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Bis(3-hydroxybenzoato-κO)bis(1*H*-imidazole-κN^3)-copper(II)

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Key indicators

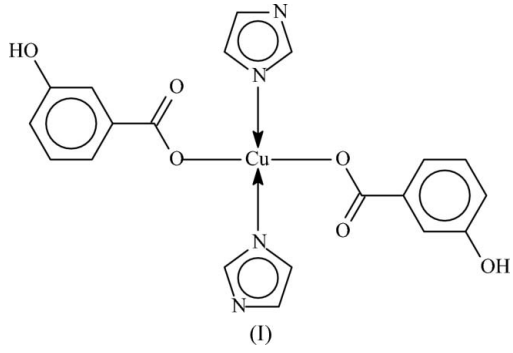
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.132
Data-to-parameter ratio = 15.2

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

The metal atom in the title compound, $[Cu(C_7H_5O_3)_2(C_3H_4N_2)_2]$, is coordinated by two O atoms (from two carboxylate anions) and two N atoms (from two *N*-heterocycles) in a square-planar geometry; it occupies a special position of site symmetry $\overline{1}$. Above and below the square are the hydroxy O atoms of adjacent molecules. This weak interaction [2.646 (2) Å] leads to the formation of a linear chain; the chains are consolidated into a layer through hydrogen bonds.

Comment

The 1:2 copper(II) bis(3-hydroxybenzoate) adduct with benzimidazole is a dihydrate having monomeric square-planar and dimeric square-pyramidal molecules within the crystal structure (Su & Xu, 2005). The use of the smaller imidazole ligand leads to the formation of the title anhydrous four-coordinate 1:2 adduct, (I). The Cu atom lies on a centre of symmetry. The geometry is distorted from square-planar towards octahedral (Table 1) as a result of the presence of the hydroxy groups of adjacent molecules; these weak interactions lead to the formation of a linear chain (Fig. 1). Adjacent chains are linked (Table 2) into layers by hydrogen bonds.



(I)

Experimental

Copper(II) acetate hydrate (4.00 g, 20 mmol), imidazole (1.36 g, 20 mmol) and 3-hydroxybenzoic acid (2.76 g, 20 mmol) were dissolved in water (50 ml). The pH of the solution was adjusted to 7 with 0.2 *M* sodium hydroxide. The solution was filtered; blue single crystals of (I) were isolated after several days.

Crystal data

$[Cu(C_7H_5O_3)_2(C_3H_4N_2)_2]$
M_r = 473.92
Monoclinic, $P2_1/c$
a = 9.299 (1) Å
b = 13.333 (1) Å
c = 8.078 (1) Å
β = 92.196 (1)°
V = 1000.80 (18) Å^3
Z = 2
D_x = 1.573 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 295 (2) K
Block, blue
0.32 × 0.22 × 0.13 mm

Data collection

Bruker APEXII area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.712, T_{max} = 0.866
6475 measured reflections
2281 independent reflections
1859 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.132
S = 1.09
2281 reflections
150 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2 + 0.451P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.978 (2)	Cu1—O1^{i}	1.980 (2)
Cu1—O1	1.980 (2)	Cu1···O3^{ii}	2.646 (2)
N1—Cu1—N1^{i}	180	N1—Cu1···O3^{ii}	88.5 (1)
N1—Cu1—O1	89.0 (1)	N1—Cu1—O3^{iii}	91.5 (1)
N1—Cu1—O1^{i}	91.1 (1)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y, z-1$; (iii) $-x+1, -y+1, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O2^{iv}	0.85 (1)	1.76 (1)	2.596 (3)	170 (4)
N2—H2N···O1^{v}	0.85 (1)	2.01 (2)	2.841 (3)	166 (4)

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

The hydroxy and amino H atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H = N—H = 0.85 (1) Å; their displacement parameters were freely refined. Other H atoms were positioned geometrically, with C—H = 0.93 Å and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; method used to solve structure: Difference Fourier synthesis, with Cu1 at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

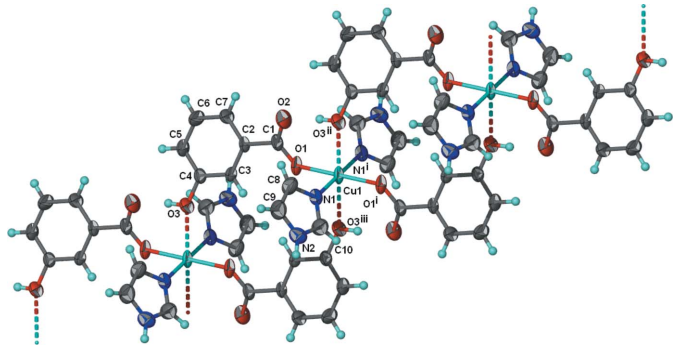


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii. Dashed lines indicate the weak interaction between Cu and the hydroxy group. Symmetry codes are given in Table 1.

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