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Poly[aquadi-μ_3-dicyanamido-di-μ_2-dicyanamido-dicopper(II)]

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Key indicators

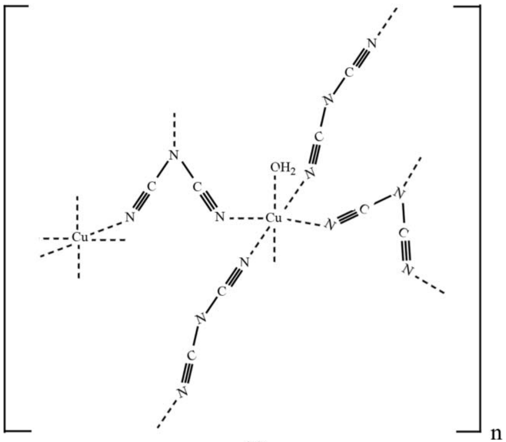
Single-crystal X-ray study
T = 100 K
Mean σ(N–C) = 0.002 Å
R factor = 0.017
wR factor = 0.047
Data-to-parameter ratio = 17.8

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

The asymmetric unit of the title compound, $[Cu_2(C_2N_3)_4(H_2O)]_n$, contains two Cu atoms with CuN_6 and CuN_4O_2 chromophores. The Cu atoms lie on inversion centres and the aqua ligands on a crystallographic twofold rotation axis. Two dicyanamide ligands link the metal ions into an infinite three-dimensional structure.

Comment

Transition metal complexes of dicyanamide anions form one-, two- and three-dimensional coordination compounds with interesting magnetic properties (Armentano *et al.*, 2006; Van Albada *et al.*, 2006; Miller, 2006; Zeng *et al.*, 2006).



(I)

The asymmetric unit of the title compound, (I) (Fig. 1), contains two Cu atoms and a water molecule in special positions, and two dicyanamide ligands. The Cu atoms lie on inversion centres and the aqua ligands on a crystallographic twofold rotation axis. Both Cu atoms are hexacoordinated, Cu1 by four N donor atoms in the equatorial plane [1.976 (1) and 2.017 (1) Å] and two water O atoms [2.390 (1) Å], and Cu12 by six N donor atoms [1.974 (1), 1.972 (1) and 2.565 (1) Å]. One of the dicyanamide anions is triply coordinating through its three N atoms. The other organic ligand bridges two metal ions through the terminal N atoms, while the central N atom acts as an acceptor of one water H atom (Table 1, Fig. 2). Along the c axis, there are chains of metal ions bridged by the O atoms of the water molecules, with $Cu\cdots Cu^i$ distances of 4.4064 (2) Å [symmetry code: (i) $1 - x, y, \frac{1}{2} - z$]. Overall, the organic ligands assemble into an infinite three-dimensional metal–organic framework.

A similar compound has been reported by Kurmoo & Kepert (1998). In that case, the dicyanamide anion is triply

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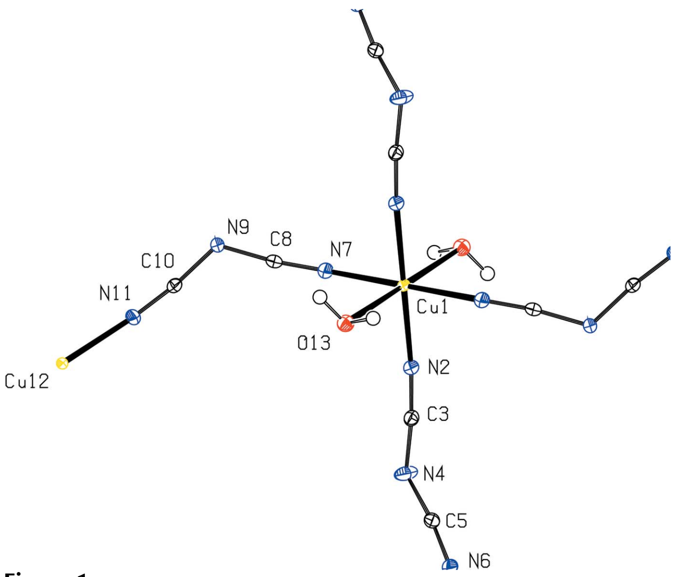

Figure 1
Part of the polymeric structure of (I), with the numbering scheme of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator ($-x$, $-y$, $-z$).

coordinating, bridging the metal ions in an infinite three-dimensional metal–organic framework with a rutile-type structure.

Experimental

A solution of $CuSO_4 \cdot 5H_2O$ (1.0 mmol) in water (3 ml) was added to a solution of KNO_2NCN (4.0 mmol) in water (10 ml) mixed with a solution of imidazole (4.0 mmol) in methanol (10 ml). The resulting green solution was left standing and after a few days blue crystals of (I) were isolated (yield *ca* 10%).

Crystal data

$[Cu_2(C_2N_3)_4(H_2O)]$
$M_r = 409.30$
Monoclinic, $C2/c$
$a = 21.8718\ (11)$ Å
$b = 6.8726\ (3)$ Å
$c = 8.8127\ (4)$ Å
$\beta = 100.199\ (4)^\circ$
$V = 1303.76\ (11)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.29$ mm^{-1}
$T = 100\ (1)$ K
$0.37 \times 0.31 \times 0.06$ mm

Data collection

Oxford Gemini R CCD area-detector diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
$T_{\min} = 0.366$, $T_{\max} = 0.889$
57505 measured reflections
1989 independent reflections
1959 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.048$
$S = 1.19$
1989 reflections
112 parameters
All H-atom parameters refined
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.35$ e Å^{-3}

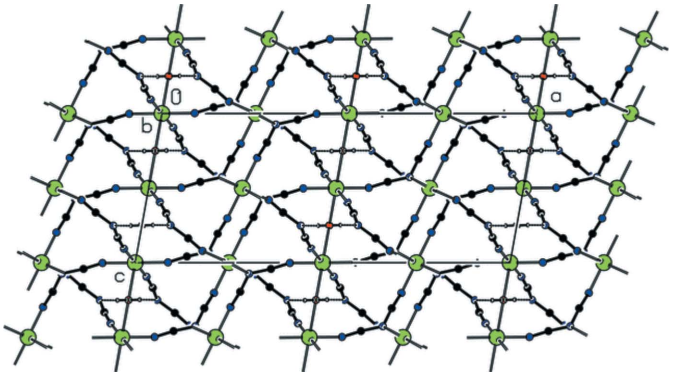

Figure 2
A packing diagram for (I), showing the hydrogen-bonding network as dashed lines.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O13—H13$\cdots$N4$^{\rm i}$	0.88 (3)	2.01 (3)	2.8538 (15)	162 (2)

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

The unique water H atom was located in a difference Fourier map and refined freely with an isotropic displacement parameter.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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