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μ-Succinato-bis[aquanitrato(1,10-phenanthroline)-copper(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.124
Data-to-parameter ratio = 11.5

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

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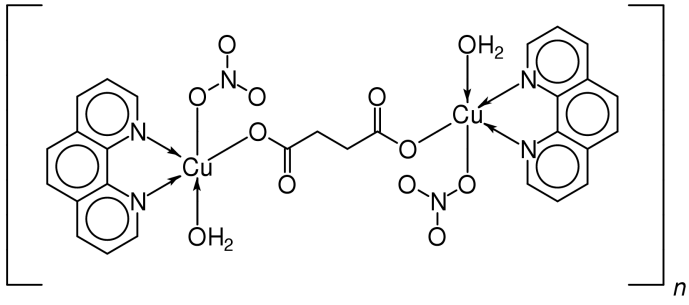
The Cu atom in the title compound, $[Cu_2(C_4H_4O_4)(NO_3)_2(C_{12}H_8N_2)_2(H_2O)_2]$, adopts an octahedral geometry that is distorted tetragonally, as seen in the copper–water [Cu—O 2.657 (4) Å] and copper–nitrate [Cu—O 2.525 (4) Å] bonds. The water molecule bridges adjacent molecules into a linear chain, and neighboring chains are linked by hydrogen bonds into a layer structure.

Comment

Copper succinate is a Lewis acid that is capable of forming complexes with nitrogen-donor ligands. For example, it has been characterized as the bis[*N*-(2-hydroxyethyl)ethylenediamine)] (Pajunen & Pajunen, 1978) and diethylenetriamine (Pajunen *et al.*, 1966) adducts, and as a decahydrated 1,10-phenanthroline adduct that cocrystallizes with copper dihydroxide (Zheng *et al.*, 2000).



(I)

Molecules of μ-succinato-bis[aquanitrato(1,10-phenanthroline)copper(II)], (I), are packed such that the water-coordinated Cu atom [$Cu—O_{water}$ = 1.984 (3) Å] at either end of the centrosymmetric molecule is water-bridged to adjacent Cu atoms [$Cu—O_{water}$ = 2.657 (4) Å] to furnish a jagged chain that runs along the *b* axis. The donor water molecule uses one of its H atoms to form an intramolecular hydrogen bond to the double-bond carbonyl O atom [O···O = 2.551 (4) Å]. The other is used to bind to the copper-bonded O atom [Cu—O = 2.525 (4) Å] of the nitrate group [$O\cdots O^{i}$ = 2.739 (5) Å; symmetry code: (i) $2-x, -y, 1-z$] to link neighboring chains into a layer structure (Fig. 1). The geometry of the Cu atom is an octahedron that is tetragonally distorted as seen in the rather long copper–water and copper–nitrate bonds.

Experimental

A solution of copper nitrate hexahydrate (0.24 g, 1 mmol) in water (5 ml) was added to a mixture of 1,10-phenanthroline (0.18 g,

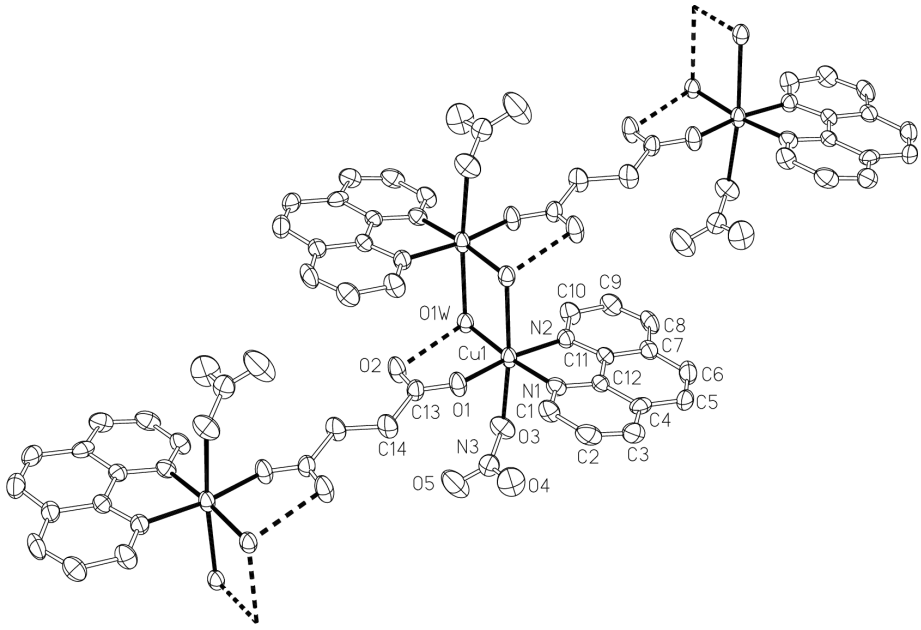


Figure 1
*ORTEP*II (Johnson, 1976) plot of the polymeric title compound at the 50% probability level. H atoms are not shown.

1 mmol) and succinic acid (0.12 g, 0.5 mmol) in a methanol–water mixture (50:50, 10 ml) to give an immediate blue solution. Blue crystals deposited from this solution after it was set aside for a week. Calculated for $C_{28}H_{24}Cu_2N_6O_{12}$: C 44.01, H 3.67, N 11.01%; found: C 43.71, H 3.95, N 10.87%.

Crystal data

$[Cu_2(C_4H_4O_4)(NO_3)_2(C_{12}H_8N_2)_2(H_2O)_2]$	$Z = 1$
$M_r = 763.61$	$D_x = 1.793$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.940$ (1) Å	Cell parameters from 22 reflections
$b = 10.351$ (2) Å	$\theta = 9$–$15°$
$c = 10.857$ (2) Å	$\mu = 1.58$ mm^{-1}
$\alpha = 69.72$ (3)°	$T = 293$ (2) K
$\beta = 81.28$ (3)°	Block, blue
$\gamma = 75.75$ (3)°	0.45 × 0.40 × 0.20 mm
$V = 707.1$ (2) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.028$
ω scans	$\theta_{max} = 25.0°$
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)	$h = -8 \rightarrow 0$
$T_{min} = 0.663$, $T_{max} = 0.728$	$k = -12 \rightarrow 11$
2711 measured reflections	$l = -12 \rightarrow 12$
2486 independent reflections	2 standard reflections
1966 reflections with $I > 2\sigma(I)$	frequency: 60 min
	intensity decay: <1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.124$	$\Delta\rho_{max} = 0.39$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.53$ e Å^{-3}
2486 reflections	
217 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.925 (3)	Cu1—O1w^i	2.657 (4)
Cu1—O3	2.525 (4)	Cu1—N1	2.012 (4)
Cu1—O1w	1.984 (3)	Cu1—N2	2.001 (4)
O1—Cu1—O3	86.4 (1)	O3—Cu1—N2	90.6 (2)
O1—Cu1—O1w	91.6 (1)	O1w—Cu1—N1	172.9 (2)
O1—Cu1—O1w^i	92.4 (1)	O1w—Cu1—N2	96.8 (2)
O1—Cu1—N1	89.8 (2)	O1w—Cu1—O1w^i	80.5 (1)
O1—Cu1—N2	171.2 (2)	O1w^i—Cu1—N1	92.5 (1)
O3—Cu1—O1w	92.5 (1)	O1w^i—Cu1—N2	91.6 (1)
O3—Cu1—O1w^i	172.8 (1)	N1—Cu1—N2	82.3 (2)
O3—Cu1—N1	94.6 (2)		

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

Data collection: *CAD*-4 *VAX*/*PC Fortran System* (Enraf–Nonius, 1988); cell refinement: *CAD*-4 *VAX*/*PC Fortran System*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); 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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References

Enraf–Nonius (1988). *CAD*-4 *VAX*/*PC Fortran System. Operator's Guide to the Enraf–Nonius CAD*-4 *Diffractometer Hardware, its Software and the Operating System*. Enraf–Nonius, Scientific Instruments Division, PO Box 483, 2600 AL Delft, The Netherlands.

Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Pajunen, A. & Pajunen, S. (1978). *Cryst. Struct. Commun.* **7**, 63–66.
Pajunen, A., Panujen, S., Kivikoski, J. & Valkonen, J. (1996). *Acta Cryst.* C**52**, 2689–2691.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Zheng, Y.-Q., Sun, J. & Lin, J.-L. (2000). *Z. Krist. New Cryst. Struct.* **215**, 533–534.