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(*N*,*N*-Dimethyldithiocarbamato-$\kappa^2 S,S'$)iodo-(1,10-phenanthroline-$\kappa^2 N,N'$)copper(II)

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Key indicators

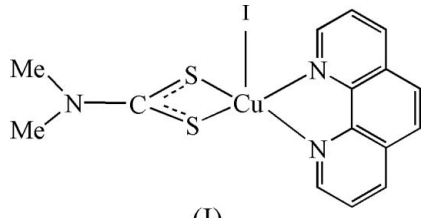
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.035
wR factor = 0.125
Data-to-parameter ratio = 20.2

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

In the title complex, $[Cu(C_3H_6NS_2)I(C_{12}H_8N_2)]$, the Cu^{II} atom is coordinated by one iodide ion, two N atoms from a phenanthroline ligand and two S atoms from a dimethyldithiocarbamate ligand in a distorted square-pyramidal environment.

Comment

The study of transition metal complexes has attracted much attention because of their fascinating structural diversity, as well as their potential applications as functional materials and enzymes (Noro *et al.*, 2000; Yaghi *et al.*, 1998). Dialkyldithiocarbamate anions, which are typical sulfur ligands, acting as monodentate, bidentate or bridging ligands, are often chosen for the preparation of a considerable structural variety of complexes (Englhardt *et al.*, 1988; Fernández *et al.*, 2000; Koh, *et al.*, 2003). We report here the crystal structure of the title mononuclear copper(II) complex, (I), containing a dimethyldithiocarbamate ligand.



(I)

The molecular structure of (I) is shown in Fig. 1. The Cu^{II} atom is five-coordinated in a distorted square-pyramidal environment by one I atom in the apical position, two N atoms from a phenanthroline ligand and two S atoms from a dimethyldithiocarbamate ligand in the basal plane (Table 1).

Experimental

A mixture of $Cu(OAc)_2{\cdot}H_2O$ (0.08 g, 0.4 mmol), $NaS_2CNMe_2{\cdot}2H_2O$ (0.09 g, 0.4 mmol), 1,10-phenanthroline (0.08 g 0.4 mmol) and $NaI{\cdot}2H_2O$ (0.07 g, 0.4 mmol) was stirred in dimethylformamide (15 ml). 2-PrOH was diffused into the resulting solution, yielding single crystals of (I).

Crystal data

$[Cu(C_3H_6NS_2)I(C_{12}H_8N_2)]$
M_r = 490.85
Monoclinic, $P2_1/n$
a = 9.0506 (5) Å
b = 11.3701 (7) Å
c = 17.1085 (11) Å
β = 94.490 (5)°
V = 1755.17 (18) Å^3
Z = 4
D_x = 1.858 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.24 mm^{-1}
T = 293 (2) K
Prism, black
0.26 × 0.25 × 0.2 mm

Data collection

Rigaku Mercury CCD diffractometer	13281 measured reflections
ω scans	4019 independent reflections
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)	3553 reflections with $I > 2\sigma(I)$
$T_{min} = 0.411$, $T_{max} = 0.520$	$R_{int} = 0.024$
	$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1032P)^2 + 0.0145P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.035$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.125$	$\Delta\rho_{max} = 0.84$ e Å^{-3}
$S = 0.92$	$\Delta\rho_{min} = -0.68$ e Å^{-3}
4019 reflections	
199 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.021 (3)	Cu1—S1	2.3111 (11)
Cu1—N3	2.034 (3)	Cu1—I1	2.9378 (5)
Cu1—S2	2.2963 (11)		
N2—Cu1—N3	81.47 (13)	S2—Cu1—S1	76.87 (4)
N2—Cu1—S2	164.03 (10)	N2—Cu1—I1	91.81 (9)
N3—Cu1—S2	97.95 (10)	N3—Cu1—I1	95.60 (10)
N2—Cu1—S1	99.50 (9)	S2—Cu1—I1	104.10 (3)
N3—Cu1—S1	164.63 (11)	S1—Cu1—I1	99.69 (3)

H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 (aromatic) or 0.96 Å (methyl) and $U_{iso}(H) = 1.2U_{eq}(C)$ (aromatic) or $1.5U_{eq}(C)$ (methyl).

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

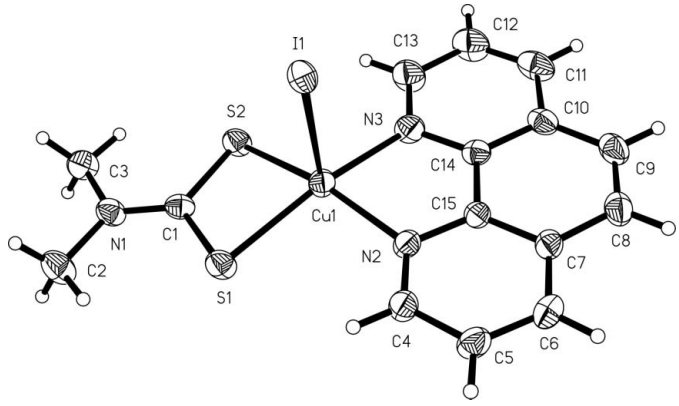


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

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