Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[tris(pyridine-κN)copper(II)]-μ-3-carboxylatophenoxyacetato-κ^2O^3:O'] trihydrate]

Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Received 7 November 2005
Accepted 21 November 2005
Online 26 November 2005

Key indicators

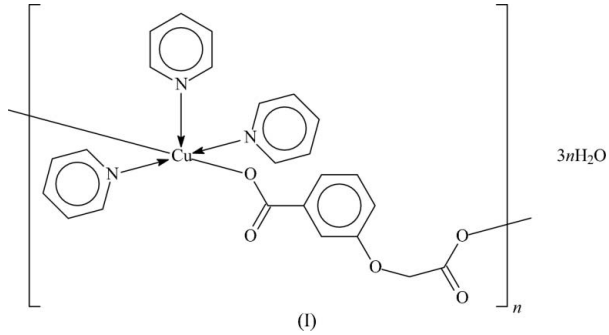
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.009 Å
R factor = 0.073
wR factor = 0.146
Data-to-parameter ratio = 17.0

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

The 3-carboxyphenoxyacetate ligand in the title compound, $[Cu(C_9H_6O_5)(C_5H_5N)_3]\cdot 3H_2O$, links adjacent tripyridinecopper(II) groups into a helical chain, which runs along the c axis of the hexagonal unit cell. The covalently bonded O atoms occupy *trans* sites in the basal plane of the square-pyramidal coordination of the Cu atom. The uncoordinated water molecules connect the chains into a three-dimensional network.

Comment

We are interested in metal complexes with carboxyphenoxyacetate because the dianion is a multidentate ligand with both rigid and flexible parts. We present here the crystal structure of the title Cu^{II} complex, (I), in which 3-carboxyphenoxyacetate plays the role of bridging ligand.



(I)

The Cu^{II} atom has a square-pyramidal coordination geometry (Fig. 1 and Table 1). The $O_2C-C_6H_4O-CH_2-CO_2$ dianion links adjacent tripyridinecopper(II) cations into a helical chain, which runs along the c axis of the hexagonal unit cell (Fig. 2). The uncoordinated water molecules connect neighboring chains into a three-dimensional network through hydrogen bonds (Table 2). In the chain, the copper shows square-pyramidal coordination, with the covalently bonded O atoms occupying *trans* sites of the basal plane.

Other $O_2CC_6H_4OCH_2-CO_2Cu$ adducts that have been characterized include the imidazole adduct, in which the ether O atom is also involved in coordination (Gao *et al.*, 2004*a*), and the benzimidazole adduct, in which the dianion functions in the μ_4-bridging mode (Gao *et al.*, 2004*b*). In this pyridine adduct, each carboxylate end of the dianion is only monodentate to copper.

Experimental

Copper dinitrate hexahydrate (1.48 g, 5 mmol) and a slight excess of pyridine (1 ml) were added to an aqueous solution of 3-carboxy-

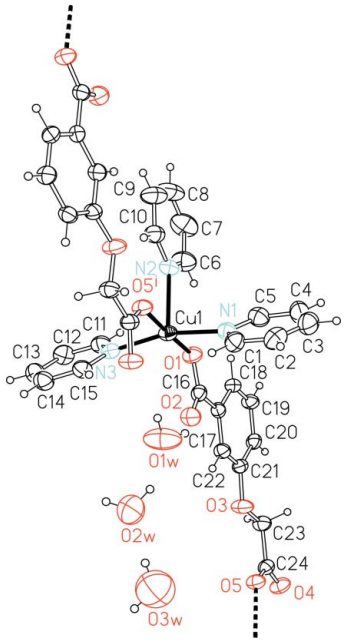


Figure 1
ORTEPII (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 30% probability level, and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1-x, -y, -\frac{1}{2}+z$.]

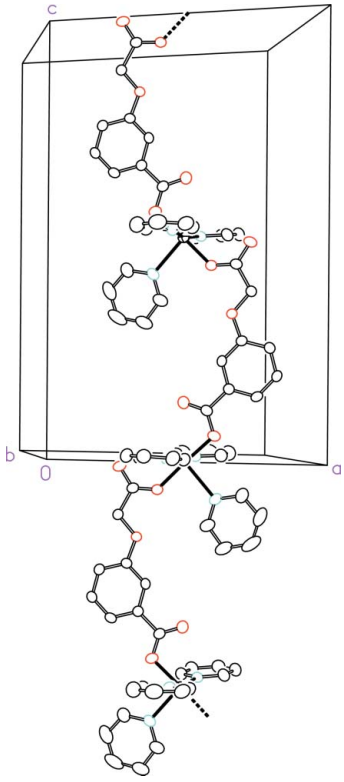


Figure 2
ORTEPII (Johnson, 1976) plot of the polymeric chain; the water molecules and H atoms are not shown.

phenoxyacetic acid (0.97 g, 5 mmol). Drops of 0.2 *M* sodium hydroxide solution were added until the pH of the solution was approximately 6. Blue block-shaped crystals of (I) were obtained after a week. Analysis calculated for $C_{24}H_{27}CuN_3O_8$: C 52.54, H 4.96, N 7.66%; found: C 52.52, H 4.98, N 6.69%.

Crystal data

$[Cu(C_9H_6O_5)(C_5H_5N)_3]\cdot 3H_2O$	Mo $K\alpha$ radiation
M_r = 549.04	Cell parameters from 26385 reflections
Hexagonal, $P6_5$	θ = 3.3–27.5°
a = 14.408 (2) Å	μ = 0.89 mm^{-1}
c = 21.630 (4) Å	T = 295 (2) K
V = 3888.6 (8) Å^3	Block, blue
Z = 6	0.37 × 0.25 × 0.19 mm
D_x = 1.407 Mg m^{-3}	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	5518 independent reflections
ω scans	4814 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.036
T_{min} = 0.591, T_{max} = 0.849	θ_{max} = 27.5°
27636 measured reflections	$h = -18 \rightarrow 18$
	$k = -18 \rightarrow 18$
	$l = -28 \rightarrow 26$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.7075P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.073	$(\Delta/\sigma)_{max}$ = 0.03
$wR(F^2)$ = 0.146	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
S = 1.24	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
5518 reflections	Absolute structure: Flack (1983), 2571 Friedel pairs
325 parameters	Flack parameter: 0.05 (2)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.952 (3)	Cu1—N2	2.332 (4)
Cu1—O5^{i}	1.951 (3)	Cu1—N3	2.055 (4)
Cu1—N1	2.057 (4)		
O1—Cu1—O5^{i}	177.5 (2)	O5^{i}—Cu1—N2	87.9 (2)
O1—Cu1—N1	89.1 (2)	O5^{i}—Cu1—N3	90.8 (1)
O1—Cu1—N2	89.7 (1)	N1—Cu1—N2	97.1 (2)
O1—Cu1—N3	89.9 (1)	N1—Cu1—N3	164.6 (2)
O5^{i}—Cu1—N1	90.8 (1)	N2—Cu1—N3	98.3 (1)

Symmetry code: (i) $-x+1, -y, z-\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O2	0.85	2.17	2.800 (6)	131
O1w—H1w2···O4^{i}	0.85	2.03	2.835 (6)	158
O2w—H2w1···O4^{ii}	0.86	2.25	2.789 (7)	121
O2w—H2*w*2···O1w	0.86	2.22	2.766 (8)	121
O3*w*—H3*w*1···O2w	0.86	1.83	2.69 (1)	170

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

C-bound H atoms were placed in calculated positions [C—H = 0.93 (aromatic) and 0.97 Å (methylene)] and included in the refinement as riding [U_{iso}(H) = 1.2U_{eq}(C)]. Water H atoms were placed in chemically sensible positions on the basis of hydrogen-bonding interactions but were not refined [U_{iso}(H) = 1.2U_{eq}(O)].

Data collection and cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku/MSC, 2002); structure solution: *SHELXS97* (Sheldrick, 1997); structure refinement : *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); publication material: *SHELXL97*.

We thank the National Natural Science Foundation of China (No. 20101003), the Scientific Fund for Remarkable

Teachers of Heilongjiang Province (No. 1054 G036) and the University of Malaya for supporting this study.

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gao, S., Gu, C.-S., Huo, L.-H., Liu, J.-W. & Zhao, J.-G. (2004*a*). *Acta Cryst.* E**60**, m1933–m1935.
Gao, S., Gu, C.-S., Huo, L.-H., Liu, J.-W. & Zhao, J.-G. (2004*b*). *Acta Cryst.* E**60**, m1936–m1938.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.