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μ-Benzene-1,4-dicarboxylato-bis[chloro-(dipyrido[3,2-*a*:2′,3′-*c*]phenazine)copper(II)]

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In the title compound, $[Cu_2Cl_2(C_8H_4O_4)(C_{18}H_{10}N_4)_2]$, the Cu^{II} atom is four-coordinated by two N atoms from one bidentate dipyrido[3,2-*a*:2′,3′-*c*]phenazine ligand, one Cl^- anion and one O atom from the benzene-1,4-dicarboxylate ligand. The complete benzene-1,4-dicarboxylate ligand is generated by inversion symmetry, leading to a dinuclear complex. Neighbouring molecules interact through π–π stacking, resulting in a two-dimensional supramolecular structure.

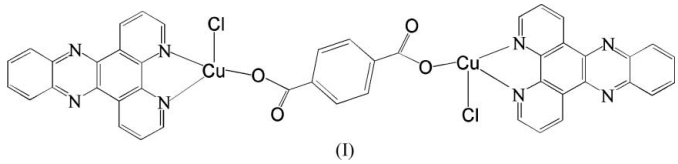
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.048
wR factor = 0.147
Data-to-parameter ratio = 15.1

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

Comment

Dipyrido[3,2-*a*:2′,3′-*c*]phenazine, $C_{18}H_{10}N_4$ (*L*), is an interesting derivative of 1,10-phenanthroline (phen). To date, the chemistry of supramolecular architectures based on *L* molecules has received little attention (Che *et al.*, 2006). As part of our ongoing studies in this area, we selected benzene-1,4-dicarboxylic acid (1,4-H_2BDC) as a linker and *L* as a secondary ligand, forming a new coordination compound, $[Cu_2Cl_2(1,4\text{-BDC})(L)_2]$, (I), which is reported here.



(I)

In compound (I), the Cu^{II} atom is four-coordinated by two N atoms from one *L* ligand, one Cl^- anion and one O atom from the 1,4-BDC dianion. An inversion centre at the 1,4-BDC ring centroid generates a dinuclear complex (Fig. 1), bridged by the 1,4-BDC ligand. The metal–ligand distances (Table 1) are normal. The different carboxylate C—O distances suggest localization of the bonding. The 1,4-BDC and *L* mean ring planes are almost perpendicular [dihedral angle = 83.29 (13)°].

Neighbouring molecules of (I) interact through π–π contacts, leading to a two-dimensional supramolecular structure (Fig. 2). The centroid-to-centroid/perpendicular distance between *L* ligands in adjacent molecules is 3.49 Å.

Experimental

Ligand *L* was synthesized according to the literature method of Dickeson & Summers (1970). A methanolic solution (4 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (8 ml) of $CuCl_2·H_2O$ (0.5 mmol) and 1,4-H_2BDC (1 mmol) with stirring. The resulting solution was filtered and allowed to stand in air at room temperature for several days, yielding blue crystals of (I) (41% yield based on Cu).

Crystal data

$[Cu_2Cl_2(C_8H_4O_4)(C_{18}H_{10}N_4)_2]$	$Z = 2$
$M_r = 926.69$	$D_x = 1.710$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.934$ (2) Å	$\mu = 1.39$ mm^{-1}
$b = 13.394$ (3) Å	$T = 292$ (2) K
$c = 14.202$ (3) Å	Block, blue
$\beta = 107.75$ (3)°	0.29 × 0.27 × 0.23 mm
$V = 1799.7$ (7) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	17350 measured reflections
	4090 independent reflections
ω scans	3015 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.043$
	$\theta_{max} = 27.5°$
$T_{min} = 0.665$, $T_{max} = 0.729$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.147$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.05$	$\Delta\rho_{max} = 1.54$ e Å^{-3}
4090 reflections	$\Delta\rho_{min} = -0.40$ e Å^{-3}
271 parameters	

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.025 (3)	Cu1—Cl1	2.2196 (11)
Cu1—N2	2.025 (3)	C19—O2	1.247 (5)
Cu1—O1	1.942 (2)	C19—O1	1.277 (4)
O1—Cu1—N1	91.96 (11)	O1—Cu1—Cl1	92.87 (8)
O1—Cu1—N2	170.38 (11)	N1—Cu1—Cl1	174.05 (8)
N1—Cu1—N2	80.66 (11)	N2—Cu1—Cl1	94.16 (8)

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron-density peak is located 2.50 Å from atom H22.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

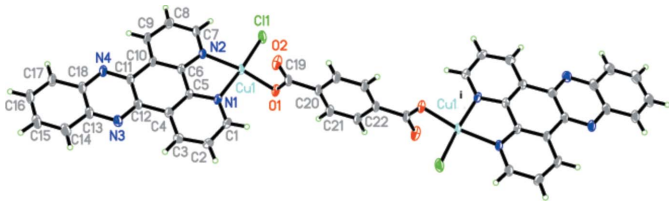


Figure 1
A view of (I), showing displacement ellipsoids at the 30% probability level and arbitrary spheres for H atoms. [Symmetry code: (i) $2 - x, -y, 1 - z$.]

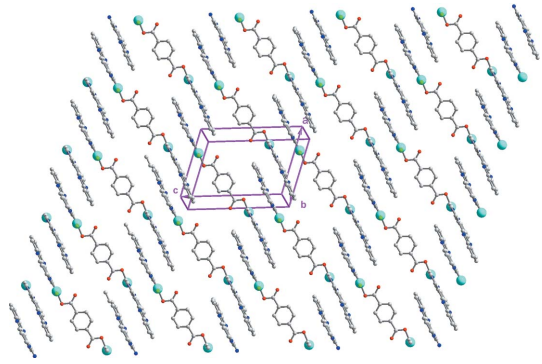


Figure 2
A view of the two-dimensional supramolecular structure of (I) arising from π–π interactions. H atoms have been omitted.

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