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Poly[[bis(dimethylamine)copper(II)]-μ-terephthalato]

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The title compound, $[Cu(C_8H_4O_4)(C_2H_7N)_2]_n$, is a two-dimensional coordination polymer. The Cu atom adopts a square-pyramidal coordination involving two *trans* dimethylamine molecules and three terephthalate O atoms. There are two distinct terephthalate dianions, both having inversion symmetry. One bonds to four Cu neighbours as a μ_4-bridge and one bonds to two Cu atoms as a μ_2-bridge. N—H···O hydrogen bonds complete the structure.

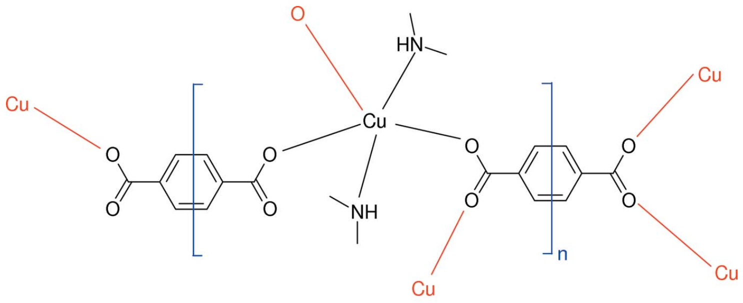
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.117
Data-to-parameter ratio = 14.4

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

Comment

This study continues our investigation of the products of solvothermal reactions of metal salts with terephthalic acid in an *N*,*N*-dimethylformamide solvent medium. Such a reaction involving manganous chloride gave $[Mn(C_8H_4O_4)(C_3H_7NO)_{0.67}]_n$ (Fu, Ren, Qiao & Ng, 2004). Reaction with cobalt(II) nitrate gave $[Co(C_8H_4O_4)(C_3H_7NO)]_n$ (Fu, Ren & Ng, 2004). Reaction with cupric(II) nitrate gave the title compound, (I), (Fig. 1), which adopts a polymeric two-dimensional layer structure.



(I)

Atom Cu1 in (I) adopts a distorted square-pyramidal coordination geometry involving two *trans* dimethylamine N atoms and three terephthalate O atoms (Table 1). The two unique terephthalate dianions are both generated by inversion symmetry from the atoms of the asymmetric unit. The C10 species bonds to four Cu neighbours as a μ_4-bridge, and the C11 molecule bonds to two Cu atoms as a μ_2-bridge (Fig. 2). Its atom O3 does not bond to Cu, and consequently this C=O bond is short. Two N—H···O hydrogen bonds (Table 2) complete the structure.

A small number of adducts of copper terephthalate have been characterized; these include the 1,10-phenanthroline (Sun *et al.*, 2000; Cano *et al.*, 1997), diethylenetriamine (Bakalbassis *et al.*, 1991) and 3-picoline (Bakalbassis *et al.*, 1992) adducts, which are complexes of ligands coordinated through their N atoms.

Experimental

Cupric nitrate (0.24 g, 1 mmol), terephthalic acid (0.40 g, 3 mmol) and dimethylformamide (10 ml) were placed in a Teflon-lined stainless steel bomb. The bomb was heated at 403 K for one month. Blue crystals of (I) were obtained on slow cooling of the bomb. CHN elemental analysis, found: C 44.9, H 5.1, N 8.3%; calculated for $C_{12}H_{18}CuN_2O_4$: C 45.3, H 5.7, N 8.8%.

Crystal data

$[Cu(C_8H_4O_4)(C_2H_7N)_2]$
$M_r = 317.83$
Monoclinic, $P2_1/c$
$a = 10.4627\ (16)$ Å
$b = 9.8602\ (14)$ Å
$c = 13.3477\ (19)$ Å
$\beta = 90.610\ (2)^\circ$
$V = 1376.9\ (3)$ Å^3
$Z = 4$
$D_x = 1.533$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.60$ mm^{-1}
$T = 298\ (2)$ K
Rod, blue
0.32 × 0.09 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.629$, $T_{\max} = 0.896$
7464 measured reflections
2532 independent reflections
1940 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 25.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.117$
$S = 1.03$
2532 reflections
176 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.2117P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.28$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.971 (2)	C10—O2	1.273 (4)
Cu1—O2	1.985 (2)	C10—O4	1.243 (4)
Cu1—O4^{i}	2.298 (2)	C11—O1	1.286 (4)
Cu1—N1	2.004 (3)	C11—O3	1.217 (4)
Cu1—N2	2.019 (3)		

Symmetry code: (i) $-x+2, -y, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2D···O4	0.91	2.19	2.974 (4)	144
N1—H1D···O3	0.91	1.94	2.777 (4)	152

H atoms were positioned geometrically, with C—H = 0.93–0.96 Å and N—H = 0.91 Å, and refined as riding, with $U_{\rm iso}(H) = 1.2U_{\rm eq}(C,N)$ or $1.5U_{\rm eq}(C_{\rm methyl})$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

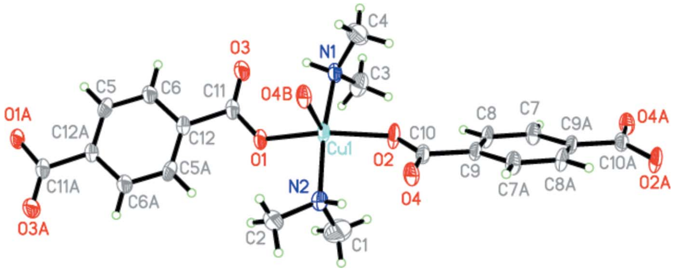


Figure 1
A view of (I), with displacement ellipsoids drawn at the 40% probability level and H atoms drawn as spheres of arbitrary radii. Atoms with the suffix A are generated by $(1-x, -y-1, -z)$ and atom O4B by $(2-x, -y, -z)$.

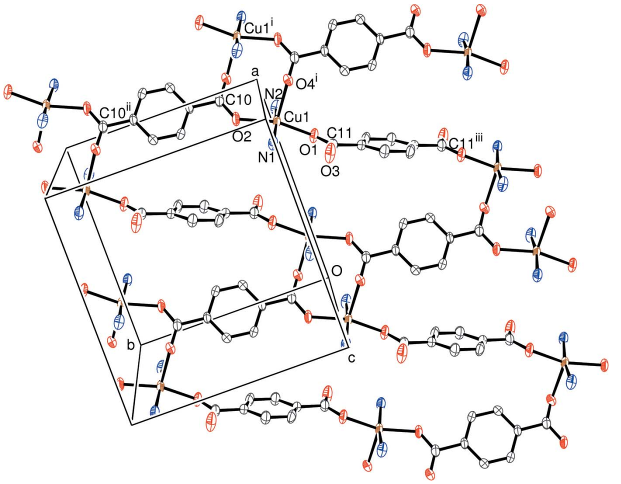


Figure 2
A view of part of an extended sheet of (I), with all H atoms and the C atoms of the dimethylamine species omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $2-x, -y, -z$; (ii) $2-x, 1-y, -z$; (iii) $1-x, 1-y, -z$.]

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m1224 Ren *et al.* • $[Cu(C_8H_4O_4)(C_2H_7N)_2]$ *Acta Cryst.* (2006). E**62**, m1223–m1224