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Bis(dicyanamido-κN^1)bis[4-(1,2,4-triazol-1-yl)phenol-κN^4]copper(II)

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In the title centrosymmetric complex, $[Cu(C_2N_3)_2(C_8H_7N_3O)_2]$, the Cu^{II} atom is coordinated by two N atoms from two 4-(1,2,4-triazol-1-yl)phenol ligands and two N atoms from two dicyanamide anions, adopting a very slightly distorted square-planar geometry. In the crystal structure, intermolecular O—H···N hydrogen bonds and π–π stacking interactions link discrete mononuclear units into a two-dimensional network. In addition, there are three weak intramolecular C—H···N hydrogen-bond interactions.

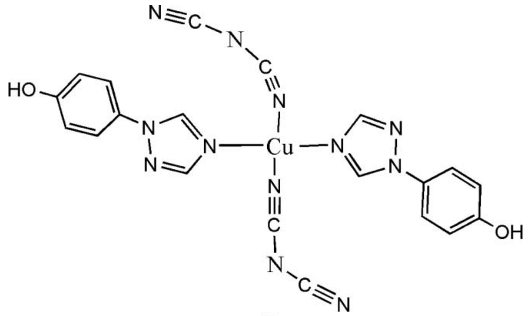
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.074
Data-to-parameter ratio = 11.2

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

Comment

Recently, 1,2,4-triazoles have attracted growing interest in the field of coordination chemistry because of their versatile bonding modes (van Diemen *et al.*, 1991) and extensive biological activity as well as their potential applications as antitumor, antibacterial, antifungal and antiviral agents (Eweiss *et al.*, 1986; Awad *et al.*, 1991). In a continuation of the study of the coordination behavior of triazole derivatives (*e.g.* Soudi *et al.*, 2006; Liu *et al.*, 2006), we report here the crystal structure of a Cu^{II} complex, (I), with mixed ligands of 4-(1,2,4-triazol-1-yl)phenol and dicyanamide.



(I)

The molecular structure of the title mononuclear complex is shown in Fig. 1 and selected bond lengths and angles are listed in Table 1. The Cu^{II} atom lies on a crystallographic center of inversion and exhibits a very slightly disorted square planar coordination geometry involving two N-atom donors from two neutral 4-(1,2,4-triazol-1-yl)phenol ligands, and two N atoms from two dicyanamide anions. Both ligands act as a typical terminal ligands, coordinating to the Cu^{II} atom in monodentate mode. There are two short non-bonded Cu1···N5$(1 - x, -\frac{1}{2} + y, \frac{1}{2} - z)$ and Cu1···N5$(x, \frac{1}{2} - y, -\frac{1}{2} + z)$ contacts of 2.884 (2) Å, which are approximately perpendicular to the CuN$_4$ coordination plane. In the molecule there are three weak weak C—H···N hydrogen bonds (Fig. 1 and Table 2).

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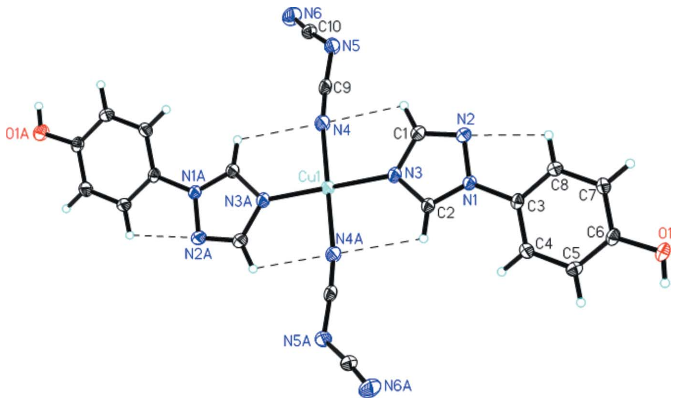

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds. [Symmetry code: (A) $-x + 1$, $-y$, $-z$.]

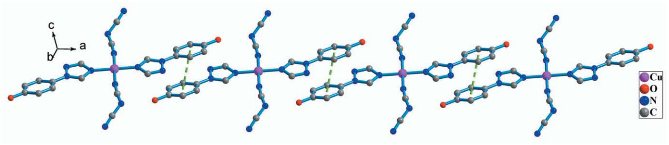

Figure 2
The one-dimensional chain of (I) formed by π–π stacking interactions (green dashed lines).

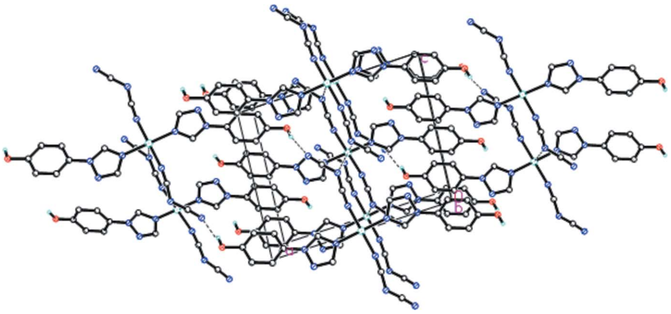

Figure 3
Part of the crystal structure of (I), showing O—H···N hydrogen bonds as dashed lines. Only H atoms involved in hydrogen bonding are shown.

In the crystal structure, intermolecular π–π stacking interactions between adjacent benzene rings, with a centroid-centroid distance of 3.540 (1) Å and parallel by symmetry, link complex molecules, forming a one-dimensional chain (Fig. 2). These chains are further assembled into a two-dimensional network through intermolecular O—H···N hydrogen bonds (Table 2 and Fig. 3).

Experimental

To a methanol solution of 4-(1,2,4-triazol-1-yl)phenol (16.1 mg, 0.1 mmol) and sodium dicyanamide (17.8 mg, 0.2 mmol) was added dropwise a solution (5 ml) of hydrated copper(II) acetate (19.9 mg, 0.1 mmol) in methanol (10 ml) with stirring. The reaction was stirred at room temperature for about 30 min and then the precipitate was filtered off, leaving the filtrate to evaporate at room temperature. Blue block-shaped crystals suitable for X-ray diffraction were obtained within 4 d in 50% yield. Analysis calculated for $C_{10}H_7Cu_{0.5}N_6O$: C 46.38, H 2.72, N 32.45%; found: C 46.42, H 2.65, N 32.60%.

Crystal data

$[Cu(C_2N_3)_2(C_8H_7N_3O)_2]$
$M_r = 517.98$
Monoclinic, $P2_1/c$
$a = 12.9515$ (17) Å
$b = 7.696$ (1) Å
$c = 10.3232$ (14) Å
$\beta = 95.548$ (2)°
$V = 1024.1$ (2) Å^3
$Z = 2$
$D_x = 1.680$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.12$ mm^{-1}
$T = 294$ (2) K
Block, blue
0.24 × 0.23 × 0.22 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.772$, $T_{\max} = 0.782$
5375 measured reflections
1801 independent reflections
1537 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.074$
$S = 1.04$
1801 reflections
161 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.4336P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N4	1.9797 (19)	Cu1—N3	1.9964 (16)
N4—Cu1—N4^{i}	180	N4—Cu1—N3	89.57 (7)
N4—Cu1—N3^{i}	90.43 (7)	N3^{i}—Cu1—N3	180

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···N2	0.93	2.48	2.804 (3)	101
C1—H1*A*···N4	0.93	2.53	2.975 (3)	110
O1—H1···N6^{ii}	0.82	1.95	2.740 (3)	162
C2—H2···N4^{i}	0.93	2.59	3.001 (3)	107

Symmetry codes: (i) $-x + 1, -y, -z$; (ii) $x - 1, y, z - 1$.

H atoms were located in difference maps, but were subsequently placed in calculated positions and treated as riding, with C—H = 0.93 Å and O—H = 0.82 Å. All H atoms were allocated displacement parameters related to those of their parent atoms [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,O)].

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); 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, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 2001) and *DIAMOND* (Brandenburg & Berndt, 1999).

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