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Aquabis(2-nitrobenzoato-κO)bis(pyridine-κN)-copper(II)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.097
Data-to-parameter ratio = 15.9

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

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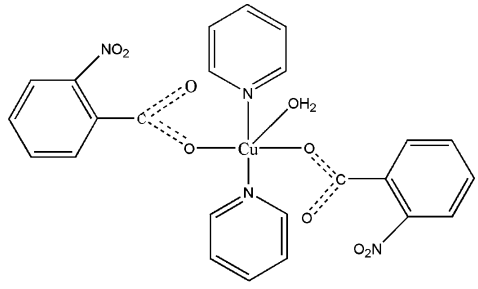
In the title complex, $[Cu(C_7H_4NO_4)_2(C_5H_5N)_2(H_2O)]$, the Cu^{II} atom has a slightly distorted square-pyramidal coordination environment, bonded to two carboxylate O atoms of two 2-nitrobenzoate ligands, two pyridine N atoms and one water O atom. O—H···O hydrogen-bonding interactions result in a chain structure.

Comment

The designed synthesis of complexes with special properties has received much attention recently (Yaghi *et al.*, 2003; Moulton & Zaworotko, 2001). The hydrothermal technique provides a powerful tool for the fabrication of such structures (Feng & Xu, 2001; Wen *et al.*, 2005). The main strategy widely used in this area is the building-block approach. In this paper, we report a new Cu^{II} complex, $[Cu(C_7H_4NO_4)_2(C_5H_5N)_2(H_2O)]$, (I), which was synthesized from 2-nitrobenzoic acid and pyridine under hydrothermal conditions.



(I)

The molecular structure of (I) is depicted in Fig. 1. The central Cu^{II} atom is five-coordinated by two carboxylate O atoms of two 2-nitrobenzoate ligands, two pyridine N atoms and one water O atom, resulting in a slightly distorted square-pyramidal coordination geometry. Two carboxylate O and two pyridine N atoms determine the basal plane, and atom Cu1 is displaced from this plane by 0.0964 (6) Å, while the water O atom occupies the apical position. The bond lengths around the Cu atom are in reasonable agreement with the values found in other Cu^{II} complexes (Cambridge Structural Database, Version 5.27, November 2005; Allen, 2002).

As shown in Fig. 2, adjacent molecules of (I) are linked *via* water-mediated hydrogen-bonding interactions to generate a one-dimensional chain propagating along the *a* axis.

Experimental

A mixture of $Cu(OH)_2$ (0.098 g, 1 mmol), 2-nitrobenzoic acid (0.335 g, 2 mmol) and distilled water (16 ml) was stirred under

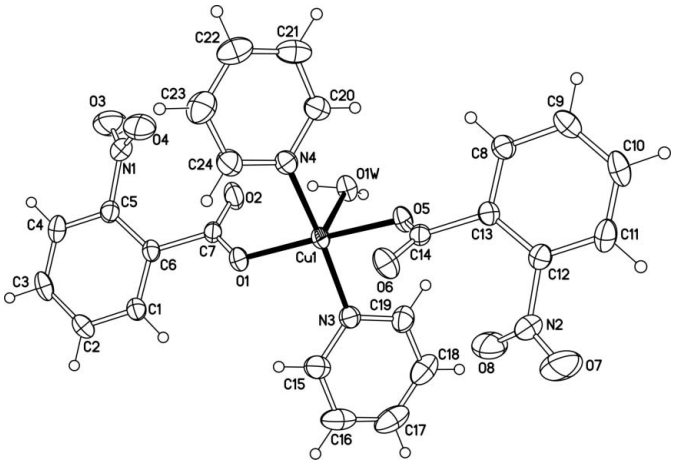


Figure 1
A view of (I), with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

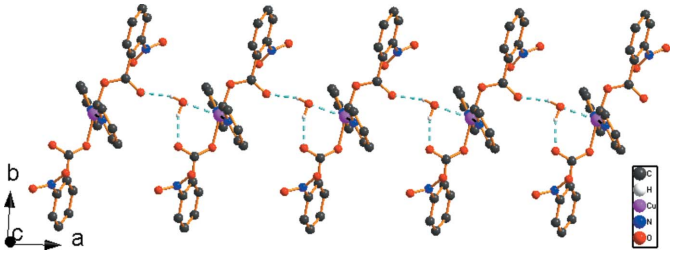


Figure 2
The one-dimensional chain structure of (I). H atoms bonded to C atoms have been omitted. Hydrogen bonds are depicted as dashed lines.

ambient conditions, and then pyridine (0.16 g, 2 mmol) was added dropwise to the suspension. The mixture was sealed in a 25 ml Teflon-lined stainless steel reactor, heated to 413 K for 60 h and then cooled to room temperature. Blue crystals of (I) were produced.

Crystal data

$[Cu(C_7H_4NO_4)_2(C_5H_5N)_2(H_2O)]$
M_r = 571.98
Triclinic, $P\overline{1}$
a = 7.4496 (15) Å
b = 10.872 (2) Å
c = 15.594 (3) Å
α = 80.14 (3)°
β = 81.45 (3)°
γ = 87.03 (3)°
V = 1230.1 (4) Å^3
Z = 2
D_x = 1.544 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 296 (2) K
Prism, blue
0.40 × 0.33 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.694, T_{max} = 0.827
12195 measured reflections
5580 independent reflections
4536 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.06
5580 reflections
351 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.1673P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O5	1.9461 (13)	Cu1—N4	2.0093 (18)
Cu1—O1	1.9647 (14)	Cu1—O1*W*	2.3700 (17)
Cu1—N3	2.0028 (17)		
O5—Cu1—O1	175.40 (6)	N3—Cu1—N4	170.68 (7)
O5—Cu1—N3	90.39 (7)	O5—Cu1—O1*W*	87.87 (6)
O1—Cu1—N3	89.64 (7)	O1—Cu1—O1*W*	96.72 (7)
O5—Cu1—N4	89.75 (7)	N3—Cu1—O1*W*	93.70 (7)
O1—Cu1—N4	89.47 (7)	N4—Cu1—O1*W*	95.62 (7)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WB*···O2	0.84 (2)	1.85 (2)	2.653 (2)	159 (3)
O1*W*—H1*WA*···O6^{i}	0.82 (2)	1.99 (2)	2.776 (2)	160 (2)

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

H atoms bonded to C atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). Water H atoms were located in a difference map and refined with distance restraints of O—H = 0.85 (2) Å and H···H = 1.30 (2) Å, with displacement parameters set to 1.5U_{eq}(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2002). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Feng, S. & Xu, R. (2001). *Acc. Chem. Res.* **34**, 239–247.
Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Wen, Y.-H., Cheng, J.-K., Feng, Y.-L., Zhang, J., Li, Z.-J. & Yao, Y.-G. (2005). *Inorg. Chim. Acta*, **358**, 3347–3354.
Yaghi, O. M., O'Keeffe, M., Ockwig, N. W., Chae, H. K., Eddaoudi, M. & Kim, J. (2003). *Nature (London)*, **423**, 705–714.