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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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Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)

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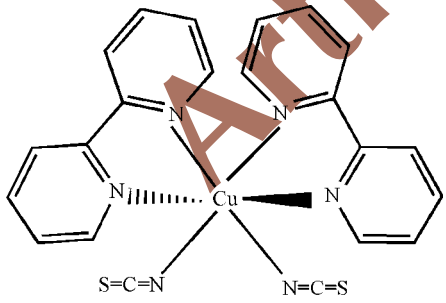
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.159; data-to-parameter ratio = 16.8.

In the molecule of the title compound, $[Cu(NCS)_2(C_{10}H_8N_2)_2]$, the Cu^{II} atom is six-coordinated by the four N atoms of two 2,2′-bipyridyl ligands and the two N atoms of two thiocyanate ligands, in a distorted octahedral arrangement. In the crystal structure, intramolecular C—H···N and intermolecular C—H···S hydrogen bonds and π–π stacking interactions, with a centroid–centroid distance of 3.573 (2) Å, lead to a supramolecular network structure.

Related literature

For a related structure, see: Zhong *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(NCS)_2(C_{10}H_8N_2)_2]$
M_r = 492.07
Orthorhombic, *Pbca*
a = 15.981 (4) Å
b = 15.997 (2) Å
c = 16.9947 (18) Å
V = 4344.7 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 273 (2) K
0.36 × 0.34 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.661, T_{max} = 0.768
28695 measured reflections
4708 independent reflections
3481 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.159
S = 1.02
4708 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.073 (2)	Cu1—N4	2.138 (2)
Cu1—N2	2.072 (2)	Cu1—N5	2.147 (2)
Cu1—N3	2.172 (2)	Cu1—N6	2.169 (2)
N1—Cu1—N2	99.34 (11)	N2—Cu1—N6	91.21 (9)
N1—Cu1—N3	91.25 (9)	N3—Cu1—N4	75.54 (8)
N1—Cu1—N4	94.60 (9)	N3—Cu1—N5	99.08 (8)
N1—Cu1—N5	90.57 (9)	N3—Cu1—N6	81.24 (8)
N1—Cu1—N6	163.33 (9)	N4—Cu1—N5	172.59 (8)
N2—Cu1—N3	164.51 (10)	N4—Cu1—N6	97.86 (8)
N2—Cu1—N4	92.26 (9)	N5—Cu1—N6	76.08 (8)
N2—Cu1—N5	92.13 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···N1	0.93	2.59	3.135 (4)	118
C12—H12···N2	0.93	2.61	3.150 (4)	117
C4—H4···S1^{i}	0.93	2.83	3.712 (3)	159

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

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: HK2290).

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supplementary materials

Acta Cryst. (2007). E**63**, m2141 [**doi:10.1107/S1600536807033181**]

Bis(2,2'-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)

H. Zhong, X.-M. Yang, Q.-Y. Luo and Y.-P. Xu

Comment

The crystal structure of bis[(2,2'-bipyridyl-κ^2N,N')bis(thiocyanato-κN)] nickel(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).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six-coordinate environment of the Cu atom is completed by the four N atoms of two 2,2'-bipyridyl ligands and two N atoms of two SCN^- ligands, in a distorted octahedral arrangement (Table 1). The Cu—N bonds [average 2.156 (4) Å] of the 2,2'-bipyridyl ligands are somewhat longer than the Cu—N bonds [average 2.073 (2) Å] for the SCN^- ligands. The two 2,2'-bipyridyl ligands are nearly perpendicular to each other, with a dihedral angle of 105.7 (4) °, as in (II).

In the crystal structure, intramolecular C—H···N and intermolecular C—H···S hydrogen bonds and π-π stacking interactions, with a centroid-centroid distance of 3.573 (2) Å [symmetry code: 2 − *x*, 1 − *y*, −*z*] lead to a supramolecular network structure (Fig. 2), as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Copper dinitrate hexahydrate (88.7 mg, 0.3 mmol), 2,2'-bipyridyl (93.6 mg, 0.6 mmol), potassium thiocyanate (58.4 mg, 0.6 mmol) and distilled water (4 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small blue 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, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

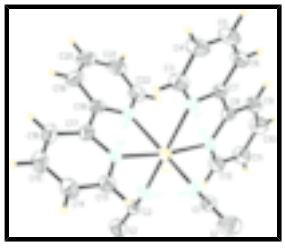

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

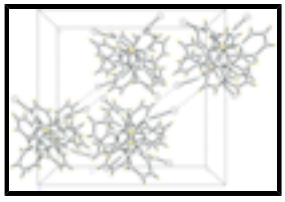

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Bis(2,2'-bipyridyl-k^2N,N')bis (isothiocyanato-kN)copper(II)

Crystal data

$[Cu(NCS)_2(C_{10}H_8N_2)_2]$	F_{000} = 2008
M_r = 492.07	D_x = 1.505 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 11573 reflections
a = 15.981 (4) Å	θ = 2.4–27.2°
b = 15.997 (2) Å	μ = 1.22 mm^{-1}
c = 16.9947 (18) Å	*T* = 273 (2) K
V = 4344.7 (13) Å^3	Block, blue
Z = 8	0.36 × 0.34 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4708 independent reflections
Radiation source: fine-focus sealed tube	3481 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 273(2) K	θ_{max} = 27.0°
φ and ω scans	θ_{min} = 2.2°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→20
T_{min} = 0.661, T_{max} = 0.768	*k* = −20→20
28695 measured reflections	*l* = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.159$

$S = 1.02$

4708 reflections

280 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1098P)^2 + 0.816P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.48$ e Å^{-3}

$\Delta\rho_{min} = -0.88$ e Å^{-3}

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	0.70224 (2)	0.38400 (2)	−0.000711 (17)	0.04902 (16)
S1	0.57516 (6)	0.51149 (7)	−0.22514 (5)	0.0814 (3)
S2	0.51121 (6)	0.22560 (5)	0.15952 (5)	0.0732 (3)
N1	0.62899 (16)	0.44609 (15)	−0.08263 (15)	0.0641 (6)
N2	0.60959 (15)	0.31786 (15)	0.05761 (16)	0.0599 (6)
N3	0.80970 (13)	0.46127 (13)	−0.02964 (14)	0.0476 (5)
N4	0.69877 (12)	0.48310 (13)	0.08362 (13)	0.0476 (5)
N5	0.72280 (12)	0.28371 (12)	−0.08243 (12)	0.0455 (5)
N6	0.79904 (12)	0.30930 (14)	0.05457 (13)	0.0480 (5)
C1	0.60600 (16)	0.47314 (16)	−0.14211 (18)	0.0523 (6)
C2	0.56808 (15)	0.28035 (15)	0.09985 (16)	0.0474 (6)
C3	0.86341 (18)	0.4456 (2)	−0.08797 (16)	0.0633 (7)
H3	0.8548	0.3983	−0.1188	0.076*
C4	0.9306 (2)	0.4959 (2)	−0.1045 (2)	0.0783 (10)
H4	0.9667	0.4837	−0.1459	0.094*
C5	0.9426 (2)	0.5644 (2)	−0.0580 (2)	0.0803 (10)
H5	0.9872	0.6003	−0.0679	0.096*
C6	0.8892 (2)	0.5806 (2)	0.00314 (18)	0.0670 (8)
H6	0.8972	0.6271	0.0350	0.080*
C7	0.82324 (17)	0.52678 (16)	0.01687 (16)	0.0489 (6)
C8	0.76310 (15)	0.53800 (15)	0.08204 (15)	0.0469 (5)
C9	0.77042 (19)	0.5995 (2)	0.13901 (18)	0.0636 (7)

H9	0.8158	0.6359	0.1382	0.076*
C10	0.7112 (2)	0.6067 (2)	0.1961 (2)	0.0753 (9)
H10	0.7167	0.6471	0.2351	0.090*
C11	0.6435 (2)	0.5541 (2)	0.19573 (18)	0.0716 (8)
H11	0.6009	0.5599	0.2326	0.086*
C12	0.64040 (18)	0.49203 (18)	0.13903 (17)	0.0584 (7)
H12	0.5956	0.4549	0.1396	0.070*
C13	0.67722 (17)	0.26890 (17)	−0.14712 (17)	0.0547 (6)
H13	0.6373	0.3082	−0.1619	0.066*
C14	0.6864 (2)	0.1988 (2)	−0.19262 (19)	0.0666 (8)
H14	0.6531	0.1902	−0.2368	0.080*
C15	0.7460 (2)	0.1416 (2)	−0.1711 (2)	0.0729 (9)
H15	0.7537	0.0933	−0.2007	0.087*
C16	0.79439 (19)	0.15602 (19)	−0.1056 (2)	0.0669 (8)
H16	0.8356	0.1179	−0.0911	0.080*
C17	0.78159 (15)	0.22705 (16)	−0.06151 (16)	0.0493 (6)
C18	0.82897 (16)	0.24607 (18)	0.01153 (16)	0.0500 (6)
C19	0.89974 (18)	0.2015 (2)	0.0339 (2)	0.0700 (8)
H19	0.9205	0.1587	0.0024	0.084*
C20	0.93845 (19)	0.2220 (2)	0.1038 (3)	0.0847 (11)
H20	0.9858	0.1929	0.1200	0.102*
C21	0.9068 (2)	0.2862 (2)	0.1499 (2)	0.0757 (10)
H21	0.9316	0.3003	0.1976	0.091*
C22	0.83809 (19)	0.32779 (19)	0.12268 (17)	0.0613 (7)
H22	0.8170	0.3714	0.1529	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0490 (2)	0.0480 (2)	0.0500 (3)	−0.00325 (13)	0.00051 (12)	−0.00126 (12)
S1	0.0734 (5)	0.1012 (7)	0.0696 (6)	−0.0093 (5)	−0.0232 (4)	0.0129 (5)
S2	0.0793 (5)	0.0683 (5)	0.0719 (5)	−0.0118 (4)	0.0254 (4)	0.0008 (4)
N1	0.0711 (15)	0.0507 (13)	0.0704 (16)	0.0035 (11)	−0.0179 (13)	0.0021 (12)
N2	0.0540 (12)	0.0548 (13)	0.0709 (15)	−0.0063 (10)	0.0088 (12)	−0.0043 (11)
N3	0.0499 (11)	0.0492 (11)	0.0436 (11)	−0.0075 (9)	0.0025 (9)	0.0016 (9)
N4	0.0483 (11)	0.0467 (11)	0.0479 (12)	−0.0038 (8)	0.0015 (9)	−0.0044 (9)
N5	0.0459 (10)	0.0440 (11)	0.0466 (12)	−0.0006 (8)	0.0016 (9)	−0.0013 (8)
N6	0.0457 (11)	0.0521 (11)	0.0461 (12)	−0.0047 (9)	−0.0010 (9)	0.0048 (9)
C1	0.0456 (12)	0.0452 (13)	0.0662 (17)	0.0010 (10)	−0.0073 (12)	−0.0093 (12)
C2	0.0421 (11)	0.0446 (12)	0.0553 (15)	−0.0001 (10)	0.0035 (11)	−0.0088 (11)
C3	0.0641 (16)	0.0734 (18)	0.0525 (16)	−0.0135 (14)	0.0119 (13)	−0.0047 (14)
C4	0.0653 (18)	0.107 (3)	0.0622 (19)	−0.0238 (18)	0.0212 (15)	−0.0014 (18)
C5	0.0658 (19)	0.089 (2)	0.086 (2)	−0.0310 (18)	0.0113 (17)	0.0048 (19)
C6	0.0610 (18)	0.0634 (19)	0.077 (2)	−0.0193 (15)	−0.0002 (14)	−0.0054 (14)
C7	0.0467 (13)	0.0478 (14)	0.0521 (14)	−0.0040 (11)	−0.0053 (11)	0.0039 (11)
C8	0.0475 (12)	0.0454 (13)	0.0478 (14)	−0.0009 (10)	−0.0080 (10)	−0.0010 (10)
C9	0.0632 (16)	0.0641 (17)	0.0634 (18)	−0.0092 (14)	−0.0088 (15)	−0.0126 (14)
C10	0.088 (2)	0.079 (2)	0.0594 (19)	−0.0027 (17)	−0.0027 (16)	−0.0273 (17)

C11	0.077 (2)	0.082 (2)	0.0558 (17)	−0.0038 (17)	0.0122 (15)	−0.0174 (15)
C12	0.0619 (15)	0.0589 (15)	0.0543 (16)	−0.0038 (13)	0.0100 (13)	−0.0064 (12)
C13	0.0552 (14)	0.0554 (15)	0.0534 (16)	−0.0037 (12)	−0.0015 (12)	−0.0039 (12)
C14	0.0797 (19)	0.0658 (18)	0.0542 (17)	−0.0080 (15)	0.0005 (15)	−0.0129 (14)
C15	0.091 (2)	0.0601 (18)	0.068 (2)	0.0047 (17)	0.0143 (18)	−0.0178 (15)
C16	0.0740 (19)	0.0532 (16)	0.073 (2)	0.0134 (14)	0.0085 (15)	−0.0066 (14)
C17	0.0483 (12)	0.0502 (14)	0.0495 (15)	0.0000 (10)	0.0095 (11)	0.0004 (11)
C18	0.0391 (12)	0.0528 (14)	0.0582 (16)	−0.0020 (11)	0.0057 (11)	0.0104 (12)
C19	0.0486 (15)	0.0728 (19)	0.089 (2)	0.0112 (14)	0.0035 (16)	0.0164 (17)
C20	0.0504 (16)	0.095 (3)	0.109 (3)	0.0042 (16)	−0.0205 (18)	0.028 (2)
C21	0.0671 (19)	0.083 (2)	0.077 (2)	−0.0152 (17)	−0.0257 (17)	0.0176 (18)
C22	0.0678 (17)	0.0612 (16)	0.0548 (16)	−0.0096 (14)	−0.0100 (14)	0.0090 (13)

Geometric parameters (Å, °)

Cu1—N1	2.073 (2)	C7—C8	1.477 (4)
Cu1—N2	2.072 (2)	C8—C9	1.386 (4)
Cu1—N3	2.172 (2)	C9—C10	1.360 (5)
Cu1—N4	2.138 (2)	C9—H9	0.9300
Cu1—N5	2.147 (2)	C10—C11	1.372 (5)
Cu1—N6	2.169 (2)	C10—H10	0.9300
S1—C1	1.616 (3)	C11—C12	1.384 (4)
S2—C2	1.619 (3)	C11—H11	0.9300
N1—C1	1.159 (4)	C12—H12	0.9300
N2—C2	1.147 (3)	C13—C14	1.370 (4)
N3—C7	1.330 (3)	C13—H13	0.9300
N3—C3	1.335 (4)	C14—C15	1.371 (5)
N4—C12	1.333 (3)	C14—H14	0.9300
N4—C8	1.352 (3)	C15—C16	1.375 (5)
N5—C13	1.340 (3)	C15—H15	0.9300
N5—C17	1.353 (3)	C16—C17	1.376 (4)
N6—C18	1.337 (4)	C16—H16	0.9300
N6—C22	1.348 (4)	C17—C18	1.486 (4)
C3—C4	1.371 (4)	C18—C19	1.390 (4)
C3—H3	0.9300	C19—C20	1.379 (5)
C4—C5	1.365 (5)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.387 (5)
C5—C6	1.370 (5)	C20—H20	0.9300
C5—H5	0.9300	C21—C22	1.366 (4)
C6—C7	1.380 (4)	C21—H21	0.9300
C6—H6	0.9300	C22—H22	0.9300
N1—Cu1—N2	99.34 (11)	N4—C8—C9	120.8 (2)
N1—Cu1—N3	91.25 (9)	N4—C8—C7	115.5 (2)
N1—Cu1—N4	94.60 (9)	C9—C8—C7	123.7 (2)
N1—Cu1—N5	90.57 (9)	C10—C9—C8	120.0 (3)
N1—Cu1—N6	163.33 (9)	C10—C9—H9	120.0
N2—Cu1—N3	164.51 (10)	C8—C9—H9	120.0
N2—Cu1—N4	92.26 (9)	C9—C10—C11	119.6 (3)
N2—Cu1—N5	92.13 (9)	C9—C10—H10	120.2

N2—Cu1—N6	91.21 (9)	C11—C10—H10	120.2
N3—Cu1—N4	75.54 (8)	C10—C11—C12	118.1 (3)
N3—Cu1—N5	99.08 (8)	C10—C11—H11	120.9
N3—Cu1—N6	81.24 (8)	C12—C11—H11	120.9
N4—Cu1—N5	172.59 (8)	N4—C12—C11	122.9 (3)
N4—Cu1—N6	97.86 (8)	N4—C12—H12	118.5
N5—Cu1—N6	76.08 (8)	C11—C12—H12	118.5
C1—N1—Cu1	160.7 (2)	N5—C13—C14	123.4 (3)
C2—N2—Cu1	168.4 (2)	N5—C13—H13	118.3
C7—N3—C3	119.0 (2)	C14—C13—H13	118.3
C7—N3—Cu1	116.26 (18)	C13—C14—C15	118.0 (3)
C3—N3—Cu1	124.71 (19)	C13—C14—H14	121.0
C12—N4—C8	118.4 (2)	C15—C14—H14	121.0
C12—N4—Cu1	124.83 (18)	C16—C15—C14	119.6 (3)
C8—N4—Cu1	116.65 (16)	C16—C15—H15	120.2
C13—N5—C17	118.3 (2)	C14—C15—H15	120.2
C13—N5—Cu1	125.43 (17)	C15—C16—C17	119.7 (3)
C17—N5—Cu1	115.91 (17)	C15—C16—H16	120.1
C18—N6—C22	118.1 (2)	C17—C16—H16	120.1
C18—N6—Cu1	115.79 (18)	N5—C17—C16	120.9 (3)
C22—N6—Cu1	125.5 (2)	N5—C17—C18	115.9 (2)
N1—C1—S1	179.2 (3)	C16—C17—C18	123.2 (3)
N2—C2—S2	178.6 (2)	N6—C18—C19	122.0 (3)
N3—C3—C4	123.1 (3)	N6—C18—C17	115.5 (2)
N3—C3—H3	118.5	C19—C18—C17	122.5 (3)
C4—C3—H3	118.5	C20—C19—C18	118.5 (3)
C5—C4—C3	117.6 (3)	C20—C19—H19	120.7
C5—C4—H4	121.2	C18—C19—H19	120.7
C3—C4—H4	121.2	C19—C20—C21	120.0 (3)
C4—C5—C6	120.2 (3)	C19—C20—H20	120.0
C4—C5—H5	119.9	C21—C20—H20	120.0
C6—C5—H5	119.9	C22—C21—C20	117.5 (3)
C5—C6—C7	119.1 (3)	C22—C21—H21	121.2
C5—C6—H6	120.4	C20—C21—H21	121.2
C7—C6—H6	120.4	N6—C22—C21	123.8 (3)
N3—C7—C6	121.0 (3)	N6—C22—H22	118.1
N3—C7—C8	115.8 (2)	C21—C22—H22	118.1
C6—C7—C8	123.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···N1	0.93	2.59	3.135 (4)	118
C12—H12···N2	0.93	2.61	3.150 (4)	117
C4—H4···S1^{i}	0.93	2.83	3.712 (3)	159

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

Fig. 1

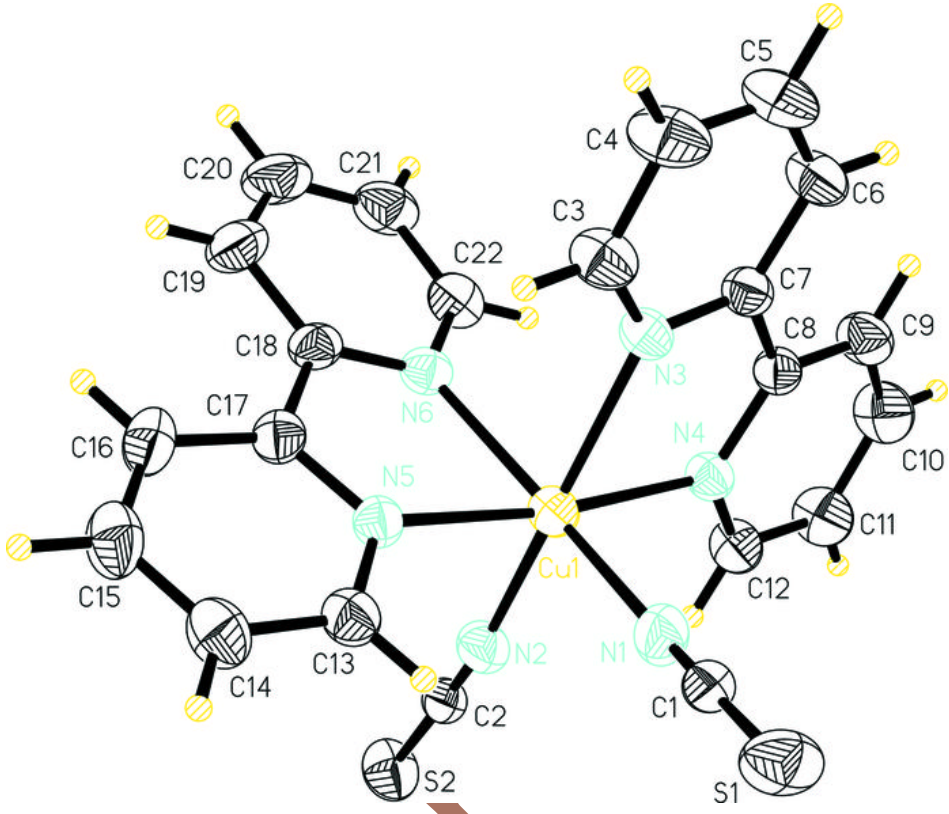

Fig. 2