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trans-Diaquabis(*N*-acetylanthranilato-*O*,*O*′)copper(II)

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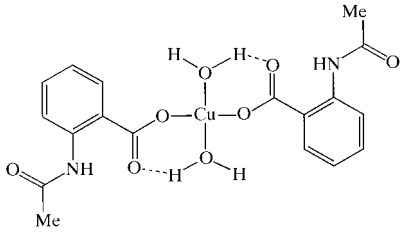
The title monomeric copper(II) complex, $[Cu(C_9H_8NO_3)_2(H_2O)_2]$, (I), shows a square-planar coordination and has an inversion centre at the Cu atom. The carboxylate group of the *N*-acetylanthranilate ion acts as a monodentate donor ligand to copper and as an acceptor of an intramolecular O—H···O hydrogen bond from the coordinated water molecule, with an O···O distance of 2.581 (2) Å.



(I)

Experimental

N-Acetylanthranilic acid (358 mg, 2.0 mmol) and $CuCO_3{\cdot}Cu(OH)_2{\cdot}H_2O$ (120 mg, 0.5 mmol) were suspended in an aqueous ethanol (1:1, 60 ml) and stirred for 3 h at 348 K. After filtration, the solution was evaporated to dryness. The green residue was dissolved in ethanol (10 ml), from which light-green crystals of (I) were grown.

Crystal data

$[Cu(C_9H_8NO_3)_2(H_2O)_2]$
M_r = 455.91
Monoclinic, $P2_1/c$
a = 5.245 (2) Å
b = 16.915 (2) Å
c = 10.461 (2) Å
β = 101.21 (2)°
V = 910.4 (4) Å^3
Z = 2
D_x = 1.663 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.6–14.9°
μ = 1.252 mm^{-1}
T = 296 K
Prism, light green
0.6 × 0.4 × 0.4 mm

Data collection

Rigaku AFC-5 diffractometer
θ–2θ scans
Absorption correction: by integration (Coppens *et al.*, 1965)
T_{min} = 0.479, T_{max} = 0.703
2918 measured reflections
2660 independent reflections
2176 reflections with $|F_o| > 3\sigma(|F_o|)$
R_{int} = 0.02
θ_{max} = 30°
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 23$
$l = -14 \rightarrow 14$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F
R = 0.052
wR = 0.058
S = 1.404
2176 reflections
133 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F) + 0.000225F^2]$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.970 (2)	O3—C15	1.285 (3)
Cu1—O5	1.952 (2)	O4—C15	1.241 (3)
O3—Cu1—O5	86.5 (1)	Cu1—O3—C15	129.2 (2)
O3—Cu1—O5^{i}	93.5 (1)	O3—C15—O4	123.6 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5B···O4^{i}	0.96	1.64	2.581 (2)	167
N6—H6···O4	0.96	1.85	2.641 (2)	138

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

The water H atoms were located in difference syntheses and the positions of the other H atoms were calculated geometrically and constrained [the C—H, N—H and O—H distances are 0.96 Å and U_{iso}(H) = 0.1 Å^2].

Data collection: *AFC/MSC Diffractometer Control System* (Rigaku Corporation, 1993); cell refinement: *AFC/MSC Diffractometer Control System* (Rigaku Corporation, 1993); data reduction: local programs; program(s) used to solve structure: *CRYSTAN-GM* (Edwards *et al.*, 1996); program(s) used to refine structure: *CRYSTAN-GM*; software used to prepare material for publication: *CRYSTAN-GM*.

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