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Diaqua(*N*-salicylidene-L-2-phenylglycinate-κ^3N,O,O')copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.025
wR factor = 0.046
Data-to-parameter ratio = 6.8

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

The title compound, $[Cu(C_{15}H_{11}NO_3)(H_2O)_2]$, was formed by the reaction of cupric perchlorate, L-α-phenylglycine and salicylaldehyde. Crystallographic analysis shows that the compound is a new Cu–Schiff base of an amino acid complex. The ligand chelates with Cu^{II} in a tridentate fashion. One water molecule is in this ligand plane and another is in an axial position. Extensive hydrogen-bonding interactions are present.

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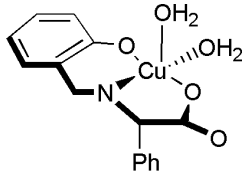
Comment

Transition metal complexes of chiral ligands attract widespread attention from the viewpoint of their structures, molecular recognition, and molecular processes (Whitesides *et al.*, 1995; Philp & Stoddart, 1996). As model systems for pyridoxal-potentiated enzymes, *N*-salicylidene-L-amino acids are being applied to synthesize a series of transition metal–chiral ligand complexes. Several *N*-salicylidene-L-amino acid–transition metal complexes have been synthesized and studied, using amino acids with different side-chain groups, such as valine (Rajak *et al.*, 1999), glutamic acid (Korhonen *et al.*, 1984), phenylalanine (Marinovich *et al.*, 1999), alanine (Warda, 1999) and methionine (Palacios *et al.*, 1989).

We report here a new Cu^{II} complex of an *N*-salicylidene-amino acid, (I), formed from copper(II), L-2-phenyl-glycine and salicylaldehyde.



(I)

The coordination of the molecule can be described as 4 + 1; each Cu^{II} ion is coordinated by the carboxylate and phenolate O atoms and amine N atom from the ligand, with bond distances of 1.950 (2), 1.932 (2) and 1.900 (2) Å, respectively, together with one water molecule at 1.960 (2) Å, forming a square-planar geometry. The axial position is occupied by another coordinated water molecule, with a Cu—O distance of 2.400 (3) Å. Except for the phenyl group, all the atoms of the organic ligand and Cu^{II} are coplanar, with an average deviation of 0.084 Å. In the crystal structure of the title compound, hydrogen-bonding interactions between the coordinated water molecules and free carboxylate and phenolate O atoms result in a two-dimensional layer structure, as shown in Fig. 2.

Experimental

A 15.0 ml methanol solution of salicylaldehyde (100 ml, 1.0 mmol) and cupric perchlorate (576 mg, 1.0 mmol) was added to a 15.0 ml suspended aqueous suspension of L-2-phenyl-glycine (150 mg, 1.0 mmol). The resulting mixture was stirred until the L-2-phenyl-glycine completely dissolved. Green prismatic single crystals of the title complex (yield 72%), suitable for X-ray diffraction analysis, were obtained by evaporation of the filtered mixture at room temperature after 6 d.

Crystal data

$[Cu(C_{15}H_{11}NO_3)(H_2O)_2]$
M_r = 352.82
Monoclinic, $P2_1$
a = 5.7870 (12) Å
b = 9.4205 (19) Å
c = 13.242 (3) Å
β = 92.81 (3)°
V = 721.0 (3) Å^3
Z = 2
D_x = 1.625 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 64 reflections
θ = 2.7–27.5°
μ = 1.54 mm^{-1}
T = 293 (2) K
Plate, green
0.40 × 0.36 × 0.16 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.565, T_{max} = 0.782
2514 measured reflections
1757 independent reflections
1509 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.5°
$h = -7 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.046
S = 0.85
1757 reflections
260 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.116
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0031 (12)
Absolute structure: Flack (1983), **xxxx** Friedel pairs **[PLEASE SUPPLY]**
Flack parameter = 0.061 (18)

Table 1
Selected geometric parameters (Å, °).

N—Cu	1.900 (2)	Cu—O5	2.400 (3)
Cu—O1	1.932 (2)	O4—H4*B*	0.81 (4)
Cu—O2	1.950 (2)	O5—H5*A*	0.75 (4)
Cu—O4	1.960 (3)	O5—H5*B*	1.13 (7)
N—Cu—O1	93.93 (10)	O2—Cu—O4	93.88 (11)
N—Cu—O2	84.43 (10)	N—Cu—O5	90.74 (10)
O1—Cu—O2	173.10 (11)	O1—Cu—O5	98.30 (11)
N—Cu—O4	174.51 (13)	O2—Cu—O5	88.44 (10)
O1—Cu—O4	87.12 (11)	O4—Cu—O5	94.45 (11)

One reflection, 001, was omitted due to extinction.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SMART* (Siemens, 1994) and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXL*97 (Siemens, 1996); software used to prepare material for publication: *SHELXL*97 (Siemens, 1996).

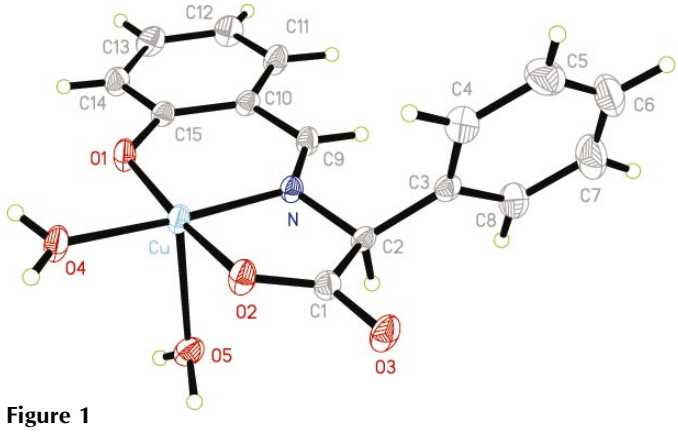


Figure 1
A displacement ellipsoid plot at the 30% probability level.

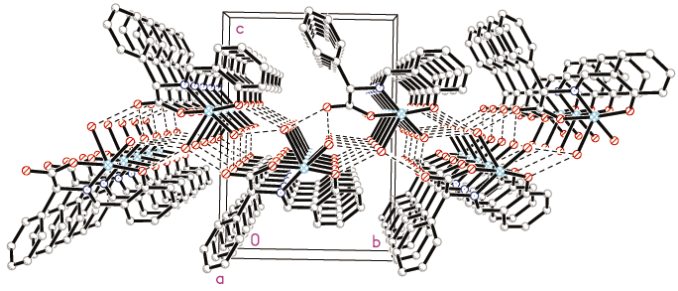


Figure 2
A view of the packing, as viewed down the *a* axis.

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