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Bis[2-(hydroxymethyl)pyridine-κ^2N,O]-dinitratocopper(II)

Feng He[a]* and Di Liu[b]

[a]School of Chemistry and Chemical Engineering, School of Pharmaceutical Science, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China, and [b]School of Pharmaceutical Science, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China

Correspondence e-mail: exstxr@zsu.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
Some non-H atoms missing
R factor = 0.025
wR factor = 0.076
Data-to-parameter ratio = 14.4

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

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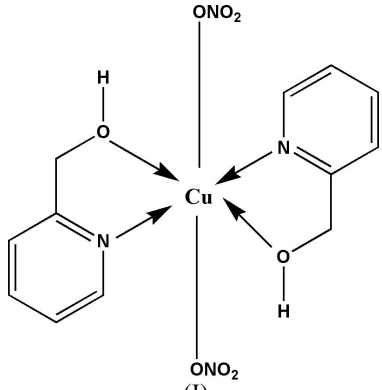
In the crystal structure of the title compound, $[Cu(NO_3)_2(C_6H_7NO)_2]$, the copper(II) ion resides at an inversion centre and it has a 4 + 2 elongated ocatahedral coordination environment. The equatorial positions are occupied by two OH groups and two N atoms from a pair of neutral 2-(hydroxymethyl)pyridine ligands, while the two axial positions are weakly ligated by two nitrate O atoms. Adjacent mononuclear copper(II) complexes are further joined together by O—H···O hydrogen bonds to form a linear chain along the a axis.

Comment

Recently, we have synthesized and characterized a series of discrete dinuclear and polymeric heterometallic copper(II)–lanthanide(III) complexes. In particular, the ligand Htza (tetrazole-1-acetic acid) coordinates with Cu^{II} and lanthanide(III) salts to form $[CuLn(tza)_4(H_2O)_5Cl]$ complexes at pH = 3.5, but forms a multinuclear heterometallic complex at higher pH values (He *et al.*, 2005). We have utilized a related ligand, namely 2-(hydroxymethyl)pyridine, to see whether similar reactions occur or not. Moreover, the title compound, (I), can be used as a so-called 'metallic ligand' reagent to bind lanthanide metal ions for the subsequent preparation of heteronuclear complexes which may exhibit large ferromagnetic interactions (Costes, Dahan & Dupuis, 2000; Costes, Dahan, Dupuis & Laurent, 2000) or quadratic non-linear optical properties (Margeat *et al.*, 2004).



(I)

The copper(II) ion in (I) has an octahedral coordination environment (Fig. 1) and adjacent mononuclear copper(II) complexes are interlinked by O—H···O(nitrato) hydrogen bonds to form a linear ribbon extending parallel to the a axis (Fig. 2).

Experimental

$Cu(NO_3)_2{\cdot}3H_2O$ (0.242 g, 1 mmol) in water (18 ml) was mixed with 2-(hydroxymethyl)pyridine (0.218 g, 2 mmol). The resulting blue solution was stirred for 5 min and then adjusted to pH 3 with 0.5 *M* of an aqueous sodium hydroxide solution. The solution was allowed to evaporate slowly at ambient temperature for 40 d. Blue polyhedral crystals were collected in 59% yield.

Crystal data

$[Cu(NO_3)_2(C_6H_7NO)_2]$
M_r = 405.82
Monoclinic, $P2_1/n$
a = 7.4402 (5) Å
b = 12.4849 (9) Å
c = 8.4844 (6) Å
β = 104.5240 (1)°
V = 762.93 (9) Å^3
Z = 4
D_x = 1.767 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3474 reflections
θ = 2.5–28.2°
μ = 1.49 mm^{-1}
T = 293 (2) K
Polyhedron, deep blue
0.39 × 0.36 × 0.23 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.593, T_{max} = 0.726
4602 measured reflections
1712 independent reflections
1593 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 27.5°
$h = -8 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.076
S = 1.05
1712 reflections
119 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.1296P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.952 (1)	Cu1—O1	1.971 (1)
N1—Cu1—N1^{i}	180	N1—Cu1—O1^{i}	97.37 (4)
N1—Cu1—O1	82.63 (4)	O1—Cu1—O1^{i}	180

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{ii}	0.84 (1)	1.75 (1)	2.5567 (16)	159 (2)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2000); software used to prepare material for publication: *SHELXL97*.

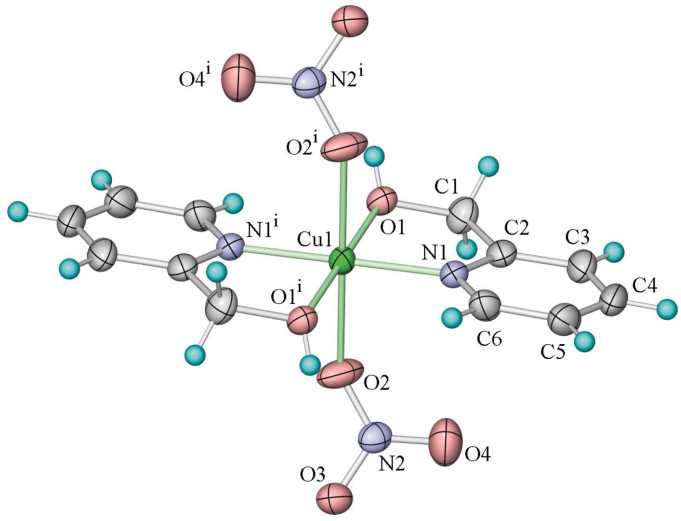


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

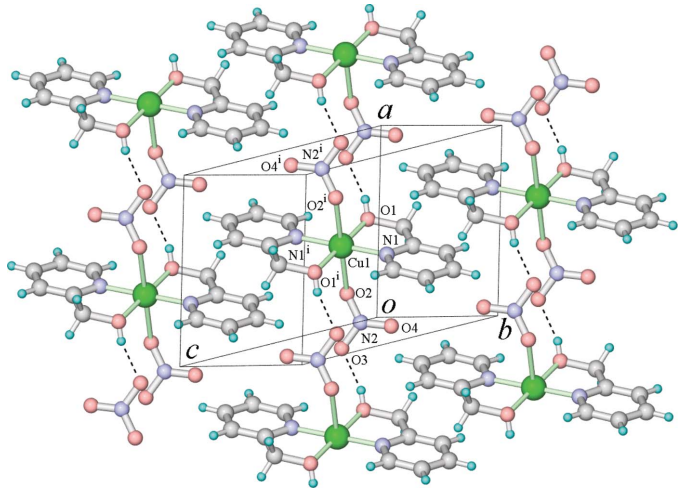


Figure 2
The crystal structure of the title compound. Dashed lines represent hydrogen bonds. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

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