catena-Poly[[aquachlorodimethylformamide-copper(II)]-μ-chloro]

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In the title complex, $[CuCl_2(C_3H_7NO)(H_2O)]_n$, each Cu^{II} atom is in a Cl$_3$O$_2$ five-coordinate environment with a slightly distorted square-pyramidal geometry. Cu atoms are linked by μ_2-Cl ions, resulting in a one-dimensional linear chain structure. In the crystal structure, intermolecular O—H···Cl hydrogen bonds link adjacent chains to form a two-dimensional network.

Comment

One strategy in the design and synthesis of coordination architectures is the building-block approach (Evans & Lin, 2002; Moulton & Zaworotko, 2001; Wen *et al.*, 2005). In our current work, we have selected the multifunctional 3,5-dihydroxybenzoic acid ligand as the main building block to construct coordination compounds. The title complex, (I), was obtained unexpectedly during an attempt to react 3,5-dihydroxybenzoic acid with CuCl$_2$ in an *N,N'*-dimethylformamide (DMF)–water mixture.
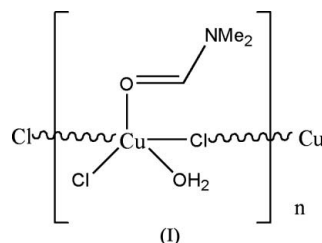

The molecular structure of (I) consists of linear chains formed *via* μ_2-Cl ligands bridging five-coordinate Cu^{II} atoms (Fig. 2). As shown in Fig. 1, the Cu^{II} atom has a slightly distorted square-pyramidal geometry, coordinated by three Cl$^-$ ions, one water molecule and one donor O atom from a DMF ligand. Selected bond lengths and angles are given in Table 1. Atoms O1, O1*W*, Cl1 and Cl2 define a square plane, and atom Cl2^i [symmetry code: (i) $x, \frac{3}{2} - y, -\frac{1}{2} - z$] occupies the apical position. The μ_2-Cl ions function as spacers between Cu^{II} atoms, with a Cu···Cu separation of 3.768 (1) Å. In the crystal structure, O—H···Cl hydrogen bonds involving water molecules and Cl$^-$ ions link adjacent chains into a two-dimensional network (Table 2 and Fig. 3).

Experimental

The title compound was prepared by mixing DMF–water (1:1 *v/v*, 20 ml) solutions of CuCl$_2$ (1 mmol) and 3,5-dihydroxybenzoic acid (1 mmol), and stirring at 353 K for 2 h. The reaction mixture was filtered and green single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after 7 d.
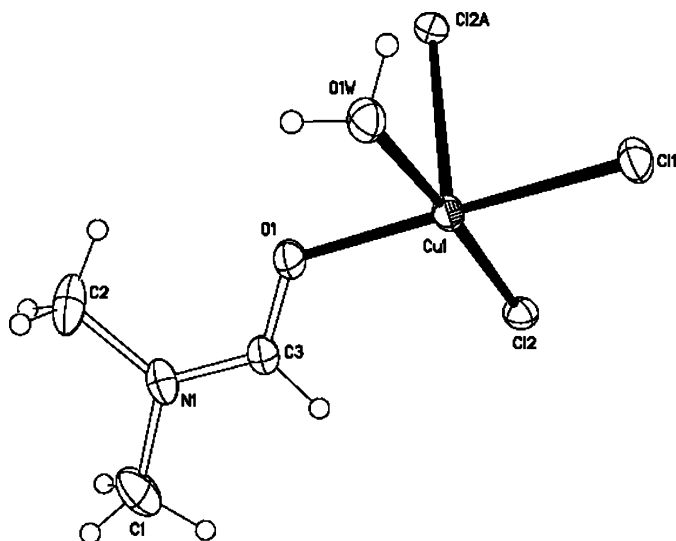
Figure 1
A view of a segment of the polymeric structure of (I), showing 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii [symmetry code: (A) $x, \frac{3}{2} - y, -\frac{1}{2} + z$].
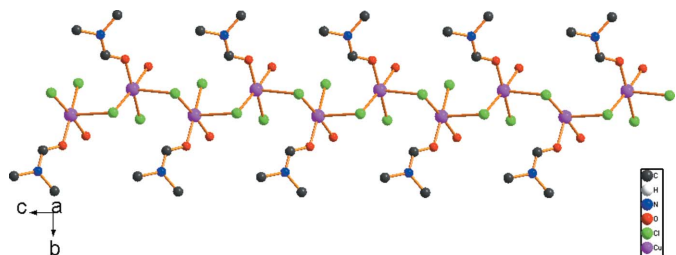
Figure 2
The one-dimensional chain structure of (I), with H atoms omitted.

Crystal data

$[CuCl_2(C_3H_7NO)(H_2O)]$
$M_r = 225.55$
Monoclinic, $P2_1/c$
$a = 9.2638\ (7)$ Å
$b = 12.5066\ (9)$ Å
$c = 6.9493\ (5)$ Å
$\beta = 98.0030\ (10)°$
$V = 797.29\ (10)$ Å^3

$Z = 4$
$D_x = 1.879$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.34$ mm^{-1}
$T = 273\ (2)$ K
Prism, green
$0.30 \times 0.28 \times 0.20$ mm

Data collection

Bruker APEX-II area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.382$, $T_{max} = 0.513$

5213 measured reflections
1885 independent reflections
1626 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.048$
$S = 1.05$
1885 reflections
90 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.1571P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
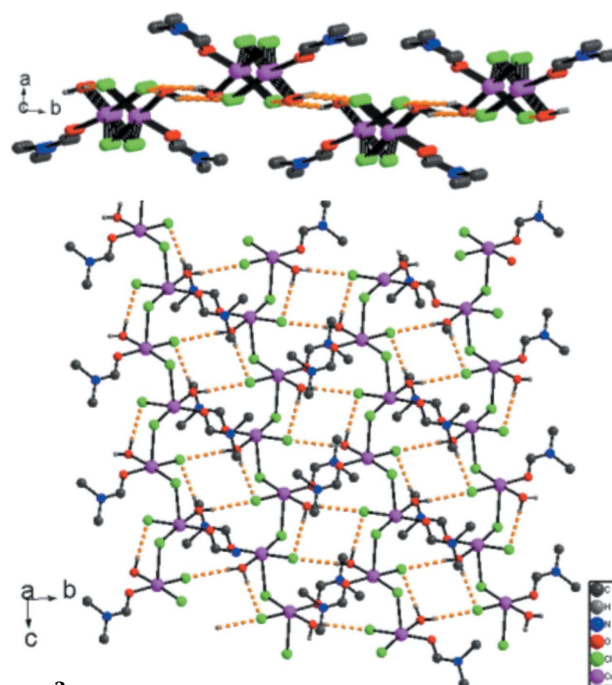
Figure 3
The packing of (I), viewed along two directions. Hydrogen bonds are depicted as dashed lines.

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9598 (11)	Cu1—Cl1	2.2970 (4)
Cu1—O1*W*	2.0028 (12)	Cu1—Cl2^i	2.6963 (5)
Cu1—Cl2	2.2529 (4)		
O1—Cu1—O1*W*	82.92 (5)	O1—Cu1—Cl2^i	92.70 (4)
O1—Cu1—Cl2	94.15 (4)	O1*W*—Cu1—Cl2^i	88.64 (4)
O1*W*—Cu1—Cl2	175.95 (4)	Cl2—Cu1—Cl2^i	94.299 (16)
O1—Cu1—Cl1	167.54 (4)	Cl1—Cu1—Cl2^i	94.964 (16)
O1*W*—Cu1—Cl1	87.45 (4)	Cu1—Cl2—Cu1^{ii}	98.777 (17)
Cl2—Cu1—Cl1	95.060 (17)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1*W*—H1*WA*$\cdots$Cl1^i	0.83 (1)	2.37 (1)	3.1907 (14)	178 (2)
O1*W*—H1*WB*$\cdots$Cl1^{iii}	0.81 (1)	2.59 (2)	3.3411 (13)	156 (2)

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

H atoms bonded to C atoms were positioned geometrically and included in the refinement in the riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C)] and methyl groups were allowed to rotate to fit the electron density [C—H = 0.96 Å and U_{iso}(H) = $1.5U_{eq}$(C)]. Water H atoms were located and refined with distance restraints of O—H = 0.85 (2) Å and H$\cdots$H = 1.30 (2) Å, with displacement parameters set at $1.5U_{eq}$(O).

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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