu1^{i}	1.971 (2)	O3—H3WA	0.86 (3)
O5—C4	1.258 (4)	O3—H3WB	0.86 (4)
O5—Cu1^{ii}	1.968 (2)	C1—C2	1.502 (4)
C4—O6	1.245 (3)	O4—H4WA	0.86 (3)
C4—C3	1.504 (4)	O4—H4WB	0.86 (3)
Cu1—O5^{iii}	1.968 (2)	C5—C3	1.388 (4)
Cu1—O1^{iv}	1.971 (2)	C5—C2^{v}	1.393 (4)
Cu1—O4	1.983 (2)	C5—H13	0.9300
Cu1—O2	2.086 (2)	C2—C5^{v}	1.393 (4)
Cu1—O3	2.268 (3)	C2—C3	1.405 (4)
C1—O1—Cu1^{i}	132.4 (2)	Cu1—O3—H3WB	108 (4)
C4—O5—Cu1^{ii}	116.65 (19)	H3WA—O3—H3WB	112 (3)
O6—C4—O5	124.0 (3)	O2—C1—O1	124.6 (3)
O6—C4—C3	119.4 (3)	O2—C1—C2	120.6 (3)
O5—C4—C3	116.6 (3)	O1—C1—C2	114.6 (3)
O5^{iii}—Cu1—O1^{iv}	115.69 (9)	Cu1—O4—H4WA	110 (3)
O5^{iii}—Cu1—O4	124.88 (9)	Cu1—O4—H4WB	125 (3)
O1^{iv}—Cu1—O4	119.42 (10)	H4WA—O4—H4WB	111 (2)

O5^{iii}—Cu1—O2	92.13 (9)	C3—C5—C2^{v}	122.0 (3)
O1^{iv}—Cu1—O2	81.88 (9)	C3—C5—H13	119.0
O4—Cu1—O2	95.50 (10)	C2^{v}—C5—H13	119.0
O5^{iii}—Cu1—O3	89.96 (9)	C5^{v}—C2—C3	119.1 (3)
O1^{iv}—Cu1—O3	93.08 (9)	C5^{v}—C2—C1	116.5 (3)
O4—Cu1—O3	87.06 (10)	C3—C2—C1	124.4 (3)
O2—Cu1—O3	174.95 (8)	C5—C3—C2	118.9 (3)
C1—O2—Cu1	133.2 (2)	C5—C3—C4	118.7 (3)
Cu1—O3—H3WA	108 (3)	C2—C3—C4	122.4 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3WA···O6^{vi}	0.86 (3)	1.933 (17)	2.767 (3)	163 (5)
O3—H3WB···O1^{vii}	0.86 (4)	2.38 (4)	3.112 (3)	143 (5)
O3—H3WB···O2^{iv}	0.86 (4)	2.01 (4)	2.748 (3)	143 (5)
O4—H4WA···O6^{vi}	0.86 (3)	1.87 (3)	2.726 (3)	173 (4)
O4—H4WB···O3^{ii}	0.86 (3)	1.89 (3)	2.744 (3)	171 (5)

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