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Di-μ-chlorido-bis[(di-2-pyridyl disulfide-κ^2N,N')copper(I)]

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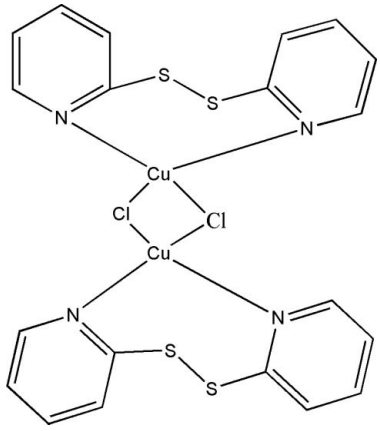
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.065; wR factor = 0.199; data-to-parameter ratio = 14.7.

In the title complex, $[Cu_2Cl_2(C_{10}H_8N_2S_2)_2]$, the asymmetric unit contains one and a half dinuclear copper complexes, one complex being arranged around an inversion center. In each complex, the Cu^I atom is coordinated by two N atoms from one di-2-pyridyl disulfide ligand and two bridging Cl atoms, and has a distorted tetrahedral geometry.

Related literature

For general background, see: Kadooka *et al.* (1976*a*,*b*); Delgado *et al.* (2006); Bell *et al.* (2000). For related literature, see: Kubo *et al.* (1998).



Experimental

Crystal data

$[Cu_2Cl_2(C_{10}H_8N_2S_2)_2]$
M_r = 638.65
Monoclinic, $P2_1/c$
a = 17.838 (3) Å
b = 9.4102 (17) Å
c = 21.309 (4) Å
β = 92.594 (3)°
V = 3573.2 (11) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 298 (2) K
0.33 × 0.19 × 0.11 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.511, T_{max} = 0.788
17489 measured reflections
6349 independent reflections
3331 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.199
S = 1.03
6349 reflections
433 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.980 (6)	Cu2—Cl3	2.393 (2)
Cu1—N2	2.028 (6)	Cu2—Cl2	2.437 (2)
Cu1—Cl1^i	2.361 (2)	Cu3—N6	2.013 (6)
Cu1—Cl1	2.450 (2)	Cu3—N5	2.015 (6)
Cu2—N4	1.990 (6)	Cu3—Cl2	2.370 (2)
Cu2—N3	2.022 (6)	Cu3—Cl3	2.427 (2)
N1—Cu1—N2	123.7 (3)	N4—Cu2—Cl2	104.46 (18)
N1—Cu1—Cl1^i	113.69 (18)	N3—Cu2—Cl2	106.35 (19)
N2—Cu1—Cl1^i	107.54 (17)	Cl3—Cu2—Cl2	102.51 (7)
N1—Cu1—Cl1	103.82 (18)	N6—Cu3—N5	120.4 (3)
N2—Cu1—Cl1	104.49 (19)	N6—Cu3—Cl2	113.55 (18)
Cl1^i—Cu1—Cl1	100.54 (7)	N5—Cu3—Cl2	107.74 (17)
N4—Cu2—N3	124.5 (2)	N6—Cu3—Cl3	103.16 (17)
N4—Cu2—Cl3	111.84 (17)	N5—Cu3—Cl3	106.90 (19)
N3—Cu2—Cl3	104.99 (18)	Cl2—Cu3—Cl3	103.49 (7)
C6—S1—S2—C5	−103.2 (4)	C25—S5—S6—C26	−105.7 (4)
C16—S3—S4—C11	104.1 (4)		

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

Data collection: *SMART* (Bruker, 1998); cell refinement and data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2183).

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supplementary materials

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Di-μ-chlorido-bis[(di-2-pyridyl disulfide-κ^2*N*,*N*')copper(I)]

L.-G. Wang

Comment

2,2'-dipyridyldisuldide possessing N-donnor and S-donnor is excellent candidates for the construction of metal complexes. Examples of crystal structure reports are copper(I) (Kadooka *et al.*, 1976*a,b*; Kubo *et al.*, 1998), copper(II) (Delgado *et al.*, 2006), cobalt(II)(Kadooka *et al.*, 1976*b*), mercury(II) (Bell *et al.*, 2000). Recently, we obtained the title novel copper complex (I) by the reaction of cuprous chloride, 2,2'-dipyridyldisuldide in a dry ethanol and acetonitrile solution, and its crystal structure is reported here.

The asymmetric unit of the title compound is build up from one and a half dinuclear copper complexes; one of the dinuclear complex being arranged around inversion center (Fig. 1). Each Cu^I is coordinated by two N atoms from one 2,2'-dipyridyldisuldide ligand, and two bridging Cl atoms, and displays a pyramidal geometry. In the centrosymmetric dinuclear complex, the Cu1···Cu1 separation is 3.076 (3) Å, whereas in the noncentrosymmetric molecule, the distance Cu2···Cu3 is slightly shorter 2.996 (1) Å.

Experimental

2,2'-dipyridyldisuldide (0.05 g,0.012 mmol), CuCl (0.18 g 0.8 mmol), were added in a mixed solvent of dry ethanol and acetonitrile, the mixture was heated for five h under reflux during the process stirring and influx were required. The resultant was then filtered to give a pure solution which was infiltrated by diethyl ether freely in a closed vessel, a weeks later some single crystals of the size suitable for X-Ray diffraction analysis precipitated.

Refinement

H atoms were placed at calculated positions and were treated as riding on their parent atoms with C—H = 0.93 Å, and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

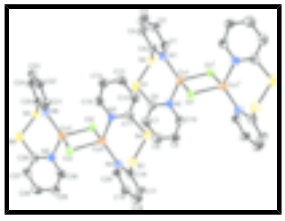


Fig. 1. Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. Symmetry code: (i) 1 − *x*, 2 − *y*, 1 − *z*).

Di-μ-chlorido-bis[(di-2-pyridyl disuldide-κ^2N,N^1)copper(I)]

Crystal data

$[Cu_2Cl_2(C_{10}H_8N_2S_2)_2]$	F_{000} = 1920
M_r = 638.65	D_x = 1.781 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6700 reflections
a = 17.838 (3) Å	θ = 1.4–26.0º
b = 9.4102 (17) Å	μ = 2.38 mm^{-1}
c = 21.309 (4) Å	T = 298 (2) K
β = 92.594 (3)º	Block, red
V = 3573.2 (11) Å^3	0.33 × 0.19 × 0.11 mm
Z = 6	

Data collection

Bruker APEXII area-detector diffractometer	6349 independent reflections
Radiation source: fine-focus sealed tube	3331 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 298(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −19→21
T_{min} = 0.511, T_{max} = 0.788	k = −11→10
17489 measured reflections	l = −25→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.066	H-atom parameters constrained
$wR(F^2)$ = 0.199	$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
6349 reflections	$\Delta\rho_{max}$ = 1.16 e Å^{-3}
433 parameters	$\Delta\rho_{min}$ = −0.47 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.44411 (5)	0.90184 (10)	0.46404 (5)	0.0569 (3)
Cu2	0.22174 (5)	1.03134 (10)	0.21276 (5)	0.0570 (3)
Cu3	0.11860 (5)	0.84980 (11)	0.13204 (5)	0.0583 (3)
Cl1	0.53561 (10)	1.0723 (2)	0.42630 (8)	0.0525 (5)
Cl2	0.12468 (11)	0.8660 (2)	0.24314 (9)	0.0574 (5)
Cl3	0.21251 (10)	1.0189 (2)	0.10053 (9)	0.0536 (5)
S1	0.28817 (12)	0.7473 (3)	0.38570 (11)	0.0695 (7)
S2	0.33945 (13)	0.6327 (2)	0.45702 (11)	0.0697 (7)
S3	0.33046 (11)	1.2986 (2)	0.22833 (10)	0.0588 (6)
S4	0.37443 (11)	1.1740 (2)	0.29946 (9)	0.0587 (6)
S5	0.01756 (12)	0.5706 (2)	0.11862 (10)	0.0610 (6)
S6	−0.01918 (12)	0.6791 (2)	0.04045 (10)	0.0652 (6)
N1	0.4784 (3)	0.7170 (6)	0.4314 (3)	0.0491 (16)
N2	0.3429 (3)	0.9894 (7)	0.4401 (3)	0.0497 (16)
N3	0.3211 (3)	0.9391 (7)	0.2374 (3)	0.0489 (16)
N4	0.1883 (3)	1.2190 (7)	0.2442 (3)	0.0472 (15)
N5	0.0181 (3)	0.9261 (7)	0.1010 (3)	0.0511 (16)
N6	0.1566 (3)	0.6636 (6)	0.0994 (3)	0.0470 (15)
C1	0.5490 (4)	0.6937 (8)	0.4137 (3)	0.053 (2)
H1	0.5816	0.7705	0.4120	0.064*
C2	0.5746 (5)	0.5611 (9)	0.3979 (4)	0.064 (2)
H2	0.6241	0.5493	0.3868	0.076*
C3	0.5268 (6)	0.4455 (10)	0.3986 (4)	0.076 (3)
H3	0.5431	0.3551	0.3880	0.092*
C4	0.4557 (6)	0.4687 (9)	0.4151 (4)	0.074 (3)
H4	0.4221	0.3932	0.4157	0.088*
C5	0.4321 (4)	0.6038 (9)	0.4311 (3)	0.054 (2)
C6	0.2844 (4)	0.9278 (9)	0.4103 (3)	0.052 (2)
C7	0.2182 (5)	1.0010 (11)	0.3922 (4)	0.068 (2)
H7	0.1783	0.9551	0.3711	0.082*
C8	0.2146 (5)	1.1429 (11)	0.4068 (4)	0.072 (3)
H8	0.1724	1.1955	0.3943	0.087*
C9	0.2724 (5)	1.2071 (9)	0.4396 (4)	0.061 (2)

H9	0.2694	1.3018	0.4516	0.073*
C10	0.3353 (4)	1.1279 (9)	0.4543 (4)	0.055 (2)
H10	0.3753	1.1730	0.4755	0.066*
C11	0.3797 (4)	0.9970 (8)	0.2701 (3)	0.049 (2)
C12	0.4435 (4)	0.9214 (10)	0.2871 (4)	0.060 (2)
H12	0.4822	0.9637	0.3112	0.072*
C13	0.4493 (4)	0.7817 (10)	0.2679 (4)	0.063 (2)
H13	0.4920	0.7285	0.2782	0.076*
C14	0.3903 (4)	0.7239 (10)	0.2334 (4)	0.061 (2)
H14	0.3923	0.6298	0.2202	0.073*
C15	0.3291 (4)	0.8041 (9)	0.2186 (3)	0.058 (2)
H15	0.2904	0.7635	0.1940	0.069*
C16	0.2350 (4)	1.3303 (8)	0.2478 (3)	0.0472 (19)
C17	0.2137 (5)	1.4648 (8)	0.2623 (4)	0.061 (2)
H17	0.2484	1.5384	0.2657	0.074*
C18	0.1379 (5)	1.4881 (10)	0.2720 (4)	0.074 (3)
H18	0.1210	1.5792	0.2806	0.088*
C19	0.0888 (5)	1.3782 (9)	0.2690 (4)	0.062 (2)
H19	0.0381	1.3923	0.2754	0.074*
C20	0.1165 (4)	1.2438 (9)	0.2562 (3)	0.056 (2)
H20	0.0836	1.1672	0.2560	0.067*
C21	0.2300 (4)	0.6443 (8)	0.0883 (3)	0.0471 (19)
H21	0.2598	0.7244	0.0837	0.056*
C22	0.2625 (4)	0.5137 (9)	0.0833 (3)	0.055 (2)
H22	0.3132	0.5051	0.0755	0.067*
C23	0.2180 (5)	0.3941 (9)	0.0902 (4)	0.063 (2)
H23	0.2391	0.3039	0.0882	0.076*
C24	0.1434 (5)	0.4090 (9)	0.0999 (3)	0.056 (2)
H24	0.1125	0.3299	0.1031	0.067*
C25	0.1149 (4)	0.5454 (8)	0.1049 (3)	0.0497 (19)
C26	−0.0330 (4)	0.8605 (9)	0.0627 (3)	0.051 (2)
C27	−0.0934 (4)	0.9273 (10)	0.0358 (4)	0.061 (2)
H27	−0.1263	0.8774	0.0089	0.074*
C28	−0.1066 (5)	1.0680 (11)	0.0479 (4)	0.073 (3)
H28	−0.1472	1.1153	0.0287	0.087*
C29	−0.0572 (5)	1.1379 (10)	0.0900 (4)	0.065 (2)
H29	−0.0652	1.2317	0.1015	0.078*
C30	0.0038 (5)	1.0631 (10)	0.1138 (4)	0.061 (2)
H30	0.0377	1.1108	0.1407	0.073*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0477 (6)	0.0528 (7)	0.0699 (7)	0.0004 (5)	0.0005 (5)	−0.0113 (5)
Cu2	0.0449 (6)	0.0503 (6)	0.0751 (7)	0.0010 (5)	−0.0038 (5)	−0.0115 (5)
Cu3	0.0449 (6)	0.0547 (7)	0.0748 (7)	0.0000 (5)	−0.0028 (5)	−0.0132 (5)
Cl1	0.0493 (12)	0.0519 (12)	0.0559 (11)	−0.0076 (9)	−0.0009 (9)	0.0004 (9)
Cl2	0.0534 (12)	0.0577 (13)	0.0608 (12)	−0.0163 (10)	0.0000 (9)	−0.0006 (10)

Cl3	0.0507 (12)	0.0505 (12)	0.0590 (12)	−0.0097 (9)	−0.0028 (9)	0.0025 (9)
S1	0.0577 (14)	0.0764 (17)	0.0740 (15)	−0.0146 (12)	−0.0002 (11)	−0.0228 (13)
S2	0.0680 (16)	0.0623 (15)	0.0811 (16)	−0.0174 (12)	0.0277 (12)	−0.0040 (13)
S3	0.0527 (13)	0.0539 (13)	0.0712 (14)	−0.0104 (10)	0.0170 (10)	0.0020 (11)
S4	0.0541 (13)	0.0649 (15)	0.0568 (12)	−0.0144 (11)	−0.0009 (10)	−0.0118 (11)
S5	0.0489 (13)	0.0576 (14)	0.0773 (14)	−0.0107 (10)	0.0141 (11)	0.0000 (12)
S6	0.0555 (14)	0.0730 (16)	0.0660 (14)	−0.0055 (11)	−0.0094 (10)	−0.0142 (12)
N1	0.042 (4)	0.046 (4)	0.060 (4)	−0.010 (3)	0.009 (3)	−0.002 (3)
N2	0.049 (4)	0.061 (5)	0.039 (3)	0.007 (3)	0.003 (3)	−0.004 (3)
N3	0.039 (4)	0.055 (4)	0.053 (4)	0.000 (3)	−0.002 (3)	−0.011 (3)
N4	0.042 (4)	0.051 (4)	0.049 (4)	−0.003 (3)	0.001 (3)	0.001 (3)
N5	0.054 (4)	0.049 (4)	0.051 (4)	0.009 (3)	0.011 (3)	0.001 (3)
N6	0.047 (4)	0.042 (4)	0.054 (4)	−0.007 (3)	0.015 (3)	−0.005 (3)
C1	0.055 (5)	0.051 (5)	0.054 (5)	0.000 (4)	0.000 (4)	−0.007 (4)
C2	0.070 (6)	0.051 (6)	0.071 (6)	0.012 (5)	0.014 (5)	−0.005 (5)
C3	0.093 (8)	0.056 (6)	0.081 (7)	0.017 (6)	0.026 (6)	−0.012 (5)
C4	0.102 (8)	0.042 (5)	0.079 (6)	−0.001 (5)	0.025 (6)	−0.007 (5)
C5	0.051 (5)	0.061 (6)	0.052 (5)	0.001 (4)	0.015 (4)	−0.001 (4)
C6	0.040 (5)	0.067 (6)	0.051 (4)	−0.008 (4)	0.012 (4)	−0.010 (4)
C7	0.058 (6)	0.088 (8)	0.059 (6)	−0.003 (5)	0.001 (4)	−0.003 (5)
C8	0.052 (6)	0.084 (8)	0.082 (6)	0.010 (5)	0.012 (5)	0.002 (6)
C9	0.061 (6)	0.060 (6)	0.063 (5)	0.016 (5)	0.014 (4)	0.000 (4)
C10	0.041 (5)	0.059 (6)	0.066 (5)	−0.002 (4)	0.005 (4)	−0.006 (4)
C11	0.045 (5)	0.064 (5)	0.040 (4)	−0.005 (4)	0.016 (4)	0.003 (4)
C12	0.034 (5)	0.081 (7)	0.063 (5)	−0.001 (4)	−0.004 (4)	−0.002 (5)
C13	0.047 (5)	0.079 (7)	0.065 (5)	0.015 (5)	0.007 (4)	0.010 (5)
C14	0.046 (5)	0.072 (6)	0.066 (5)	0.018 (4)	0.006 (4)	−0.002 (5)
C15	0.050 (5)	0.065 (6)	0.056 (5)	0.003 (4)	−0.004 (4)	−0.012 (4)
C16	0.052 (5)	0.045 (5)	0.045 (4)	−0.003 (4)	0.008 (4)	−0.005 (4)
C17	0.076 (6)	0.038 (5)	0.072 (6)	−0.009 (4)	0.018 (5)	−0.008 (4)
C18	0.077 (7)	0.063 (6)	0.082 (7)	0.008 (5)	0.019 (5)	−0.006 (5)
C19	0.065 (6)	0.065 (6)	0.055 (5)	0.015 (5)	0.013 (4)	−0.004 (4)
C20	0.060 (6)	0.051 (5)	0.058 (5)	−0.007 (4)	0.004 (4)	−0.001 (4)
C21	0.046 (5)	0.050 (5)	0.046 (4)	−0.005 (4)	0.009 (4)	−0.008 (4)
C22	0.046 (5)	0.058 (6)	0.062 (5)	0.003 (4)	0.006 (4)	−0.012 (4)
C23	0.079 (7)	0.052 (6)	0.057 (5)	0.013 (5)	−0.003 (5)	−0.005 (4)
C24	0.064 (6)	0.044 (5)	0.058 (5)	−0.004 (4)	0.007 (4)	−0.003 (4)
C25	0.050 (5)	0.050 (5)	0.049 (4)	−0.010 (4)	0.005 (4)	−0.001 (4)
C26	0.034 (4)	0.076 (6)	0.044 (4)	−0.002 (4)	0.007 (3)	−0.006 (4)
C27	0.050 (5)	0.079 (7)	0.054 (5)	−0.005 (5)	−0.006 (4)	0.011 (5)
C28	0.051 (6)	0.082 (7)	0.085 (7)	0.015 (5)	0.005 (5)	0.020 (6)
C29	0.063 (6)	0.066 (6)	0.068 (6)	0.006 (5)	0.016 (5)	0.012 (5)
C30	0.054 (5)	0.075 (7)	0.055 (5)	0.012 (5)	0.002 (4)	0.003 (5)

Geometric parameters (Å, °)

Cu1—N1	1.980 (6)	C4—H4	0.9300
Cu1—N2	2.028 (6)	C6—C7	1.405 (11)
Cu1—Cl1^{i}	2.361 (2)	C7—C8	1.374 (12)

Cu1—Cl1	2.450 (2)	C7—H7	0.9300
Cu2—N4	1.990 (6)	C8—C9	1.360 (11)
Cu2—N3	2.022 (6)	C8—H8	0.9300
Cu2—Cl3	2.393 (2)	C9—C10	1.370 (10)
Cu2—Cl2	2.437 (2)	C9—H9	0.9300
Cu2—Cu3	2.9959 (14)	C10—H10	0.9300
Cu3—N6	2.013 (6)	C11—C12	1.378 (10)
Cu3—N5	2.015 (6)	C12—C13	1.381 (11)
Cu3—Cl2	2.370 (2)	C12—H12	0.9300
Cu3—Cl3	2.427 (2)	C13—C14	1.370 (11)
Cl1—Cu1^{i}	2.361 (2)	C13—H13	0.9300
S1—C6	1.779 (8)	C14—C15	1.353 (10)
S1—S2	2.046 (4)	C14—H14	0.9300
S2—C5	1.786 (8)	C15—H15	0.9300
S3—C16	1.796 (7)	C16—C17	1.361 (10)
S3—S4	2.044 (3)	C17—C18	1.393 (11)
S4—C11	1.783 (8)	C17—H17	0.9300
S5—C25	1.790 (8)	C18—C19	1.355 (12)
S5—S6	2.037 (3)	C18—H18	0.9300
S6—C26	1.791 (8)	C19—C20	1.390 (10)
N1—C1	1.348 (9)	C19—H19	0.9300
N1—C5	1.349 (9)	C20—H20	0.9300
N2—C6	1.331 (9)	C21—C22	1.366 (10)
N2—C10	1.347 (9)	C21—H21	0.9300
N3—C15	1.341 (9)	C22—C23	1.389 (11)
N3—C11	1.345 (9)	C22—H22	0.9300
N4—C20	1.336 (9)	C23—C24	1.363 (10)
N4—C16	1.338 (9)	C23—H23	0.9300
N5—C30	1.345 (10)	C24—C25	1.386 (10)
N5—C26	1.346 (9)	C24—H24	0.9300
N6—C25	1.346 (9)	C26—C27	1.352 (10)
N6—C21	1.353 (8)	C27—C28	1.371 (12)
C1—C2	1.376 (10)	C27—H27	0.9300
C1—H1	0.9300	C28—C29	1.392 (12)
C2—C3	1.383 (12)	C28—H28	0.9300
C2—H2	0.9300	C29—C30	1.373 (11)
C3—C4	1.350 (11)	C29—H29	0.9300
C3—H3	0.9300	C30—H30	0.9300
C4—C5	1.386 (11)		
N1—Cu1—N2	123.7 (3)	C8—C9—C10	118.0 (8)
N1—Cu1—Cl1^{i}	113.69 (18)	C8—C9—H9	121.0
N2—Cu1—Cl1^{i}	107.54 (17)	C10—C9—H9	121.0
N1—Cu1—Cl1	103.82 (18)	N2—C10—C9	124.4 (8)
N2—Cu1—Cl1	104.49 (19)	N2—C10—H10	117.8
Cl1^{i}—Cu1—Cl1	100.54 (7)	C9—C10—H10	117.8
N4—Cu2—N3	124.5 (2)	N3—C11—C12	122.8 (8)
N4—Cu2—Cl3	111.84 (17)	N3—C11—S4	120.5 (6)
N3—Cu2—Cl3	104.99 (18)	C12—C11—S4	116.5 (6)

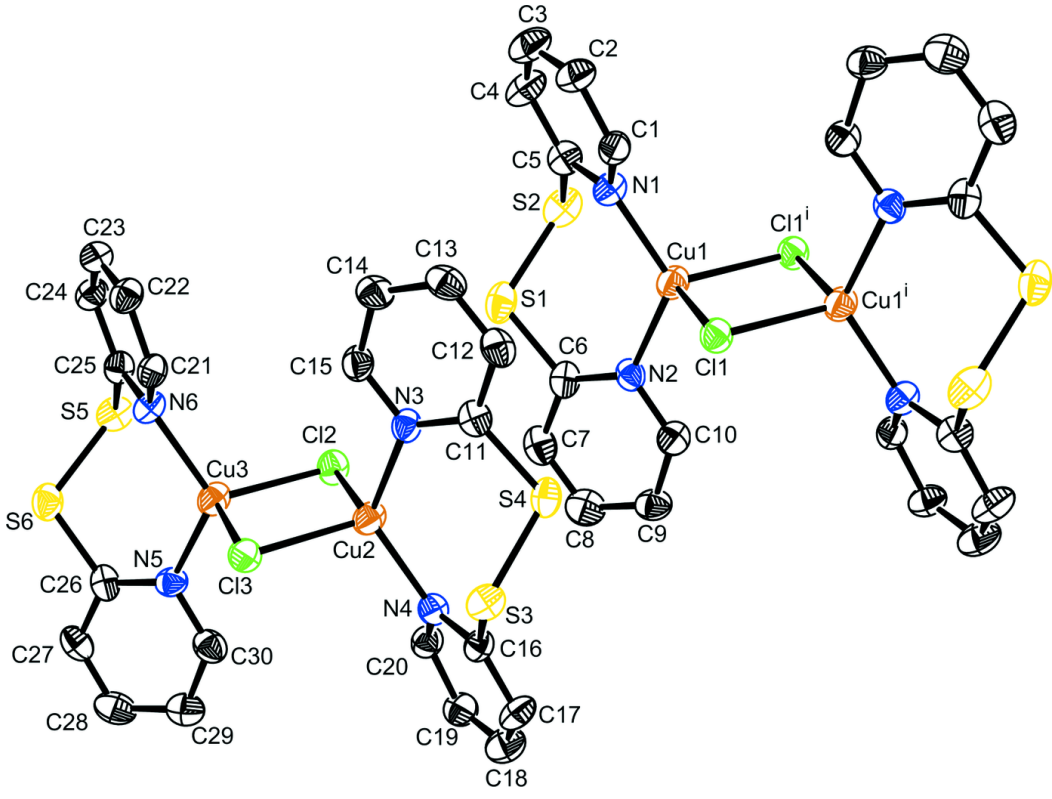
N4—Cu2—Cl2	104.46 (18)	C11—C12—C13	119.0 (8)
N3—Cu2—Cl2	106.35 (19)	C11—C12—H12	120.5
Cl3—Cu2—Cl2	102.51 (7)	C13—C12—H12	120.5
N6—Cu3—N5	120.4 (3)	C14—C13—C12	118.1 (8)
N6—Cu3—Cl2	113.55 (18)	C14—C13—H13	120.9
N5—Cu3—Cl2	107.74 (17)	C12—C13—H13	120.9
N6—Cu3—Cl3	103.16 (17)	C15—C14—C13	119.7 (9)
N5—Cu3—Cl3	106.90 (19)	C15—C14—H14	120.1
Cl2—Cu3—Cl3	103.49 (7)	C13—C14—H14	120.1
C6—S1—S2	107.8 (3)	N3—C15—C14	123.6 (8)
C5—S2—S1	103.9 (3)	N3—C15—H15	118.2
C16—S3—S4	105.1 (3)	C14—C15—H15	118.2
C11—S4—S3	107.5 (3)	N4—C16—C17	124.1 (7)
C25—S5—S6	102.2 (3)	N4—C16—S3	116.8 (5)
C26—S6—S5	107.7 (3)	C17—C16—S3	119.0 (6)
C1—N1—C5	116.7 (7)	C16—C17—C18	117.6 (8)
C1—N1—Cu1	123.3 (5)	C16—C17—H17	121.2
C5—N1—Cu1	119.8 (5)	C18—C17—H17	121.2
C6—N2—C10	116.3 (7)	C19—C18—C17	120.1 (9)
C6—N2—Cu1	127.9 (6)	C19—C18—H18	119.9
C10—N2—Cu1	115.8 (5)	C17—C18—H18	119.9
C15—N3—C11	116.6 (7)	C18—C19—C20	118.0 (8)
C15—N3—Cu2	115.6 (5)	C18—C19—H19	121.0
C11—N3—Cu2	127.8 (5)	C20—C19—H19	121.0
C20—N4—C16	116.9 (7)	N4—C20—C19	123.3 (8)
C20—N4—Cu2	121.6 (5)	N4—C20—H20	118.4
C16—N4—Cu2	121.2 (5)	C19—C20—H20	118.4
C30—N5—C26	115.7 (7)	N6—C21—C22	123.6 (7)
C30—N5—Cu3	116.7 (5)	N6—C21—H21	118.2
C26—N5—Cu3	127.1 (5)	C22—C21—H21	118.2
C25—N6—C21	116.5 (6)	C21—C22—C23	118.3 (8)
C25—N6—Cu3	119.6 (5)	C21—C22—H22	120.8
C21—N6—Cu3	121.4 (5)	C23—C22—H22	120.8
N1—C1—C2	122.8 (8)	C24—C23—C22	119.9 (8)
N1—C1—H1	118.6	C24—C23—H23	120.0
C2—C1—H1	118.6	C22—C23—H23	120.0
C1—C2—C3	119.9 (8)	C23—C24—C25	118.1 (8)
C1—C2—H2	120.1	C23—C24—H24	121.0
C3—C2—H2	120.1	C25—C24—H24	121.0
C4—C3—C2	117.6 (8)	N6—C25—C24	123.6 (7)
C4—C3—H3	121.2	N6—C25—S5	116.6 (6)
C2—C3—H3	121.2	C24—C25—S5	119.8 (6)
C3—C4—C5	120.9 (9)	N5—C26—C27	123.2 (8)
C3—C4—H4	119.6	N5—C26—S6	120.0 (6)
C5—C4—H4	119.6	C27—C26—S6	116.6 (6)
N1—C5—C4	122.1 (8)	C26—C27—C28	120.7 (8)
N1—C5—S2	117.0 (6)	C26—C27—H27	119.7
C4—C5—S2	120.8 (7)	C28—C27—H27	119.7
N2—C6—C7	123.3 (8)	C27—C28—C29	117.9 (8)

N2—C6—S1	121.1 (6)	C27—C28—H28	121.1
C7—C6—S1	115.4 (6)	C29—C28—H28	121.1
C8—C7—C6	117.4 (8)	C30—C29—C28	117.6 (9)
C8—C7—H7	121.3	C30—C29—H29	121.2
C6—C7—H7	121.3	C28—C29—H29	121.2
C9—C8—C7	120.4 (9)	N5—C30—C29	124.8 (8)
C9—C8—H8	119.8	N5—C30—H30	117.6
C7—C8—H8	119.8	C29—C30—H30	117.6
N4—Cu2—Cu3—N6	178.2 (3)	Cu1—N1—C1—C2	172.4 (6)
N3—Cu2—Cu3—N6	−7.0 (3)	N1—C1—C2—C3	1.4 (13)
Cl3—Cu2—Cu3—N6	83.4 (2)	C1—C2—C3—C4	0.0 (13)
Cl2—Cu2—Cu3—N6	−98.6 (2)	C2—C3—C4—C5	−0.4 (14)
N4—Cu2—Cu3—N5	6.7 (3)	C1—N1—C5—C4	1.8 (11)
N3—Cu2—Cu3—N5	−178.4 (3)	Cu1—N1—C5—C4	−173.1 (6)
Cl3—Cu2—Cu3—N5	−88.0 (2)	C1—N1—C5—S2	178.0 (5)
Cl2—Cu2—Cu3—N5	90.0 (2)	Cu1—N1—C5—S2	3.2 (8)
N4—Cu2—Cu3—Cl2	−83.3 (2)	C3—C4—C5—N1	−0.5 (14)
N3—Cu2—Cu3—Cl2	91.5 (2)	C3—C4—C5—S2	−176.6 (7)
Cl3—Cu2—Cu3—Cl2	−178.07 (9)	S1—S2—C5—N1	72.0 (6)
N4—Cu2—Cu3—Cl3	94.8 (2)	S1—S2—C5—C4	−111.7 (7)
N3—Cu2—Cu3—Cl3	−90.4 (2)	C10—N2—C6—C7	1.8 (11)
Cl2—Cu2—Cu3—Cl3	178.07 (9)	Cu1—N2—C6—C7	−175.6 (6)
N1—Cu1—Cl1—Cu1^{i}	−117.82 (19)	C10—N2—C6—S1	177.3 (5)
N2—Cu1—Cl1—Cu1^{i}	111.39 (18)	Cu1—N2—C6—S1	−0.1 (9)
Cl1^{i}—Cu1—Cl1—Cu1^{i}	0.0	S2—S1—C6—N2	42.7 (6)
N6—Cu3—Cl2—Cu2	109.55 (19)	S2—S1—C6—C7	−141.5 (6)
N5—Cu3—Cl2—Cu2	−114.5 (2)	N2—C6—C7—C8	−0.5 (12)
Cl3—Cu3—Cl2—Cu2	−1.55 (7)	S1—C6—C7—C8	−176.2 (6)
N4—Cu2—Cl2—Cu3	118.35 (17)	C6—C7—C8—C9	−2.2 (13)
N3—Cu2—Cl2—Cu3	−108.39 (18)	C7—C8—C9—C10	3.4 (13)
Cl3—Cu2—Cl2—Cu3	1.56 (7)	C6—N2—C10—C9	−0.5 (11)
N4—Cu2—Cl3—Cu3	−112.90 (19)	Cu1—N2—C10—C9	177.2 (6)
N3—Cu2—Cl3—Cu3	109.4 (2)	C8—C9—C10—N2	−2.1 (12)
Cl2—Cu2—Cl3—Cu3	−1.53 (7)	C15—N3—C11—C12	−3.8 (11)
N6—Cu3—Cl3—Cu2	−116.99 (19)	Cu2—N3—C11—C12	176.5 (6)
N5—Cu3—Cl3—Cu2	115.18 (19)	C15—N3—C11—S4	−178.2 (5)
Cl2—Cu3—Cl3—Cu2	1.58 (7)	Cu2—N3—C11—S4	2.1 (9)
C6—S1—S2—C5	−103.2 (4)	S3—S4—C11—N3	−46.4 (6)
C16—S3—S4—C11	104.1 (4)	S3—S4—C11—C12	138.9 (5)
C25—S5—S6—C26	−105.7 (4)	N3—C11—C12—C13	2.7 (12)
N2—Cu1—N1—C1	138.7 (6)	S4—C11—C12—C13	177.3 (6)
Cl1^{i}—Cu1—N1—C1	−87.8 (6)	C11—C12—C13—C14	−1.0 (12)
Cl1—Cu1—N1—C1	20.4 (6)	C12—C13—C14—C15	0.7 (12)
N2—Cu1—N1—C5	−46.8 (7)	C11—N3—C15—C14	3.5 (11)
Cl1^{i}—Cu1—N1—C5	86.7 (6)	Cu2—N3—C15—C14	−176.8 (6)
Cl1—Cu1—N1—C5	−165.1 (5)	C13—C14—C15—N3	−2.0 (13)
N1—Cu1—N2—C6	12.4 (7)	C20—N4—C16—C17	−0.4 (11)

Cl1^{i}—Cu1—N2—C6	−123.5 (6)	Cu2—N4—C16—C17	172.6 (6)
Cl1—Cu1—N2—C6	130.3 (6)	C20—N4—C16—S3	−177.4 (5)
N1—Cu1—N2—C10	−165.0 (5)	Cu2—N4—C16—S3	−4.3 (8)
Cl1^{i}—Cu1—N2—C10	59.1 (5)	S4—S3—C16—N4	−69.1 (6)
Cl1—Cu1—N2—C10	−47.1 (5)	S4—S3—C16—C17	113.7 (6)
N4—Cu2—N3—C15	170.8 (5)	N4—C16—C17—C18	−2.2 (12)
Cl3—Cu2—N3—C15	−58.6 (6)	S3—C16—C17—C18	174.7 (6)
Cl2—Cu2—N3—C15	49.6 (6)	C16—C17—C18—C19	2.3 (13)
Cu3—Cu2—N3—C15	−3.8 (6)	C17—C18—C19—C20	0.1 (13)
N4—Cu2—N3—C11	−9.5 (7)	C16—N4—C20—C19	3.0 (10)
Cl3—Cu2—N3—C11	121.2 (6)	Cu2—N4—C20—C19	−170.0 (6)
Cl2—Cu2—N3—C11	−130.6 (6)	C18—C19—C20—N4	−2.9 (12)
Cu3—Cu2—N3—C11	175.9 (5)	C25—N6—C21—C22	−0.9 (10)
N3—Cu2—N4—C20	−143.4 (5)	Cu3—N6—C21—C22	161.1 (6)
Cl3—Cu2—N4—C20	88.7 (5)	N6—C21—C22—C23	−0.1 (11)
Cl2—Cu2—N4—C20	−21.4 (6)	C21—C22—C23—C24	1.8 (11)
Cu3—Cu2—N4—C20	30.8 (6)	C22—C23—C24—C25	−2.3 (11)
N3—Cu2—N4—C16	43.8 (6)	C21—N6—C25—C24	0.3 (11)
Cl3—Cu2—N4—C16	−84.0 (5)	Cu3—N6—C25—C24	−162.0 (6)
Cl2—Cu2—N4—C16	165.9 (5)	C21—N6—C25—S5	−179.2 (5)
Cu3—Cu2—N4—C16	−141.9 (5)	Cu3—N6—C25—S5	18.4 (8)
N6—Cu3—N5—C30	−165.7 (5)	C23—C24—C25—N6	1.3 (11)
Cl2—Cu3—N5—C30	61.9 (5)	C23—C24—C25—S5	−179.2 (6)
Cl3—Cu3—N5—C30	−48.7 (5)	S6—S5—C25—N6	61.2 (6)
Cu2—Cu3—N5—C30	5.6 (6)	S6—S5—C25—C24	−118.3 (6)
N6—Cu3—N5—C26	5.9 (7)	C30—N5—C26—C27	2.9 (11)
Cl2—Cu3—N5—C26	−126.5 (6)	Cu3—N5—C26—C27	−168.7 (6)
Cl3—Cu3—N5—C26	122.8 (6)	C30—N5—C26—S6	178.4 (5)
Cu2—Cu3—N5—C26	177.2 (5)	Cu3—N5—C26—S6	6.8 (9)
N5—Cu3—N6—C25	−56.6 (6)	S5—S6—C26—N5	43.0 (6)
Cl2—Cu3—N6—C25	73.3 (6)	S5—S6—C26—C27	−141.2 (6)
Cl3—Cu3—N6—C25	−175.4 (5)	N5—C26—C27—C28	−1.5 (12)
Cu2—Cu3—N6—C25	132.1 (5)	S6—C26—C27—C28	−177.1 (6)
N5—Cu3—N6—C21	142.0 (5)	C26—C27—C28—C29	−1.9 (12)
Cl2—Cu3—N6—C21	−88.2 (5)	C27—C28—C29—C30	3.6 (12)
Cl3—Cu3—N6—C21	23.1 (6)	C26—N5—C30—C29	−1.0 (11)
Cu2—Cu3—N6—C21	−29.4 (6)	Cu3—N5—C30—C29	171.5 (6)
C5—N1—C1—C2	−2.3 (11)	C28—C29—C30—N5	−2.2 (13)

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Fig. 1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