Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Dimethyldithiocarbamato-κ^2S,S')-iodido(1,10-phenanthroline-κ^2N,N')-copper(II)

Le-Qing Fan and Ji-Huai Wu*

Institute of Materials Physical Chemistry, Huaqiao University, and The Key Laboratory for the College of Materials Science and Engineering, Huaqiao University of Fujian Higher Education, Quanzhou, Fujian 362021, People's Republic of China
Correspondence e-mail: jhwu@hqu.edu.cn

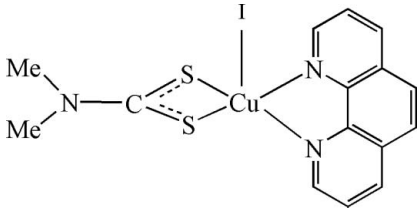
Received 9 May 2007; accepted 23 May 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.050; wR factor = 0.144; data-to-parameter ratio = 20.0.

In the title complex, $[Cu(C_3H_6NS_2)I(C_{12}H_8N_2)]$, each 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. There are two molecules in the asymmetric unit.

Related literature

For related literature, see: Engelhardt *et al.* (1998); Fernández *et al.* (2000); Koh *et al.* (2003); Noro *et al.* (2000); Yaghi *et al.* (1998).



Experimental

Crystal data

$[Cu(C_3H_6NS_2)I(C_{12}H_8N_2)]$
M_r = 490.85
Monoclinic, $P2_1/c$
a = 14.2931 (13) Å
b = 17.4948 (13) Å
c = 14.6359 (16) Å
β = 107.790 (4)°
V = 3484.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.26 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.08 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.547, T_{max} = 1.000 (expected range = 0.421–0.770)
25019 measured reflections
7942 independent reflections
6762 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.07
7942 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.037 (4)	Cu2—N5	2.042 (4)
Cu1—N2	2.043 (4)	Cu2—N6	2.051 (4)
Cu1—S1	2.3015 (14)	Cu2—S4	2.3040 (15)
Cu1—S2	2.3032 (16)	Cu2—S3	2.3078 (15)
Cu1—I1	2.9334 (8)	Cu2—I2	2.8421 (8)
N3—Cu1—N2	81.32 (16)	N5—Cu2—N6	81.00 (17)
N3—Cu1—S1	164.60 (12)	N5—Cu2—S4	158.11 (13)
N2—Cu1—S1	100.36 (12)	N6—Cu2—S4	98.62 (13)
N3—Cu1—S2	98.25 (12)	N5—Cu2—S3	97.36 (12)
N2—Cu1—S2	167.68 (13)	N6—Cu2—S3	164.24 (13)
S1—Cu1—S2	76.82 (5)	S4—Cu2—S3	77.04 (5)
N3—Cu1—I1	87.74 (11)	N5—Cu2—I2	95.88 (12)
N2—Cu1—I1	91.36 (12)	N6—Cu2—I2	98.70 (12)
S1—Cu1—I1	107.45 (4)	S4—Cu2—I2	105.76 (5)
S2—Cu1—I1	100.94 (5)	S3—Cu2—I2	97.07 (5)

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*.

This work was supported financially by the National Natural Science Foundation of China (grant Nos. 50572030 and 50372022) and the Research Fund of Huaqiao University (grant No. 06BS216)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2086).

References

Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Engelhardt, L. M., Healy, P. C., Shephard, R. M., Skelton, B. W. & White, A. H. (1998). *Inorg. Chem.* **27**, 2371–2373.
Fernández, E. J., López-de-Luzuriaga, J. M., Monge, M., Olmos, E., Laguna, A., Villacampa, M. D. & Jones, P. G. (2000). *J. Cluster Sci.* **11**, 153–166.
Koh, Y. W., Lai, C. S., Du, A. Y., Tiekink, E. R. T. & Loh, K. P. (2003). *Chem. Mater.* **15**, 4544–4554.
Noro, S.-I., Kitagawa, S., Kondo, M. & Seki, K. (2000). *Angew. Chem. Int. Ed.* **39**, 2081–2084.
Rigaku (2000). *CrystalClear*. Version 1.3. Rigaku Corporation, Akishima, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yaghi, O. M., Li, H., Davis, C., Richardson, D. & Groy, T. L. (1998). *Acc. Chem. Res.* **31**, 474–484.

  doi:10.1107/S1600536807025093

supplementary materials

Acta Cryst. (2007). E**63**, m1768 [**doi:10.1107/S1600536807025093**]

(Dimethyldithiocarbamato-κ^2S,S')iodido(1,10-phenanthroline-κ^2N,N')copper(II)

L.-Q. Fan and J.-H. Wu

Comment

Research into transition metal complexes has been rapidly expanding 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). Dialkyldithiocarbamates 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 (Engelhardt *et al.*, 1998; Fernández *et al.*, 2000; Koh, *et al.*, 2003). We report here the crystal structure of the title copper(II) complex, (I), contanining a dimethyldithiocarbamate ligand.

The molecular structure of (I) is shown in Fig. 1. In (1), there are two crystallographically independent Cu^{II} atoms in the asymmetric unit. Both are 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 $Cu(Ac)_2{\cdot}H_2O$ (0.16 g, 0.8 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 DMF (15 ml). 2-PrOH was diffused into the resulting solution, yielding single crystals of (I).

Refinement

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

Figures

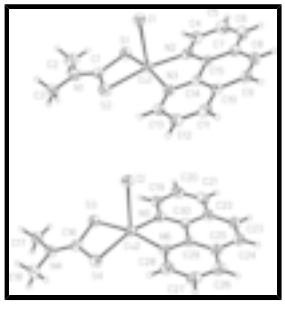


Fig. 1. The molecular structure of (I) with 30% probability displacement ellipsoids.

(Dimethyldithiocarbamato-κ^2S,S')iodido(1,10-phenanthroline-κ^2N,N')copper(II)

Crystal data

$[Cu(C_3H_6NS_2)I(C_{12}H_8N_2)]$	F_{000} = 1912
M_r = 490.85	D_x = 1.871 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8049 reflections
a = 14.2931 (13) Å	θ = 3.1–27.5º
b = 17.4948 (13) Å	μ = 3.26 mm^{-1}
c = 14.6359 (16) Å	T = 293 (2) K
β = 107.790 (4)º	Prism, black
V = 3484.8 (6) Å^3	0.30 × 0.20 × 0.08 mm
Z = 8	

Data collection

Rigaku Mercury CCD diffractometer	7942 independent reflections
Radiation source: Sealed Tube	6762 reflections with $I > 2\sigma(I)$
Monochromator: Graphite Monochromator	R_{int} = 0.034
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	h = −18→18
T_{min} = 0.547, T_{max} = 1.000	k = −22→21
25019 measured reflections	l = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 1.0573P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.002
7942 reflections	$\Delta\rho_{max}$ = 0.82 e Å^{-3}
397 parameters	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.54618 (5)	0.55197 (3)	0.86587 (5)	0.04700 (17)
Cu2	1.00225 (5)	0.61593 (4)	1.33013 (5)	0.04827 (17)
S1	0.42686 (10)	0.63047 (8)	0.89036 (11)	0.0543 (3)
S2	0.62636 (10)	0.66705 (8)	0.90659 (12)	0.0591 (4)
S3	0.93575 (10)	0.73224 (8)	1.35167 (11)	0.0558 (3)
S4	1.13164 (10)	0.69918 (8)	1.34873 (12)	0.0579 (4)
I1	0.51765 (3)	0.54788 (2)	0.65876 (2)	0.05071 (12)
I2	0.90939 (2)	0.60430 (2)	1.12905 (2)	0.05199 (12)
N1	0.5001 (3)	0.7725 (2)	0.9289 (3)	0.0521 (10)
N2	0.4799 (3)	0.4479 (2)	0.8607 (3)	0.0465 (10)
N3	0.6662 (3)	0.4841 (2)	0.8832 (3)	0.0416 (9)
N4	1.0712 (3)	0.8404 (3)	1.3710 (3)	0.0510 (10)
N5	0.9043 (3)	0.5482 (2)	1.3688 (3)	0.0473 (10)
N6	1.0793 (3)	0.5152 (2)	1.3508 (3)	0.0469 (9)
C1	0.5151 (4)	0.7001 (3)	0.9117 (3)	0.0472 (11)
C2	0.4034 (5)	0.7993 (4)	0.9317 (5)	0.0711 (17)
H2A	0.3583	0.7571	0.9198	0.107*
H2B	0.3791	0.8377	0.8834	0.107*
H2C	0.4096	0.8207	0.9937	0.107*
C3	0.5778 (5)	0.8294 (3)	0.9439 (5)	0.0749 (18)
H3A	0.6370	0.8052	0.9405	0.112*
H3B	0.5895	0.8525	1.0058	0.112*
H3C	0.5583	0.8680	0.8951	0.112*
C4	0.3883 (4)	0.4299 (4)	0.8548 (4)	0.0570 (13)
H4A	0.3467	0.4686	0.8623	0.068*
C5	0.3513 (4)	0.3560 (4)	0.8379 (5)	0.0671 (16)
H5A	0.2869	0.3457	0.8359	0.081*
C6	0.4106 (4)	0.2989 (4)	0.8242 (4)	0.0610 (14)
H6A	0.3860	0.2497	0.8099	0.073*
C7	0.5091 (4)	0.3148 (3)	0.8317 (3)	0.0462 (11)
C8	0.5770 (4)	0.2601 (3)	0.8185 (4)	0.0554 (13)
H8A	0.5562	0.2099	0.8038	0.066*
C9	0.6703 (4)	0.2786 (3)	0.8267 (4)	0.0535 (13)

H9A	0.7125	0.2412	0.8169	0.064*
C10	0.7056 (3)	0.3541 (3)	0.8500 (3)	0.0418 (10)
C11	0.8032 (4)	0.3790 (3)	0.8621 (4)	0.0535 (13)
H11A	0.8498	0.3448	0.8537	0.064*
C12	0.8281 (4)	0.4522 (3)	0.8859 (4)	0.0541 (13)
H12A	0.8926	0.4681	0.8961	0.065*
C13	0.7583 (4)	0.5039 (3)	0.8952 (4)	0.0493 (12)
H13A	0.7770	0.5544	0.9104	0.059*
C14	0.6403 (3)	0.4106 (3)	0.8620 (3)	0.0403 (10)
C15	0.5401 (3)	0.3899 (3)	0.8508 (3)	0.0399 (10)
C16	1.0494 (4)	0.7674 (3)	1.3596 (4)	0.0472 (11)
C17	0.9991 (4)	0.8958 (3)	1.3836 (5)	0.0611 (15)
H17A	0.9393	0.8697	1.3812	0.092*
H17B	0.9861	0.9332	1.3332	0.092*
H17C	1.0248	0.9207	1.4446	0.092*
C18	1.1674 (5)	0.8703 (4)	1.3727 (4)	0.0644 (15)
H18A	1.2080	0.8291	1.3636	0.097*
H18B	1.1981	0.8944	1.4334	0.097*
H18C	1.1592	0.9070	1.3221	0.097*
C19	0.8178 (4)	0.5667 (3)	1.3776 (4)	0.0552 (13)
H19A	0.7989	0.6177	1.3718	0.066*
C20	0.7540 (4)	0.5129 (4)	1.3954 (4)	0.0632 (15)
H20A	0.6930	0.5276	1.3997	0.076*
C21	0.7825 (4)	0.4377 (4)	1.4065 (4)	0.0639 (15)
H21A	0.7407	0.4012	1.4189	0.077*
C22	0.8737 (4)	0.4156 (3)	1.3991 (4)	0.0526 (12)
C23	0.9109 (5)	0.3398 (3)	1.4089 (4)	0.0621 (15)
H23A	0.8731	0.3008	1.4230	0.075*
C24	0.9981 (5)	0.3224 (3)	1.3988 (4)	0.0632 (15)
H24A	1.0189	0.2718	1.4045	0.076*
C25	1.0607 (4)	0.3806 (3)	1.3791 (4)	0.0545 (13)
C26	1.1541 (5)	0.3669 (4)	1.3700 (4)	0.0632 (15)
H26A	1.1796	0.3176	1.3762	0.076*
C27	1.2073 (4)	0.4269 (4)	1.3520 (5)	0.0658 (16)
H27A	1.2692	0.4188	1.3452	0.079*
C28	1.1676 (4)	0.5006 (4)	1.3439 (4)	0.0566 (13)
H28A	1.2050	0.5411	1.3331	0.068*
C29	1.0272 (4)	0.4564 (3)	1.3691 (3)	0.0428 (10)
C30	0.9323 (4)	0.4743 (3)	1.3794 (3)	0.0445 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0428 (3)	0.0411 (3)	0.0588 (4)	0.0056 (3)	0.0181 (3)	0.0003 (2)
Cu2	0.0419 (3)	0.0429 (3)	0.0619 (4)	0.0020 (3)	0.0187 (3)	−0.0001 (3)
S1	0.0478 (7)	0.0519 (8)	0.0675 (9)	0.0064 (6)	0.0240 (7)	−0.0016 (6)
S2	0.0477 (7)	0.0509 (8)	0.0796 (10)	0.0029 (6)	0.0205 (7)	−0.0107 (7)
S3	0.0461 (7)	0.0467 (7)	0.0772 (10)	0.0027 (6)	0.0227 (7)	−0.0037 (6)

S4	0.0466 (7)	0.0477 (8)	0.0833 (10)	−0.0005 (6)	0.0256 (7)	−0.0080 (6)
I1	0.0524 (2)	0.0530 (2)	0.0486 (2)	−0.00187 (15)	0.01823 (16)	0.00498 (13)
I2	0.0470 (2)	0.0554 (2)	0.0538 (2)	0.00504 (15)	0.01572 (16)	−0.00251 (14)
N1	0.057 (3)	0.048 (2)	0.050 (2)	0.009 (2)	0.015 (2)	−0.0111 (18)
N2	0.040 (2)	0.054 (3)	0.047 (2)	0.0056 (18)	0.0154 (18)	0.0077 (17)
N3	0.037 (2)	0.041 (2)	0.046 (2)	0.0029 (17)	0.0121 (17)	0.0036 (16)
N4	0.054 (3)	0.046 (2)	0.054 (3)	0.000 (2)	0.018 (2)	−0.0049 (18)
N5	0.040 (2)	0.051 (2)	0.051 (2)	0.0074 (18)	0.0141 (18)	0.0005 (18)
N6	0.042 (2)	0.047 (2)	0.051 (2)	0.0045 (19)	0.0133 (19)	−0.0004 (18)
C1	0.048 (3)	0.051 (3)	0.042 (3)	0.009 (2)	0.012 (2)	−0.003 (2)
C2	0.070 (4)	0.071 (4)	0.073 (4)	0.022 (3)	0.024 (3)	−0.017 (3)
C3	0.081 (4)	0.051 (4)	0.087 (5)	−0.003 (3)	0.016 (4)	−0.017 (3)
C4	0.047 (3)	0.064 (4)	0.065 (4)	0.003 (3)	0.024 (3)	0.008 (3)
C5	0.049 (3)	0.074 (4)	0.083 (4)	−0.010 (3)	0.026 (3)	0.011 (3)
C6	0.056 (3)	0.057 (3)	0.070 (4)	−0.015 (3)	0.021 (3)	0.007 (3)
C7	0.052 (3)	0.043 (3)	0.043 (3)	−0.004 (2)	0.015 (2)	0.0082 (19)
C8	0.067 (4)	0.045 (3)	0.055 (3)	−0.006 (3)	0.019 (3)	0.002 (2)
C9	0.063 (3)	0.042 (3)	0.053 (3)	0.010 (2)	0.015 (3)	0.000 (2)
C10	0.042 (3)	0.044 (3)	0.038 (2)	0.006 (2)	0.010 (2)	0.0034 (18)
C11	0.049 (3)	0.060 (3)	0.054 (3)	0.013 (3)	0.019 (2)	0.008 (2)
C12	0.037 (3)	0.057 (3)	0.068 (4)	0.002 (2)	0.016 (2)	0.003 (2)
C13	0.041 (3)	0.047 (3)	0.056 (3)	−0.004 (2)	0.010 (2)	0.002 (2)
C14	0.041 (2)	0.041 (2)	0.039 (2)	0.005 (2)	0.011 (2)	0.0055 (17)
C15	0.040 (2)	0.045 (3)	0.035 (2)	0.002 (2)	0.0122 (19)	0.0066 (17)
C16	0.050 (3)	0.048 (3)	0.043 (3)	0.005 (2)	0.013 (2)	−0.002 (2)
C17	0.061 (4)	0.049 (3)	0.075 (4)	0.005 (3)	0.023 (3)	−0.007 (3)
C18	0.065 (4)	0.061 (4)	0.072 (4)	−0.015 (3)	0.028 (3)	−0.011 (3)
C19	0.047 (3)	0.056 (3)	0.065 (3)	0.001 (2)	0.019 (3)	−0.003 (2)
C20	0.043 (3)	0.075 (4)	0.075 (4)	−0.004 (3)	0.023 (3)	−0.010 (3)
C21	0.053 (3)	0.069 (4)	0.073 (4)	−0.018 (3)	0.023 (3)	−0.006 (3)
C22	0.057 (3)	0.052 (3)	0.047 (3)	−0.006 (3)	0.013 (2)	−0.001 (2)
C23	0.072 (4)	0.049 (3)	0.064 (4)	−0.007 (3)	0.019 (3)	0.002 (2)
C24	0.078 (4)	0.045 (3)	0.062 (4)	0.004 (3)	0.015 (3)	−0.001 (2)
C25	0.057 (3)	0.050 (3)	0.052 (3)	0.010 (3)	0.011 (3)	−0.004 (2)
C26	0.061 (4)	0.067 (4)	0.056 (3)	0.021 (3)	0.010 (3)	−0.002 (3)
C27	0.051 (3)	0.075 (4)	0.073 (4)	0.018 (3)	0.022 (3)	−0.003 (3)
C28	0.048 (3)	0.066 (4)	0.059 (3)	0.006 (3)	0.021 (3)	0.004 (3)
C29	0.045 (3)	0.046 (3)	0.035 (2)	0.003 (2)	0.010 (2)	−0.0011 (18)
C30	0.041 (3)	0.047 (3)	0.044 (3)	0.002 (2)	0.009 (2)	−0.004 (2)

Geometric parameters (Å, °)

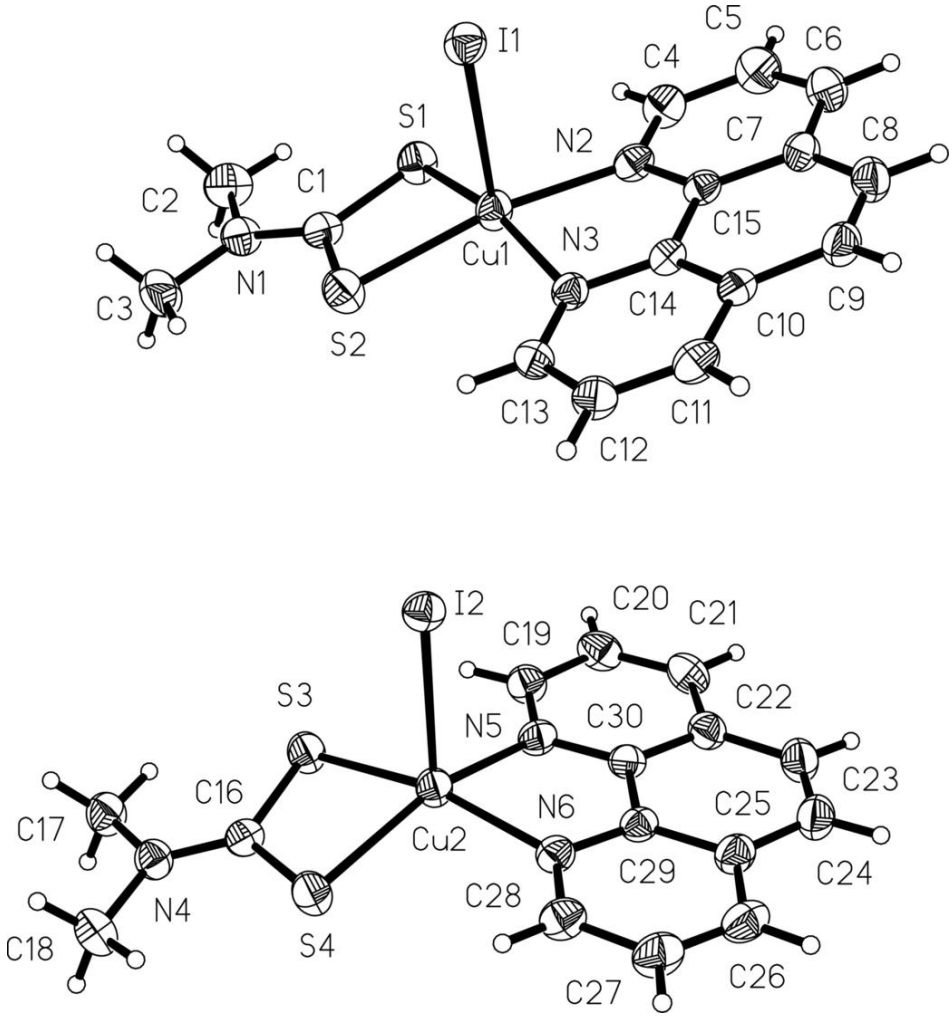
Cu1—N3	2.037 (4)	C7—C15	1.388 (7)
Cu1—N2	2.043 (4)	C7—C8	1.417 (8)
Cu1—S1	2.3015 (14)	C8—C9	1.342 (8)
Cu1—S2	2.3032 (16)	C8—H8A	0.9300
Cu1—I1	2.9334 (8)	C9—C10	1.419 (7)
Cu2—N5	2.042 (4)	C9—H9A	0.9300
Cu2—N6	2.051 (4)	C10—C14	1.405 (6)

Cu2—S4	2.3040 (15)	C10—C11	1.420 (7)
Cu2—S3	2.3078 (15)	C11—C12	1.346 (8)
Cu2—I2	2.8421 (8)	C11—H11A	0.9300
S1—C1	1.712 (6)	C12—C13	1.384 (7)
S2—C1	1.714 (5)	C12—H12A	0.9300
S3—C16	1.708 (6)	C13—H13A	0.9300
S4—C16	1.716 (5)	C14—C15	1.437 (7)
N1—C1	1.323 (6)	C17—H17A	0.9600
N1—C3	1.458 (8)	C17—H17B	0.9600
N1—C2	1.472 (7)	C17—H17C	0.9600
N2—C4	1.322 (6)	C18—H18A	0.9600
N2—C15	1.368 (6)	C18—H18B	0.9600
N3—C13	1.321 (6)	C18—H18C	0.9600
N3—C14	1.349 (6)	C19—C20	1.388 (8)
N4—C16	1.312 (7)	C19—H19A	0.9300
N4—C18	1.464 (7)	C20—C21	1.372 (9)
N4—C17	1.467 (7)	C20—H20A	0.9300
N5—C19	1.322 (7)	C21—C22	1.395 (8)
N5—C30	1.348 (6)	C21—H21A	0.9300
N6—C28	1.322 (6)	C22—C30	1.411 (7)
N6—C29	1.344 (6)	C22—C23	1.419 (8)
C2—H2A	0.9600	C23—C24	1.335 (8)
C2—H2B	0.9600	C23—H23A	0.9300
C2—H2C	0.9600	C24—C25	1.441 (9)
C3—H3A	0.9600	C24—H24A	0.9300
C3—H3B	0.9600	C25—C26	1.402 (8)
C3—H3C	0.9600	C25—C29	1.403 (7)
C4—C5	1.391 (9)	C26—C27	1.368 (9)
C4—H4A	0.9300	C26—H26A	0.9300
C5—C6	1.364 (9)	C27—C28	1.399 (8)
C5—H5A	0.9300	C27—H27A	0.9300
C6—C7	1.406 (7)	C28—H28A	0.9300
C6—H6A	0.9300	C29—C30	1.443 (7)
N3—Cu1—N2	81.32 (16)	C8—C9—C10	121.1 (5)
N3—Cu1—S1	164.60 (12)	C8—C9—H9A	119.4
N2—Cu1—S1	100.36 (12)	C10—C9—H9A	119.4
N3—Cu1—S2	98.25 (12)	C14—C10—C9	118.9 (5)
N2—Cu1—S2	167.68 (13)	C14—C10—C11	115.7 (5)
S1—Cu1—S2	76.82 (5)	C9—C10—C11	125.4 (5)
N3—Cu1—I1	87.74 (11)	C12—C11—C10	119.7 (5)
N2—Cu1—I1	91.36 (12)	C12—C11—H11A	120.2
S1—Cu1—I1	107.45 (4)	C10—C11—H11A	120.2
S2—Cu1—I1	100.94 (5)	C11—C12—C13	120.4 (5)
N5—Cu2—N6	81.00 (17)	C11—C12—H12A	119.8
N5—Cu2—S4	158.11 (13)	C13—C12—H12A	119.8
N6—Cu2—S4	98.62 (13)	N3—C13—C12	122.3 (5)
N5—Cu2—S3	97.36 (12)	N3—C13—H13A	118.9
N6—Cu2—S3	164.24 (13)	C12—C13—H13A	118.9
S4—Cu2—S3	77.04 (5)	N3—C14—C10	123.6 (4)

N5—Cu2—I2	95.88 (12)	N3—C14—C15	117.4 (4)
N6—Cu2—I2	98.70 (12)	C10—C14—C15	119.0 (4)
S4—Cu2—I2	105.76 (5)	N2—C15—C7	123.5 (4)
S3—Cu2—I2	97.07 (5)	N2—C15—C14	116.0 (4)
C1—S1—Cu1	85.00 (17)	C7—C15—C14	120.5 (4)
C1—S2—Cu1	84.90 (19)	N4—C16—S3	122.9 (4)
C16—S3—Cu2	84.50 (18)	N4—C16—S4	123.1 (4)
C16—S4—Cu2	84.44 (19)	S3—C16—S4	114.0 (3)
C1—N1—C3	121.5 (5)	N4—C17—H17A	109.5
C1—N1—C2	121.3 (5)	N4—C17—H17B	109.5
C3—N1—C2	117.2 (5)	H17A—C17—H17B	109.5
C4—N2—C15	117.3 (5)	N4—C17—H17C	109.5
C4—N2—Cu1	130.8 (4)	H17A—C17—H17C	109.5
C15—N2—Cu1	111.4 (3)	H17B—C17—H17C	109.5
C13—N3—C14	118.2 (4)	N4—C18—H18A	109.5
C13—N3—Cu1	129.1 (4)	N4—C18—H18B	109.5
C14—N3—Cu1	111.5 (3)	H18A—C18—H18B	109.5
C16—N4—C18	122.4 (5)	N4—C18—H18C	109.5
C16—N4—C17	120.7 (5)	H18A—C18—H18C	109.5
C18—N4—C17	117.0 (5)	H18B—C18—H18C	109.5
C19—N5—C30	118.5 (5)	N5—C19—C20	122.7 (5)
C19—N5—Cu2	128.8 (4)	N5—C19—H19A	118.7
C30—N5—Cu2	112.5 (3)	C20—C19—H19A	118.7
C28—N6—C29	117.9 (5)	C21—C20—C19	118.9 (5)
C28—N6—Cu2	129.6 (4)	C21—C20—H20A	120.5
C29—N6—Cu2	112.4 (3)	C19—C20—H20A	120.5
N1—C1—S1	124.2 (4)	C20—C21—C22	120.5 (5)
N1—C1—S2	122.6 (4)	C20—C21—H21A	119.8
S1—C1—S2	113.2 (3)	C22—C21—H21A	119.8
N1—C2—H2A	109.5	C21—C22—C30	116.2 (5)
N1—C2—H2B	109.5	C21—C22—C23	125.5 (5)
H2A—C2—H2B	109.5	C30—C22—C23	118.3 (5)
N1—C2—H2C	109.5	C24—C23—C22	122.3 (6)
H2A—C2—H2C	109.5	C24—C23—H23A	118.8
H2B—C2—H2C	109.5	C22—C23—H23A	118.8
N1—C3—H3A	109.5	C23—C24—C25	121.3 (6)
N1—C3—H3B	109.5	C23—C24—H24A	119.4
H3A—C3—H3B	109.5	C25—C24—H24A	119.4
N1—C3—H3C	109.5	C26—C25—C29	117.1 (6)
H3A—C3—H3C	109.5	C26—C25—C24	124.5 (5)
H3B—C3—H3C	109.5	C29—C25—C24	118.4 (5)
N2—C4—C5	123.3 (6)	C27—C26—C25	119.3 (6)
N2—C4—H4A	118.4	C27—C26—H26A	120.4
C5—C4—H4A	118.4	C25—C26—H26A	120.4
C6—C5—C4	119.1 (5)	C26—C27—C28	119.2 (6)
C6—C5—H5A	120.4	C26—C27—H27A	120.4
C4—C5—H5A	120.4	C28—C27—H27A	120.4
C5—C6—C7	119.8 (5)	N6—C28—C27	123.0 (6)
C5—C6—H6A	120.1	N6—C28—H28A	118.5

C7—C6—H6A	120.1	C27—C28—H28A	118.5
C15—C7—C6	116.9 (5)	N6—C29—C25	123.5 (5)
C15—C7—C8	118.5 (5)	N6—C29—C30	116.8 (4)
C6—C7—C8	124.5 (5)	C25—C29—C30	119.7 (5)
C9—C8—C7	121.9 (5)	N5—C30—C22	123.2 (5)
C9—C8—H8A	119.1	N5—C30—C29	116.9 (4)
C7—C8—H8A	119.1	C22—C30—C29	119.9 (5)

Fig. 1


I1
C5
C6
C4
S1
N2
C7
C8
C1
C2
C15
N3
Cu1
N1
C3
C14
C9
C10
S2
C13
C11
C12
I2
C20
C21
C19
S3
C22
N5
C30
C23
C16
N6
C25
C17
Cu2
C29
C24
C28
N4
C18
S4
C27
C26