Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{2-[2-(isopropylamino)ethyliminomethyl]-4-nitrophenolato}copper(II) dinitrate

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Received 7 January 2007
Accepted 11 January 2007

In the title mononuclear copper(II) complex, $[Cu(C_{12}H_{17}N_3O_3)_2](NO_3)_2$, the Cu^{II} ion, lying on an inversion centre, is four-coordinated in a square-planar geometry by two phenolate O atoms and two imine N atoms from two Schiff base ligands. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds, forming a network.

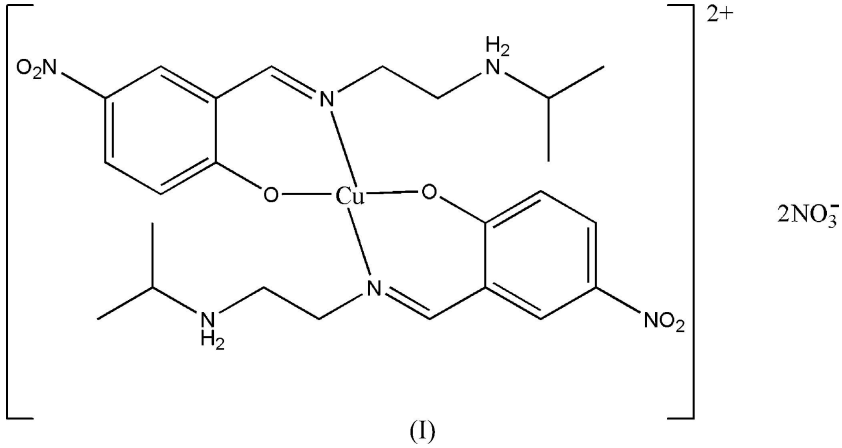
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.123
Data-to-parameter ratio = 16.4

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

Comment

Over the last few years, there has been a great effort to identify the biological role of copper, primarily through techniques associated with the interface of biology, biochemistry and coordination chemistry (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). An extensive effort has been made to prepare and characterize a variety of copper(II) coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination number four, five, and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). As an extension of our study on the crystal structures of copper(II) complexes, the title copper(II) complex, (I), is reported here.



(I)

Compound (I) consists of a mononuclear copper(II) complex cation and two nitrate anions (Fig. 1). The Cu^{II} ion in the cation, lying on an inversion centre, is four-coordinated by two phenolate O atoms and two imine N atoms from two Schiff base ligands, forming a square-planar geometry. All the bond lengths and angles (Table 1) subtended at the Cu centre

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are typical and comparable with those in other Schiff base–copper(II) complexes (Hebbachi & Benali-Cherif, 2005; Butcher *et al.*, 2003; Elmali *et al.*, 2000; Warda *et al.*, 1997).

In the crystal structure, molecules are linked by intermolecular N—H···O hydrogen bonds (Table 2), forming a network (Fig. 2).

Experimental

5-Nitrosalicylaldehyde (1.0 mmol, 167.2 mg), *N*-isopropyl-1,2-diaminoethane (1.0 mmol, 102.3 mg) and $Cu(NO_3)_2{\cdot}3H_2O$ (0.5 mmol, 121.0 mg) were dissolved in methanol (80 ml). The mixture was stirred at room temperature for about 1 h, giving a deep-blue solution. After allowing the solution to stand in air for two weeks, blue block-shaped crystals of (I) formed.

Crystal data

$[Cu(C_{12}H_{17}N_3O_3)_2](NO_3)_2$
M_r = 690.13
Monoclinic, $P2_1/n$
a = 7.710 (1) Å
b = 21.608 (2) Å
c = 9.075 (1) Å
β = 95.434 (2)°
V = 1505.1 (3) Å^3
Z = 2
D_x = 1.523 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 298 (2) K
Block, blue
0.18 × 0.12 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.869, T_{max} = 0.954
11622 measured reflections
3394 independent reflections
2630 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.123
S = 1.04
3394 reflections
207 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.6314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.895 (2)	Cu1—N1	2.007 (2)
O1—Cu1—O1^{i}	180	O1—Cu1—N1	91.55 (8)
O1—Cu1—N1^{i}	88.45 (8)	N1^{i}—Cu1—N1	180

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O5^{ii}	0.90	2.05	2.933 (4)	167
N2—H2A···O4^{iii}	0.90	1.97	2.808 (3)	155

Symmetry codes: (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$.

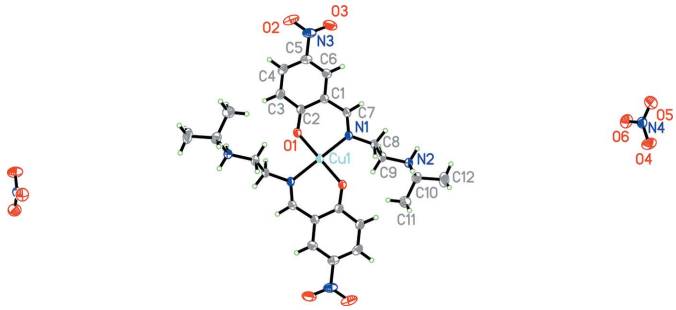

Figure 1
The structure of the component ions of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position $(2-x, 2-y, 1-z)$.

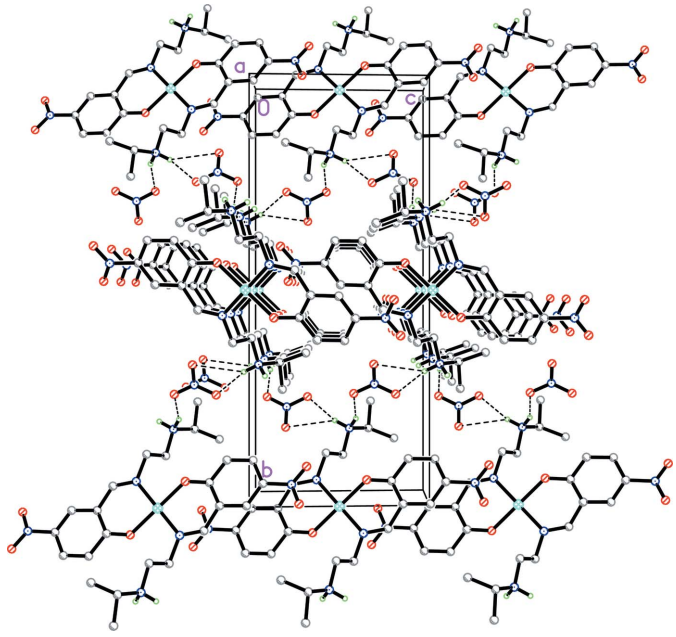

Figure 2
The molecular packing of (I). Intermolecular N—H···O hydrogen bonds are shown as dashed lines.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 or N—H = 0.90 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This project was financially supported by the the Science and Technology Plan of Huzhou (No. 2006YZ08).

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