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trans-Bis(dicyanamido-*N*)-*trans*-bis(imidazole-*N*′)copper(II)

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Key indicators

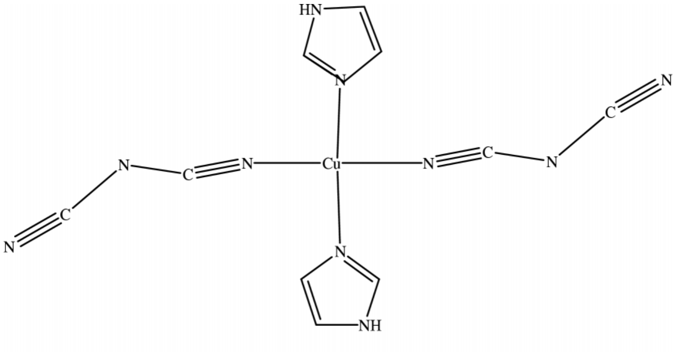
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.053
wR factor = 0.133
Data-to-parameter ratio = 12.1

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 complex, $[Cu\{N(CN)_2\}_2(C_3H_4N_2)_2]$, is reported. The Cu^{II} atom is tetragonally coordinated by two N atoms from two imidazole (iz) ligands and by two N atoms from two terminally bonded dicyanamide (dca) anions. The Cu—N distances are in the range 1.984 (4)–1.988 (5) Å. The Cu atom lies on an inversion centre.

Comment

Dicyanamide, $[N(CN)_2]^-$, was selected since its coordination versatility ranges from being monodentate to μ_4-coordination. Also, many complexes containing dicyanamide have been reported, such as $(CH_3)_2Tl[[N(CN)_2]$ (Chow & Britton, 1975), $[Cu(phen)_2\{N(CN)_2\}_2]$ (Potocnák *et al.*, 1995), $[Ni\{N(CN)_2\}_2(C_4H_6N_2)_4]$ (Kozísek *et al.*, 1996), $[Ag_2\{N(CN)_2\}_2\{P(Ph)_3\}_2]$ (Bessler *et al.*, 2000), $[Zn\{N(CN)_2\}_2]$ (Manson *et al.*, 1998) and $[Mn\{N(CN)_2\}_2]$ (Batten *et al.*, 1999). We report here the crystal structure of the title compound, $[Cu(N(CN)_2)_2(C_3H_4N_2)_2]$, (I), whose structure is composed of discrete molecules.



(I)

The Cu atom is four-coordinated by two N atoms from two *trans*-bonded dicyanamide anions and two N atoms of two *trans*-bonded imidazole ligands. The Cu—N$_{dca}$ (Cu1—N3) bond length is 1.988 (5) Å, which is comparable to the corresponding values in $[Cu(C_{12}H_8N_2)\{N(CN)_2\}][C(CN)_3]$ (Potocnák *et al.*, 1995) and the Cu—N$_{iz}$ (Cu1—N4) bond length is 1.984 (4) Å. The N$_{iz}$—Cu1—N$_{iz}$ and N$_{dca}$—Cu1—N$_{dca}$ bond angles are exactly 180°. The N$_{iz}$—Cu1—N$_{dca}$ bond angles are almost exactly 90°. The five atoms Cu1, N3, N3^i, N4 and N4^i are coplanar [symmetry code: (i) $-x$, $-y$, $-z$]. In summary, the Cu atom exhibits almost perfect tetragonal coordination.

Experimental

To an aqueous solution (20 ml) of $Cu_2Cl_2.2H_2O$ (0.085 g, 0.5 mmol), sodium dicyanamide (0.09 g, 1 mmol) was added. After stirring the

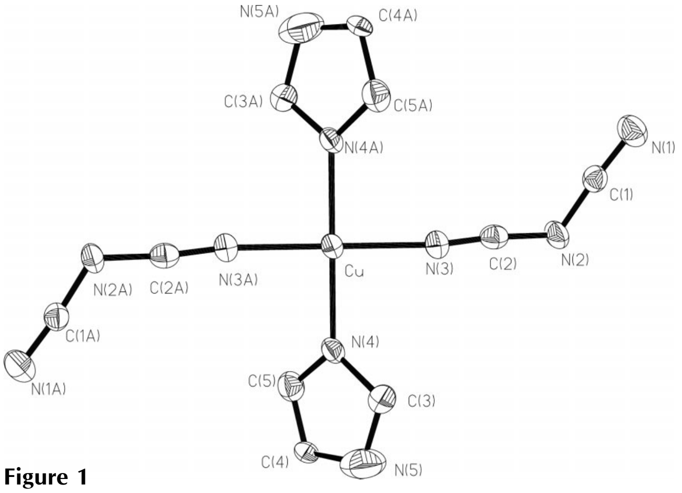


Figure 1
The structure of the title molecule with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (*A*) $-x, -y, -z$.]

mixture for about 30 min, a DMF solution (10 ml) of imidazole (0.07 g, 0.5 mmol) was added. This mixture was stirred and heated for 1 h, then filtered while hot. Well-shaped crystals were obtained from the mother liquor by slow evaporation at room temperature over a period of several days.

Crystal data

$[\mathrm{Cu(C_2N_3)_2(C_3H_4N_2)_2}]$
$M_r = 165.90$
Monoclinic, $P2_1/c$
$a = 9.2024$ (11) Å
$b = 7.5897$ (9) Å
$c = 9.7251$ (11) Å
$\beta = 101.790$ (2)°
$V = 664.90$ (13) Å^3
$Z = 2$
$D_x = 1.657$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 97 reflections
$\theta = 2.3$–25.1°
$\mu = 1.65$ mm^{-1}
$T = 293$ (2) K
Plate, blue
0.28 × 0.21 × 0.18 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.502$, $T_{\max} = 0.549$
3295 measured reflections
1173 independent reflections
817 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.053$
$\theta_{\max} = 25.1°$
$h = -10 \rightarrow 9$
$k = -9 \rightarrow 7$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.133$
$S = 1.02$
1173 reflections
97 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 1.5680P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.53$ e Å^{-3}
$\Delta\rho_{\min} = -0.50$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N4	1.984 (4)	C3—N5	1.363 (8)
Cu—N3	1.988 (5)	C3—N4	1.364 (7)
C1—N1	1.153 (6)	C4—C5	1.307 (7)
C1—N2	1.300 (7)	C4—N5	1.340 (8)
C2—N3	1.155 (7)	C5—N4	1.316 (7)
C2—N2	1.309 (7)		
N4^{i}—Cu—N4	180.0	C4—C5—N4	112.9 (5)
N4^{i}—Cu—N3	90.15 (18)	C1—N2—C2	120.1 (5)
N4—Cu—N3	89.85 (18)	C2—N3—Cu	168.8 (5)
N3^{i}—Cu—N3	180.0	C5—N4—C3	105.4 (5)
N1—C1—N2	174.0 (6)	C5—N4—Cu	128.1 (4)
N3—C2—N2	174.3 (6)	C3—N4—Cu	126.5 (4)
N5—C3—N4	107.2 (5)	C4—N5—C3	108.2 (5)
C5—C4—N5	106.2 (5)		

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

H-atom positions were generated geometrically and the H atoms were allowed to ride on their respective parent C atoms.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SMART*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

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