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Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*d*)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*e*)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*f*)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*g*)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*a*)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*h*)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*b*)	10.1107/S1600536807056498	XIRJEO
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*i*)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-κ^2N,N')-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)

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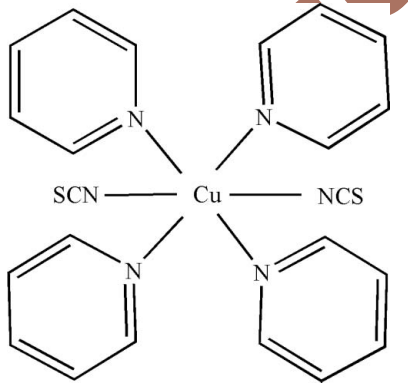
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.116; data-to-parameter ratio = 17.1.

In the molecule of the title complex, $[Cu(NCS)_2(C_5H_5N)_4]$, the Cu^{II} atom is bonded in a distorted octahedral arrangement to two N atoms of two SCN^- and four N atoms of four pyridine ligands. A crystallographic twofold rotation axis passes through the Cu atom, and the N and *para*-C atoms of two *trans* pyridine rings. In the crystal structure, weak π–π stacking interactions cause the formation of a supramolecular network structure.

Related literature

For a related structure see: Zhong *et al.* (2007).



Experimental

Crystal data

$[Cu(NCS)_2(C_5H_5N)_4]$
M_r = 496.10
Monoclinic, $C2/c$
a = 10.890 (4) Å
b = 14.737 (5) Å
c = 14.692 (4) Å
β = 90.517 (6)°
V = 2357.9 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 273 (2) K
0.25 × 0.16 × 0.07 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.763, T_{max} = 0.925
7961 measured reflections
2465 independent reflections
1680 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.03
2465 reflections
144 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.159 (2)	Cu1—N3	2.119 (3)
Cu1—N2	2.158 (3)	Cu1—N4	2.038 (2)
N1—Cu1—N2	89.68 (6)	N2—Cu1—N3	180
N1—Cu1—N3	90.32 (6)	N2—Cu1—N4	88.66 (7)
N1—Cu1—N4	90.02 (10)	N3—Cu1—N4	91.34 (7)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2232).

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supplementary materials

Acta Cryst. (2007). E**63**, m1445 [**doi:10.1107/S160053680701879X**]

Tetrakis(pyridine-*κN*)bis(thiocyanato-*κN*)copper(II)

H. Zhong, X.-R. Zeng, X.-M. Yang and Q.-Y. Luo

Comment

The crystal structure of Tetrakis(pyridine-*N*)dithiocyanatocobalt(II),(II), has previously been reported (Zhong *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We herein report the crystal structure of (I).

In the molecule of (I), (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The two N atoms of two SCN^- and four N atoms of four pyridine ligands are coordinated to the Cu atom, in a distorted octahedral arrangement (Table 1). A crystallographic twofold rotation axis passes through the Cu atom, and the N and *para*-C atoms of two *trans* pyridine rings·The planar pyridine rings A (N1/C1—C5), B (N2/C6A/C7A/C6—C8) and C (N3/C9A/C10A/C9—C11) are nearly perpendicular to each other, with dihedral angles of A/B = 110.72 (5), A/C = 87.11 (7) and B/C = 87.22 (5)°, as in (II).

In the crystal structure, the weak π-π stacking interactions, involving the adjacent pyridine rings with centroid-centroid distance of 3.481 (7) %A [symmetry code: 1 − *x*, 2 − *y*, 1 − *z*], cause the formation of a supramolecular network structure (Fig. 2). The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a Teflon-lined Parr bomb (23 ml), which was then sealed. Copper dinitrate trihydrate (72.5 mg, 0.3 mmol), potassium thiocyanate (58.3 mg, 0.6 mmol), pyridine (2.5 ml), and distilled water (6 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure for 4 d at 393 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small green crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

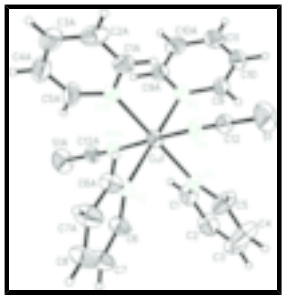


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): 2 − *x*, *y*, *z*].

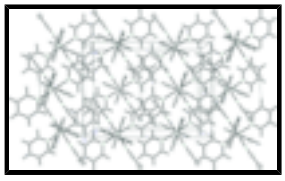


Fig. 2. A packing diagram for (I). The π-π interactions are shown as dashed lines.

Tetrakis(pyridine-κ*N*)bis(thiocyanato-κ*N*)copper(II)

Crystal data

$[Cu(NCS)_2(C_5H_5N)_4]$	F_{000} = 1020
M_r = 496.10	D_x = 1.398 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2304 reflections
a = 10.890 (4) Å	θ = 2.3–23.8°
b = 14.737 (5) Å	μ = 1.12 mm^{-1}
c = 14.692 (4) Å	*T* = 273 (2) K
β = 90.517 (6)°	Block, green
V = 2357.9 (13) Å^3	0.25 × 0.16 × 0.07 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	2465 independent reflections
Radiation source: fine-focus sealed tube	1680 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 273(2) K	θ_{max} = 26.7°
φ and ω scans	θ_{min} = 2.3°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −13→13
T_{min} = 0.763, T_{max} = 0.925	*k* = −18→18
7961 measured reflections	*l* = −18→18

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.116$

$S = 1.03$

2465 reflections

144 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 1.9905P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.29$ e Å^{-3}

$\Delta\rho_{min} = -0.38$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0010 (3)

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	1.0000	0.64045 (3)	0.2500	0.0502 (2)
S1	1.36255 (10)	0.63311 (8)	0.06607 (9)	0.1004 (4)
N1	0.8932 (2)	0.63964 (15)	0.12550 (16)	0.0510 (6)
N2	1.0000	0.4940 (2)	0.2500	0.0511 (8)
N3	1.0000	0.7842 (2)	0.2500	0.0503 (8)
N4	1.1577 (2)	0.63721 (17)	0.17641 (17)	0.0578 (6)
C1	0.7736 (3)	0.6587 (2)	0.1248 (2)	0.0699 (9)
H1	0.7389	0.6816	0.1776	0.084*
C2	0.6990 (3)	0.6459 (3)	0.0496 (3)	0.0875 (12)
H2	0.6161	0.6608	0.0520	0.105*
C3	0.7470 (5)	0.6116 (3)	−0.0275 (3)	0.0940 (13)
H3	0.6981	0.6007	−0.0786	0.113*
C4	0.8669 (4)	0.5941 (4)	−0.0278 (3)	0.1117 (17)
H4	0.9030	0.5713	−0.0801	0.134*
C5	0.9372 (3)	0.6093 (3)	0.0476 (2)	0.0875 (12)
H5	1.0210	0.5976	0.0442	0.105*

C6	0.9018 (3)	0.4462 (2)	0.2236 (2)	0.0640 (8)
H6	0.8313	0.4777	0.2064	0.077*
C7	0.8990 (4)	0.3538 (3)	0.2204 (3)	0.0889 (12)
H7	0.8297	0.3238	0.1985	0.107*
C8	1.0000	0.3054 (4)	0.2500	0.0995 (19)
H8	1.0000	0.2423	0.2500	0.119*
C9	1.0416 (3)	0.8318 (2)	0.1787 (2)	0.0584 (8)
H9	1.0711	0.8003	0.1286	0.070*
C10	1.0425 (3)	0.9244 (2)	0.1763 (2)	0.0740 (9)
H10	1.0716	0.9547	0.1253	0.089*
C11	1.0000	0.9729 (4)	0.2500	0.0814 (15)
H11	1.0000	1.0360	0.2500	0.098*
C12	1.2431 (2)	0.63577 (19)	0.13021 (19)	0.0502 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0419 (3)	0.0570 (3)	0.0519 (3)	0.000	0.01060 (19)	0.000
S1	0.0726 (7)	0.1203 (9)	0.1094 (9)	0.0010 (6)	0.0537 (6)	0.0005 (7)
N1	0.0466 (13)	0.0534 (14)	0.0531 (14)	0.0006 (11)	0.0031 (10)	−0.0012 (11)
N2	0.0443 (18)	0.0478 (19)	0.061 (2)	0.000	0.0023 (15)	0.000
N3	0.0452 (18)	0.054 (2)	0.0521 (19)	0.000	0.0015 (14)	0.000
N4	0.0434 (13)	0.0701 (17)	0.0600 (15)	0.0017 (11)	0.0138 (11)	−0.0002 (12)
C1	0.0517 (19)	0.088 (3)	0.070 (2)	0.0120 (16)	0.0027 (15)	0.0121 (17)
C2	0.052 (2)	0.106 (3)	0.104 (3)	−0.004 (2)	−0.0178 (19)	0.026 (3)
C3	0.101 (3)	0.095 (3)	0.085 (3)	−0.002 (2)	−0.039 (2)	−0.014 (2)
C4	0.098 (3)	0.163 (5)	0.074 (3)	0.035 (3)	−0.021 (2)	−0.042 (3)
C5	0.066 (2)	0.133 (4)	0.064 (2)	0.027 (2)	−0.0068 (17)	−0.029 (2)
C6	0.0515 (18)	0.058 (2)	0.082 (2)	−0.0034 (15)	−0.0025 (15)	0.0017 (17)
C7	0.070 (2)	0.061 (2)	0.135 (4)	−0.0104 (19)	−0.017 (2)	0.000 (2)
C8	0.094 (4)	0.049 (3)	0.155 (6)	0.000	−0.014 (4)	0.000
C9	0.0595 (19)	0.0592 (19)	0.0566 (18)	−0.0025 (15)	0.0032 (14)	0.0063 (15)
C10	0.086 (2)	0.064 (2)	0.071 (2)	−0.0089 (19)	−0.0028 (18)	0.0155 (18)
C11	0.097 (4)	0.053 (3)	0.093 (4)	0.000	−0.010 (3)	0.000
C12	0.0442 (16)	0.0526 (17)	0.0538 (16)	0.0050 (12)	0.0063 (12)	−0.0005 (13)

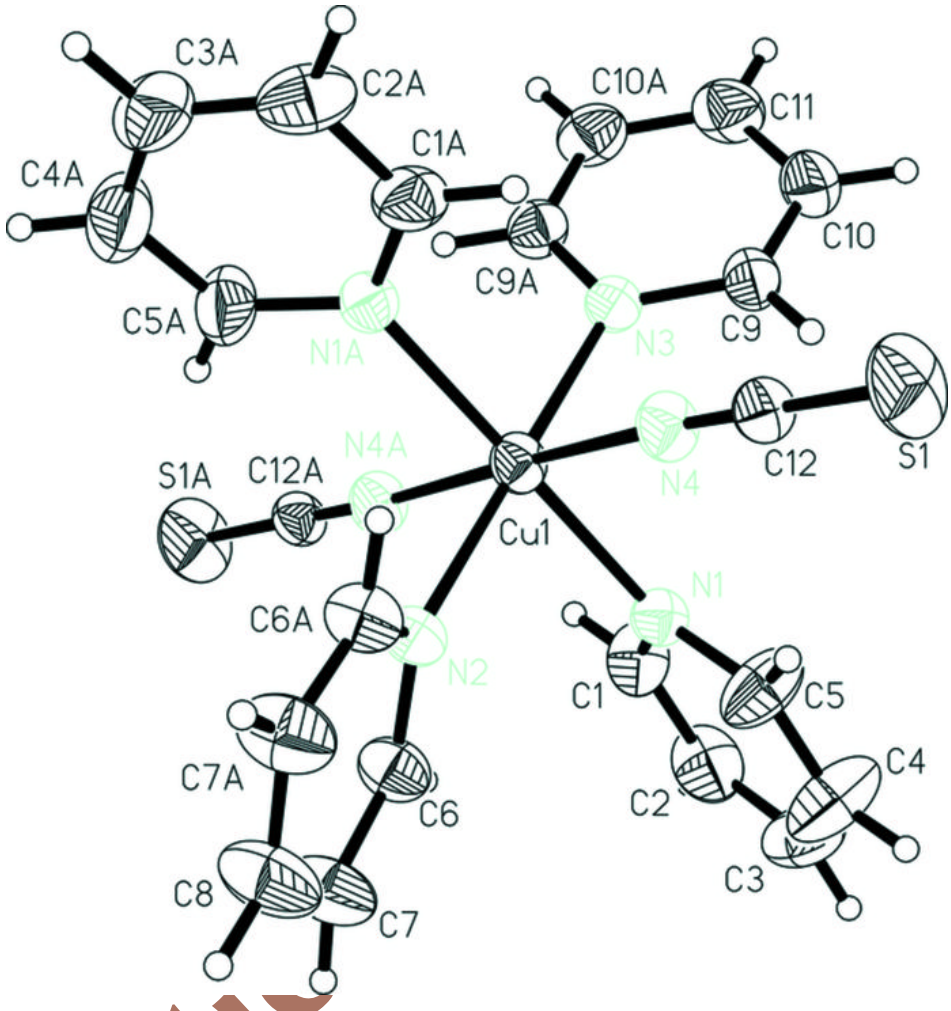
Geometric parameters (Å, °)

Cu1—N1	2.159 (2)	C3—C4	1.331 (6)
Cu1—N2	2.158 (3)	C3—H3	0.9300
Cu1—N3	2.119 (3)	C4—C5	1.359 (5)
Cu1—N4	2.038 (2)	C4—H4	0.9300
Cu1—N4^{i}	2.038 (2)	C5—H5	0.9300
Cu1—N1^{i}	2.159 (2)	C6—C7	1.362 (5)
S1—C12	1.613 (3)	C6—H6	0.9300
N1—C5	1.323 (4)	C7—C8	1.378 (5)
N1—C1	1.332 (4)	C7—H7	0.9300
N2—C6	1.336 (3)	C8—C7^{i}	1.378 (5)

N2—C6^{i}	1.336 (3)	C8—H8	0.9300
N3—C9^{i}	1.343 (3)	C9—C10	1.365 (5)
N3—C9	1.343 (3)	C9—H9	0.9300
N4—C12	1.157 (4)	C10—C11	1.381 (4)
C1—C2	1.379 (5)	C10—H10	0.9300
C1—H1	0.9300	C11—C10^{i}	1.381 (4)
C2—C3	1.351 (6)	C11—H11	0.9300
C2—H2	0.9300		
N1—Cu1—N2	89.68 (6)	C1—C2—H2	120.2
N1—Cu1—N3	90.32 (6)	C4—C3—C2	117.5 (4)
N1—Cu1—N4	90.02 (10)	C4—C3—H3	121.2
N2—Cu1—N3	180.000 (1)	C2—C3—H3	121.2
N2—Cu1—N4	88.66 (7)	C3—C4—C5	120.7 (4)
N3—Cu1—N4	91.34 (7)	C3—C4—H4	119.6
N4^{i}—Cu1—N4	177.31 (14)	C5—C4—H4	119.6
N4^{i}—Cu1—N3	91.34 (7)	N1—C5—C4	123.7 (4)
N4^{i}—Cu1—N2	88.66 (7)	N1—C5—H5	118.1
N4^{i}—Cu1—N1^{i}	90.02 (10)	C4—C5—H5	118.1
N4—Cu1—N1^{i}	89.97 (10)	N2—C6—C7	123.7 (3)
N3—Cu1—N1^{i}	90.32 (6)	N2—C6—H6	118.1
N2—Cu1—N1^{i}	89.68 (6)	C7—C6—H6	118.1
N4^{i}—Cu1—N1	89.97 (10)	C6—C7—C8	119.3 (4)
N1^{i}—Cu1—N1	179.37 (12)	C6—C7—H7	120.4
C5—N1—C1	115.2 (3)	C8—C7—H7	120.4
C5—N1—Cu1	122.6 (2)	C7^{i}—C8—C7	117.6 (5)
C1—N1—Cu1	121.6 (2)	C7^{i}—C8—H8	121.2
C6—N2—C6^{i}	116.2 (4)	C7—C8—H8	121.2
C6—N2—Cu1	121.88 (18)	N3—C9—C10	123.0 (3)
C6^{i}—N2—Cu1	121.88 (18)	N3—C9—H9	118.5
C9^{i}—N3—C9	117.0 (4)	C10—C9—H9	118.5
C9^{i}—N3—Cu1	121.49 (19)	C9—C10—C11	119.6 (3)
C9—N3—Cu1	121.49 (19)	C9—C10—H10	120.2
C12—N4—Cu1	176.1 (3)	C11—C10—H10	120.2
N1—C1—C2	123.2 (3)	C10^{i}—C11—C10	117.7 (5)
N1—C1—H1	118.4	C10^{i}—C11—H11	121.1
C2—C1—H1	118.4	C10—C11—H11	121.1
C3—C2—C1	119.6 (4)	N4—C12—S1	179.6 (3)
C3—C2—H2	120.2		

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

Fig. 1


C3A
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C10A
C11
C1A
C4A
C10
C9A
C5A
N1A
N3
C9
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S1A
C12A
N4
C12
S1
Cu1
N1
C6A
N2
C1
C5
C4
C7A
C6
C2
C8
C3
C7

Fig. 2