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Bis(2,2′-bipyridine *N*-oxide)bis(dicyanamido)-copper(II)

Jian-Fang Dai,[a] Fu-Ying Liu,[b] Hui Liu,[a] Bai-Wang Sun[a]* and Yi-Hong Wang[a]

[a]Department of Chemistry and, Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China, and [b]Department of Chemistry, Key Laboratory of Medicinal Chemistry, for Natural Resource, Ministry of Education, Yunnan University, Kunming 650091, People's Republic of China

Correspondence e-mail: chmsunbw@seu.edu.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.083
Data-to-parameter ratio = 15.8

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

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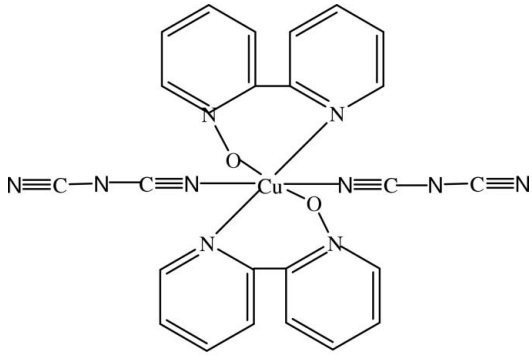
In the centrosymmetric title compound, $[Cu(C_2N_3)_2(C_{10}H_8N_2O)_2]$, the Cu^{II} atom adopts a distorted octahedral geometry, with the equatorial plane formed by two O atoms and two N atoms of two chelating 2,2′-bipyridine *N*-oxide ligands. The axial positions are occupied by N atoms of two monodentate dicyanamide anions.

Comment

O,*O*′- and *N*,*O*′-chelating derivatives of bipy, such as 2,2′-bipyridine *N*,*N*′-dioxide and 2,2′-bipyridine *N*-oxide have attracted much interest (van Albada *et al.*, 2003; Anderson *et al.*, 1999; Baran *et al.*, 1993; Paulus *et al.*, 1992) in forming a new class of molecule-based magnetic materials. The 2,2′-bipyridine *N*,*N*′-dioxide ligand is expected to be a good *O*-donor since it possesses resonance-contributing O atoms. To the best of our knowledge, only a few crystal structures with 2,2′-bipyridine *N*,*N*′-dioxide (abbreviated as bpyNO) have been reported (van Albada *et al.*, 2003, 2006).



(I)

In the centrosymmetric title compound, (I), the Cu ion has an axially elongated octahedral geometry. As shown in Fig. 1, the Cu atom is surrounded by two bpyNO molecules which form the equatorial plan. The axial positions are occupied by N atoms of two monodentate dicyanamido anions (Table 1). The presence of the N—O group in bpyNO destroys the coplanarity of the pyridine rings and results in a Cu1—O1—N1—C5 torsion angle of 54.08 (15)°. The crystal structure is stabilized by stacking of the pyridine rings (Fig. 2), with distances of 3.3831 (5) Å and centroid-to-centroid distances of 4.108 Å. In addition, C4—H4*A*···N4^{ii} hydrogen-bonding interactions (Table 2) stabilize the crystal packing.

Experimental

An ethanol (5 ml) solution of bpyNO (34.44 mg, 0.2 mmol) was added slowly to an aqueous solution (5 ml) of $CuCl_2{\cdot}2H_2O$ (34.01 mg,

0.2 mmol), followed by an aqueous solution (5 ml) of $NaN(CN)^2$ (35.61 mg, 0.4 mol). After three weeks, well shaped green polyhedral crystals of (I) were obtained from the mother liquor.

Crystal data

$[Cu(C_2N_3)_2(C_{10}H_8N_2O)_2]$
M_r = 540.01
Monoclinic, $P2_1/c$
a = 10.206 (2) Å
b = 8.0840 (16) Å
c = 13.638 (3) Å
β = 92.56 (3)°
V = 1124.1 (4) Å^3
Z = 2
D_x = 1.595 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 298 (2) K
Block, green
0.18 × 0.16 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.830, T_{max} = 0.856
9715 measured reflections
2667 independent reflections
2376 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 28.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.083
S = 1.01
2667 reflections
169 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.381P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0076 (13)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9620 (12)	Cu1—N4	2.5052 (17)
Cu1—N2	2.0156 (13)		
O1—Cu1—N2	86.73 (5)	O1^i—Cu1—N4	91.66 (5)
O1^i—Cu1—N2	93.27 (5)	N2—Cu1—N4	92.46 (6)
O1—Cu1—N4	88.34 (5)	N2^i—Cu1—N4	87.54 (6)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···N4^{ii}	0.93	2.47	3.386 (2)	169

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

H atoms bound to C atoms were placed in idealized positions and allowed to ride during subsequent refinement, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

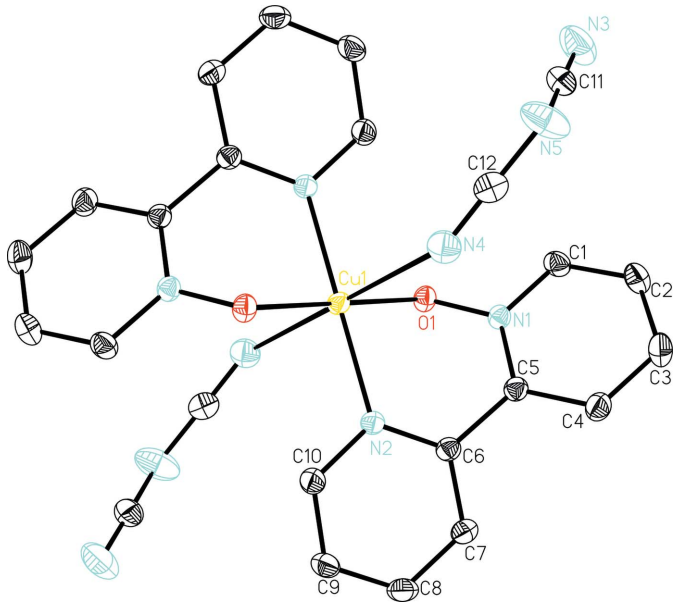


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry code for unlabelled atoms: $1-x, -y, 1-z$.

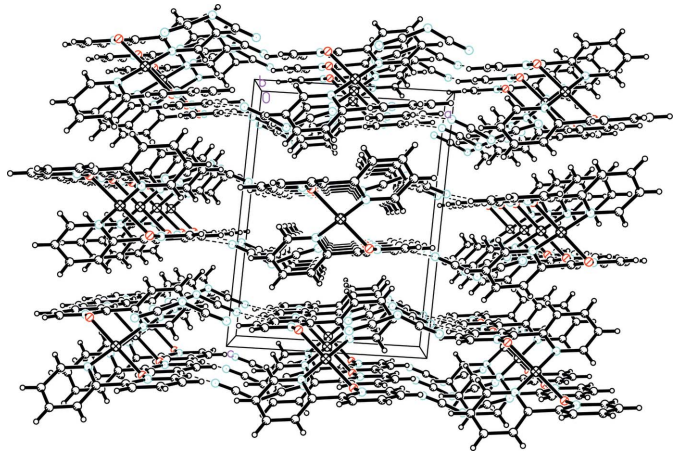


Figure 2
View of (I) along the *b*-axis direction, showing the stacking of the pyridine rings. Hydrogen bonds are shown as dashed lines.

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