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The infinite one-dimensional polymer *catena*-poly[[aquabis(*p*-nitrobenzoato-κO)copper(II)]-μ-1,4-diazabicyclo[2.2.2]octane-$\kappa^2 N$:N']

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.074
wR factor = 0.164
Data-to-parameter ratio = 9.9

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

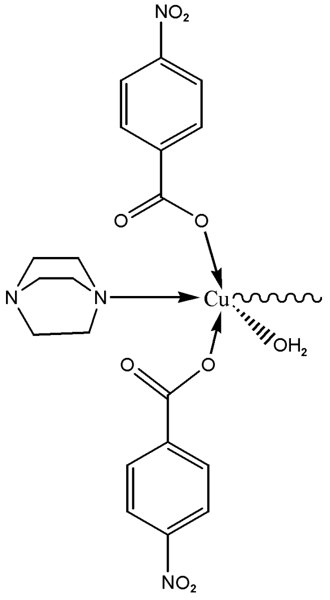
The crystal structure of the title compound, $[Cu(C_7H_4NO_4)_2(C_6H_{12}N_2)(H_2O)]_n$, contains a one-dimensional polymeric chain running along the *a* axis. Both *p*-nitrobenzoate groups are monodentate ligands and dabco (1,4-diazabicyclo[2.2.2]octane) acts as an end-to-end bridging ligand. The Cu atom has a slightly distorted square-pyramidal (SQP) coordination involving two N atoms of the dabco ligand, two O atoms from the carboxylate group of the *p*-nitrobenzoate anions and one water ligand. The point symmetry of the copper(II) polyhedron with the *p*-nitrobenzoate anion ligands is *mm*, these ligands lying on mirror planes. The chains are crosslinked by hydrogen bonds involving the coordinated water molecule to form layers parallel to (101).

Comment

In attempts to build molecular materials with interesting properties, such as catalysis, clathration, *etc*., much attention has been paid to the synthesis of one-, two- and three-dimensional structures. Rigid bridging ligands are frequently employed to construct these materials (Abrahams *et al.*, 1994; Fujita *et al.*, 1994). Triethylenediamine was selected because it is a suitable compound for the formation of coordination polymers *via* μ-N:N' coordination of two metal cations. Triethylenediamine has a very versatile coordination behaviour, since it can form bridges between metallic centres, generating varied and sometimes surprising molecular architectures (Zhu *et al.*, 2003). However, factors influencing the formation of coordination polymers are still not well understood, in spite of the fact that the self-assembly of these architectures has been documented to be highly influenced by various factors, such as the nature of the metal ions (Carlucci *et al.*, 1995), molecular templates (Tong *et al.*, 1998) and experimental conditions (Tong *et al.*, 1998). Much work is required to extend the knowledge of the relevant structural types and to establish proper synthetic strategies leading to the desired species. We report here the structure of a new copper(II)–1,4-diazabicyclo[2.2.2]octane coordination complex, (I).

The molecular structure of (I) is shown in Fig. 1 and Table 1 gives selected structural parameters. Each Cu atom has a slightly distorted square-pyramidal coordination. The square basal plane is defined by two O atoms from two *p*-nitrobenzoate anions and two 1,4-diazabicyclo[2.2.2]octane (dabco) N atoms. The Cu atom is displaced from the basal plane by 0.3164 (9) Å towards atom O1*W*. The point symmetry of the copper(II) polyhedron with the *p*-nitrobenzoate anion ligands is *mm*. These ligands lie on mirror planes. The Cu—O(*p*-nitrobenzoate) bond length is 1.962 (5) Å, and the Cu—O(H_2O) bond length is 2.254 (9) Å.

Dabco acts as a bridging ligand linking Cu atoms in an end-to-end coordination mode [N2—Cu1—N2 = 178.8 (4)°], generating almost linear chains, with a Cu···Cu separation of 6.820 (5) Å. The Cu1—N2 bond length of 2.102 (6) Å is consistent with those in related compounds [Cu—N = 2.093 (2) Å; Sieroń, 2003]. Compound (I) forms an infinite one-dimensional chain extending along the *a* axis. A two-dimensional network structure is formed *via* O—H···O interactions [O···O = 2.719 (8) Å] between the carboxylate O atoms and the coordinated water H atoms.



(I)

Experimental

All reagents and solvents were used as obtained without further purification. CuO (1 mmol, 80 mg), *p*-nitrobenzoic acid (2 mmol, 334 mg) and 1,4-diazabicyclo[2.2.2]octane (1 mmol, 112 mg) were dissolved in an aqueous ammonia solution (10 ml, 30%), and the mixture was stirred for about 20 min at room temperature. The resulting clear blue solution was kept in air and, after slow evaporation of the solvent over a period of a week, large green crystals of (I) formed at the bottom of the vessel. The crystals were isolated, washed three times with water and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 43%). Elemental analysis found: C 45.88, H 4.08, N 10.59%; calculated for $C_{20}H_{22}CuN_4O_9$: C 45.67, H 4.22, N 10.65%.

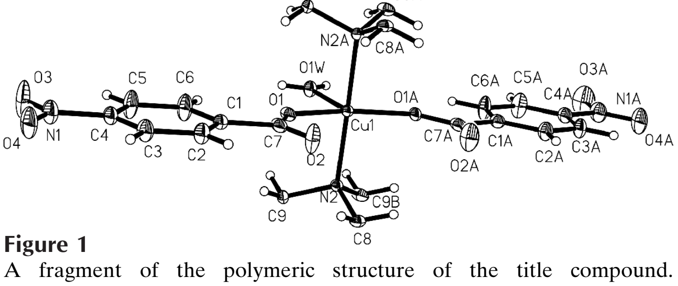


Figure 1
A fragment of the polymeric structure of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. [Symmetry codes: (*A*) $\frac{1}{2} - x$, $\frac{3}{2} - y$, z; (*B*) x, $\frac{3}{2} - y$, z; (*C*) $\frac{1}{2} - x$, y, z.]

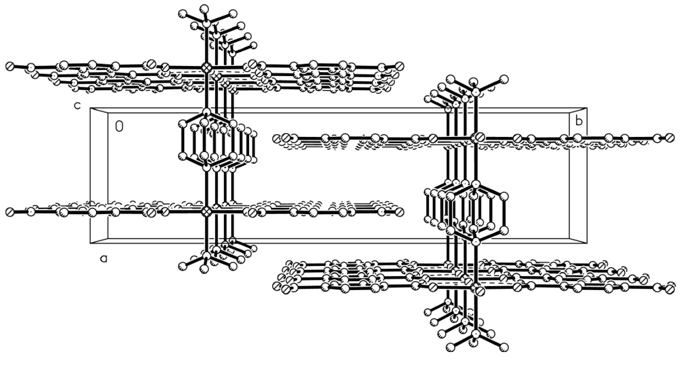


Figure 2
The crystal packing of (I), viewed along the *c* axis.

Crystal data

$[Cu(C_7H_4NO_4)_2(C_6H_{12}N_2)(H_2O)]$
$M_r = 525.96$
Orthorhombic, *Pmmn*
$a = 6.8202$ (14) Å
$b = 25.024$ (5) Å
$c = 6.1958$ (12) Å
$V = 1057.4$ (4) Å^3
$Z = 2$
$D_x = 1.652$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 1000 reflections
$\theta = 2.5$–24.4°
$\mu = 1.10$ mm^{-1}
$T = 293$ (2) K
Block, green
0.41 × 0.30 × 0.26 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.700$, $T_{max} = 0.750$
4939 measured reflections

1041 independent reflections
1000 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 7$
$k = -29 \rightarrow 29$
$l = -6 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.164$
$S = 1.38$
1041 reflections
105 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 7.5254P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2^{i}	0.78 (9)	1.94 (10)	2.722 (8)	175 (11)

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

The H atoms bonded to atoms C9, C2, C3, C5 and C6 were placed in calculated positions, with C—H distances of 0.97 or 0.96 Å and $U_{iso}(H) = 1.2U_{eq}$ of the parent atom. Atoms H8*C* and H8*B* were placed in calculated positions with $U_{iso}(H) = 1.5U_{eq}(C8)$. The C-bound H atoms were refined as riding. Atom H1*W* was found in a difference electron-density map and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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