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catena-Poly[[bis(4-cyanobenzoato-κO)copper(II)]-di-μ-3-aminopyridine-$\kappa^2 N^1$:N^3;$\kappa^2 N^3$:N^1]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.057
wR factor = 0.132
Data-to-parameter ratio = 11.9

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

In the title complex, $[Cu(C_8H_4NO_2)_2(C_5H_6N_2)_2]_n$, the two crystallographically distinct Cu atoms each lie on an inversion centre and are coordinated by N atoms from four 3-aminopyridine ligands, two from the amino groups and two from the pyridine rings. The octahedral coordination about each Cu atom is completed by two carboxylate O atoms from different 4-cyanobenzoate ligands. The 3-aminopyridines serve as bridging ligands, linking adjacent Cu atoms into one-dimensional chains. In the crystal structure, weak N—H⋯O hydrogen-bonding interactions form a two-dimensional layer structure.

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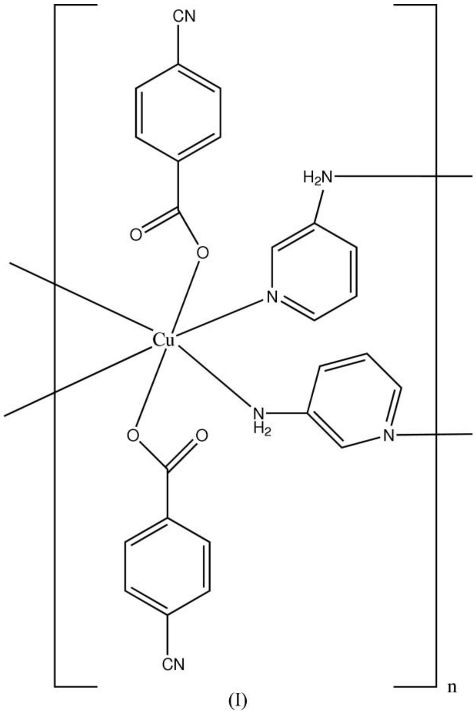
Comment

4-Cyanobenzoate metal complexes have been extensively studied in our laboratory in recent years and have provided some interesting structural assemblies (He & Zhu, 2003*a*; He *et al.*, 2003, 2005). Despite using a similar synthetic procedure to that which produced the monomeric cobalt complex diaquabis(3-aminopyridine)bis(4-cyanobenzoato)cobalt(II) dihydrate (He & Zhu, 2003*b*), we find that the copper salt yields the title coordination polymer, (I).



(I)

In the title complex, there are two crystallographically independent Cu atoms in the asymmetric unit and each lies on an inversion centre. Each Cu atom is coordinated by N atoms

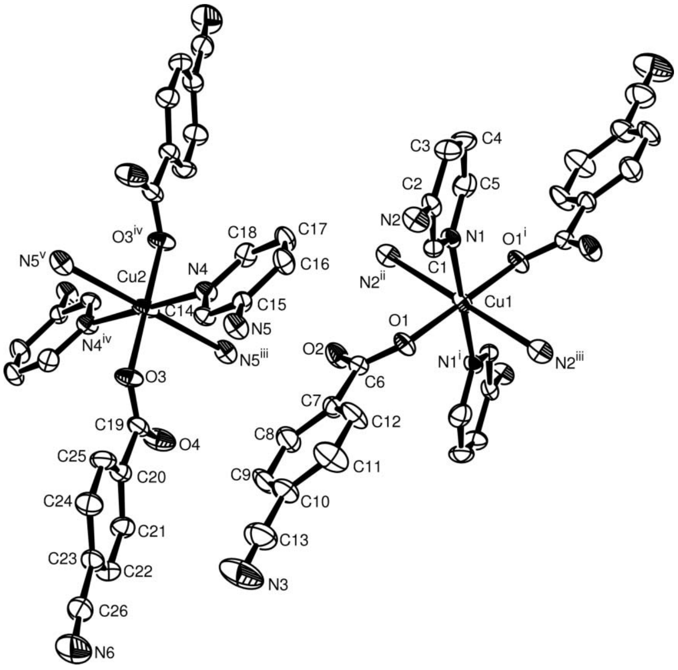


Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Symmetry codes (i): $2 - x, 1 - y, -z$; (ii): $1 + x, y, z$; (iii) $1 - x, 1 - y, -z$; (iv) $2 - x, 1 - y, 1 - z$; (v): $1 - x, 1 - y, 1 - z$.

from four 3-aminopyridine ligands, two from the amino groups and two from the pyridine rings. The octahedral coordination about each Cu is completed by two carboxylate O atoms from individual monodentate 4-cyanobenzoato ligands (Fig. 1 and Table 1). The 3-aminopyridine ligands act as μ_2-bridging ligands linking adjacent Cu1 or Cu2 atoms into approximately parallel one-dimensional chains along the *a* axis (Fig. 2). Moreover, there are intramolecular hydrogen bonds within the chains and a weak N5—H5*A*···O2 intermolecular interaction generates a two-dimensional layer structure and stabilizes the crystal packing (Table 2).

Experimental

Crystals were grown using three layers of solutions in a narrow tube. The bottom layer comprised 5 ml of water containing 0.10 mol l^{-1} $Cu(CH_3COO)_2 \cdot H_2O$, the middle layer 3 ml of CH_3OH/H_2O (1:1 *v*/*v*) solvent and the upper layer 5 ml of CH_3OH containing 0.12 mol/l 4-cyanobenzoic acid and 0.12 mol l^{-1} 3-aminopyridine. After 2 d, green plate-shaped crystals of (I) were obtained.

Crystal data

$[Cu(C_8H_4NO_2)_2(C_5H_6N_2)_2]$
$M_r = 544.02$
Triclinic, $P\overline{1}$
$a = 6.3906$ (9) Å
$b = 13.613$ (2) Å
$c = 15.466$ (3) Å
$\alpha = 63.894$ (3)°
$\beta = 81.922$ (4)°
$\gamma = 80.455$ (3)°
$V = 1188.0$ (3) Å^3
$Z = 2$
$D_x = 1.521$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 1217 reflections
$\theta = 5.3$–44.8°
$\mu = 0.97$ mm^{-1}
$T = 295$ (2) K
Plate, green
0.46 × 0.22 × 0.05 mm

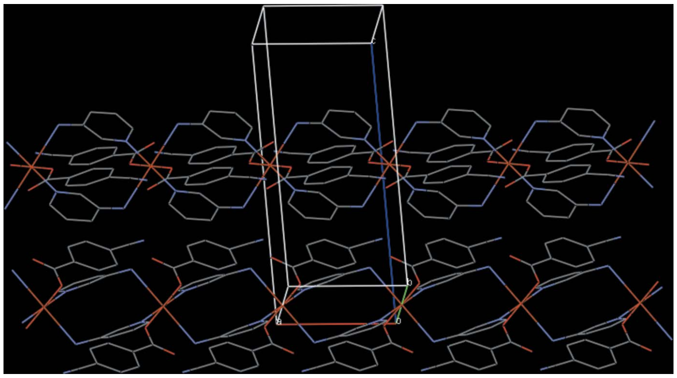


Figure 2
A view of the approximately parallel one-dimensional chains formed along the *a* axis in (I). H atoms have been omitted for clarity.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.666$, $T_{max} = 0.951$
6040 measured reflections
4151 independent reflections
2697 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 25.1°$
$h = -7 \rightarrow 7$
$k = -16 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.132$
$S = 0.98$
4151 reflections
349 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.945 (3)	Cu2—O3	1.949 (3)
Cu1—N1	2.036 (4)	Cu2—N4	2.063 (4)
Cu1—N2^{i}	2.604 (4)	Cu2—N5^{i}	2.689 (5)
O1—Cu1—N1	88.41 (14)	O3—Cu2—N4	88.82 (14)
O1^{ii}—Cu1—N1	91.59 (14)	O3^{iii}—Cu2—N4	91.18 (14)
O1—Cu1—N2^{i}	89.92 (13)	O3—Cu2—N5^{i}	93.43 (14)
O1^{ii}—Cu1—N2^{i}	90.08 (13)	O3^{iii}—Cu2—N5^{i}	86.57 (14)
N1—Cu1—N2^{i}	86.04 (14)	N4—Cu2—N5^{i}	85.57 (14)
N1^{ii}—Cu1—N2^{i}	93.96 (14)	N4^{iii}—Cu2—N5^{i}	94.43 (14)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{iv}	0.90 (4)	2.03 (2)	2.903 (5)	164 (5)
N5—H5*A*···O2^{iv}	0.89 (5)	2.26 (5)	3.122 (5)	165 (5)
N5—H5*B*···O4^{iv}	0.89 (5)	2.00 (5)	2.871 (5)	165 (5)

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

C-bound H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. N-bound H atoms were located in difference Fourier maps and refined with a distance restraint of N—H = 0.90 (1) Å with $U_{\rm iso}$(H) = 0.08 Å^2.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Bruker (2002). *SADABS* (Version 2.03), *SAINT* (Version 6.02a) and *SMART* (Version 5.618). Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

He, H.-Y., Ma, A.-Q. & Zhu, L.-G. (2003). *Acta Cryst.* E**59**, m333–m335.

He, H.-Y. & Zhu, L.-G. (2003*a*). *Acta Cryst.* E**59**, o174–o176.

He, H.-Y. & Zhu, L.-G. (2003*b*). *Acta Cryst.* E**59**, m1192–m1193.

He, H.-Y., Zhu, L.-G. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m311–m313.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.