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Bis[*N*-(4-hydroxybenzyl)-D,L-alaninato]-copper(II) tetrahydrate

Ben-Yong Lou, Ying Xu, Da-Qiang Yuan, Lei Han and Mao-Chun Hong*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: loubenyong@ms.fjirsm.ac.cn

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.094
Data-to-parameter ratio = 15.1

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

The title complex has a mononuclear structure, $[Cu(C_{10}H_{12}NO_3)_2]\cdot 4H_2O$, which is a centrosymmetric unit with both D and L-sala ligands [sala = *N*-(4-hydroxybenzyl)alanine] coordinated to the Cu^{II} center. Hydrogen bonding results in a three-dimensional supramolecular structure.

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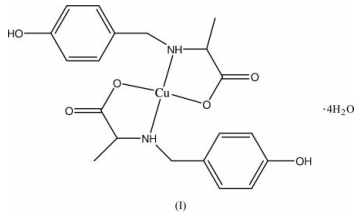
Comment

The study of copper complexes with ligands derived from amino acids has been given considerable attention (Koh *et al.*, 1996; Yang *et al.*, 2004). In our study of the preparation of copper complexes, a mononuclear compound, (I), was obtained and its synthesis and structure are reported here.



(I)

The crystallographic analysis reveals that (I) is a mononuclear unit, in which each copper ion is in an N_2O_2 four-coordinate environment with a regular square-planar geometry, as shown in Fig. 1. Both D and L-sala ligands [sala = *N*-(4-hydroxybenzyl)alanine] coordinate to the Cu^{II} center through the carboxyl O and the imine N atoms. Selected distances and angles are listed in Table 1.

The solvent water molecules form a complicated hydrogen-bonded network with the uncoordinated O atoms of carboxyl groups and phenolate O atoms, giving a three-dimensional supramolecular structure, as shown in Fig. 2.

Experimental

A mixture of *N*-(4-hydroxybenzyl)-D,L-alanine (0.040 g, 0.2 mmol) and NaOH (0.008 g, 0.2 mmol) was stirred in water (10 ml), and a solution of $CuCl_2\cdot 2H_2O$ (0.017 g, 0.1 mmol) in water (10 ml) was added. The solution was kept in air and, after several days, blue crystals were obtained in 80% yield.

Crystal data

$[Cu(C_{10}H_{12}NO_3)_2]\cdot 4H_2O$
M_r = 524.02
Monoclinic, $P2_1/c$
a = 11.5535 (19) Å
b = 9.3028 (11) Å
c = 11.6612 (19) Å
β = 110.097 (9)°
V = 1177.0 (3) Å^3
Z = 2
D_x = 1.479 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2484 reflections
θ = 3.1–27.5°
μ = 0.99 mm^{-1}
T = 173 (2) K
Prism, blue
0.15 × 0.10 × 0.05 mm

Data collection

Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.866, T_{max} = 0.952
8837 measured reflections
2603 independent reflections
2124 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°
$h = -12 \rightarrow 14$
$k = -12 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.094
S = 1.03
2603 reflections
172 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.9404 (17)	O1—C9	1.254 (3)
Cu1—N1	2.0096 (18)	O2—C9	1.262 (3)
O2—Cu1—N1	85.81 (7)	C9—O2—Cu1	115.28 (15)
O2—Cu1—N1^{i}	94.19 (7)	C8—N1—Cu1	108.66 (13)
O2^{i}—Cu1—N1^{i}	85.81 (7)	N1—C7—C4	113.7 (2)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O5^{ii}	0.83 (4)	1.80 (4)	2.611 (3)	167 (3)
O5—H7···O1^{iii}	0.76 (3)	1.96 (3)	2.714 (3)	168 (3)
O5—H10···O4^{iv}	0.82 (4)	1.83 (4)	2.639 (3)	169 (3)
O4—H4···O3^{v}	0.74 (4)	1.97 (4)	2.714 (3)	172 (4)
O4—H9···O1	0.88 (4)	1.97 (5)	2.839 (3)	168 (4)

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

The H atoms of C—H and N—H were positioned geometrically (C—H = 0.95–1.00 Å). They were constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(parent atom). The H atoms of O—H were located in difference Fourier maps.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

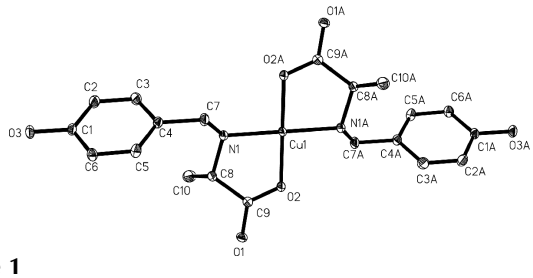


Figure 1
The structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level. The hydrogen atoms and uncoordinated water molecules have been omitted. The suffix *A* corresponds to symmetry code (i) in Table 1.

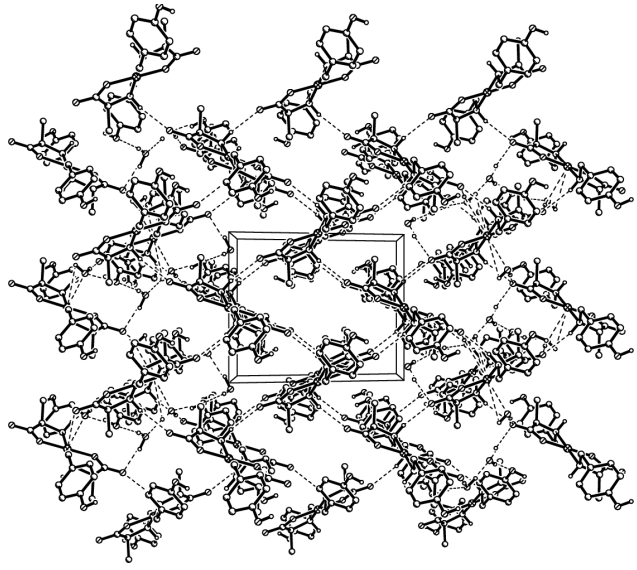


Figure 2
The three-dimensional packing of the title complex. Dashed lines indicate the hydrogen bonds.

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