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# *catena*-Poly[copper(I)-di-$\mu$-chlorido-copper(I)-bis[$\mu$-bis(pyrimidin-2-yl-sulfanyl)methane-$\kappa^2N:N'$]]

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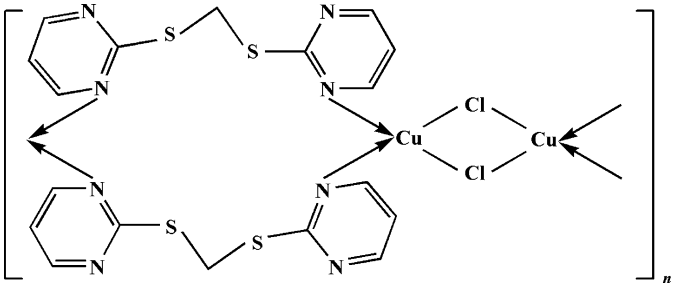
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.041; $wR$ factor = 0.101; data-to-parameter ratio = 15.7.

The flexible heterocyclic thioether ligand bis(pyrimidin-2-yl-sulfanyl)methane in the centrosymmetric title compound, $[Cu_2Cl_2(C_9H_8N_4S_2)_2]_n$, links $Cu_2Cl_2$ dimers into a chain. The chains are linked into a three-dimensional network through C—H···Cl hydrogen bonds. The $Cu^I$ atom is in a slightly distorted tetrahedral coordination environment.

## Related literature

For details of metal complexes of bis(pyrimidin-2-ylsulfanyl)-methane, see: Hou *et al.* (2005); Zheng *et al.* (2003). For complexes of other flexible thioether ligands, see: Bu *et al.* (2003); Hong *et al.* (2000); Zheng *et al.* (2005). For those with heterocyclic components, see: Peng *et al.* (2006); Song *et al.* (2005). For synthesis of the title compound, see: Xu *et al.* (1997).



## Experimental

### *Crystal data*

$[Cu_2Cl_2(C_9H_8N_4S_2)_2]$
$M_r$ = 670.61
Monoclinic, $C2/c$
$a$ = 12.3432 (13) Å
$b$ = 13.2611 (14) Å
$c$ = 15.5179 (17) Å
$\beta$ = 98.992 (2)°
$V$ = 2508.8 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.27 mm$^{-1}$
$T$ = 293 (2) K
0.20 × 0.18 × 0.15 mm

### *Data collection*

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.660, $T_{max}$ = 0.727
6900 measured reflections
2422 independent reflections
2032 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.101
$S$ = 1.06
2422 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2···Cl1$^{i}$ | 0.93 | 2.67 | 3.537 (4) | 155 |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); 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: SJ2325).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2314 [ **doi:10.1107/S160053680703913X** ]

# *catena*-Poly[copper(I)-di-$\mu$-chlorido-copper(I)-bis[$\mu$-bis(pyrimidin-2-ylsulfanyl)methane-$\kappa^2N$:$N'$]]

**W.-J. Shi and Z.-Q. Gong**

## Comment

Heterocyclic flexible thioethers containing nitrogen and sulfur donors have attracted much attention because of the flexibility and conformational freedoms. Previously, a series of flexible thioethers were designed, and the investigations on the formation of Ag(I) complexes with these ligands have been reported (Bu *et al.*, 2003; Hong *et al.*, 2000; Zheng *et al.*, 2003; Zheng *et al.*, 2005), while those on the $Cu^I$ complexes with heterocyclic flexible thioether ligands were much more sporadic (Peng *et al.*, 2006; Song *et al.*, 2005).

In the title compound, 1, Fig. 1, two chloride ions are each bound to two symmetry related $Cu^I$ centers forming a $Cu_2Cl_2$ core. Within these cores the $Cu^I$ centres are separated by a distance of 2.991 (3) Å. The dihedral angle between the two pyrimidyl rings is 83.9 (2) °, with interplanar angles between the S1—C1—S2 plane and the N1 and N3 pyrimidyl rings of the ligand 106.5 (2) ° and 73 (1) °, respectively.

There are weak intermolecular C—H···Cl interactions in the adjacent chain, furnishing a three-dimensional supramolecular array (Fig. 2).

## Experimental

The ligand bis(pyrimidin-2-ylsulfanyl)methane was synthesized according to the reported procedure (Xu *et al.*, 1997). Equimolar quantities (0.05 mmol) of solid CuCl (5.0 mg) was added to MeCN solution (7 ml) of the ligand (12.0 mg), the mixture was stirred until a small amount of precipitate was formed. The precipitate was filtered off, and the filtrate was allowed to stand at room temperature for two weeks, well shaped yellow crystals were obtained. Yield: 5.0 mg (30%).

## Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, $U_{iso}$=1.2$U_{eq}$ (C) for aromatic and 0.97 Å, $U_{iso}$ = 1.2$U_{eq}$ (C) for $CH_2$ atoms.

## Figures

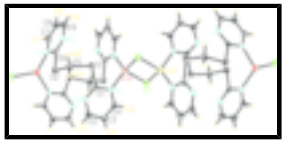

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level, Only the asymmetric unit and one of the symmetry related copper atoms are labelled. [symmetry code: (I) 3/2 − $x$, 1/2 − $y$, 1 − $z$].

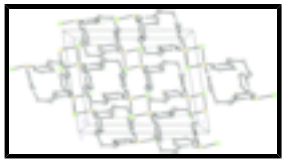

Fig. 2. A view of title compound, showing the extended three-dimensional structure linked by C—H···Cl hydrogen interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level, and H atoms are drawn as spheres of arbitrary radii.

**_catena_-Poly[copper(I)-di-μ-chlorido-copper(I)- bis[μ-bis(pyrimidin-2-ylsulfanyl)methane-κ$^2$*N*:*N*']]**

*Crystal data*

| | |
|---|---|
| $[Cu_2Cl_2(C_9H_8N_4S_2)_2]$ | $F_{000}$ = 1344 |
| $M_r$ = 670.61 | $D_x$ = 1.775 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 1888 reflections |
| *a* = 12.3432 (13) Å | θ = 2.5–23.6º |
| *b* = 13.2611 (14) Å | μ = 2.27 mm$^{-1}$ |
| *c* = 15.5179 (17) Å | *T* = 293 (2) K |
| β = 98.992 (2)º | Block, yellow |
| *V* = 2508.8 (5) Å$^3$ | 0.20 × 0.18 × 0.15 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEX area-detector diffractometer | 2422 independent reflections |
| Radiation source: fine-focus sealed tube | 2032 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.029 |
| *T* = 293(2) K | $\theta_{max}$ = 26.0º |
| φ and ω scans | $\theta_{min}$ = 2.3º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −15→13 |
| $T_{min}$ = 0.660, $T_{max}$ = 0.727 | *k* = −16→16 |
| 6900 measured reflections | *l* = −19→16 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.041 | H-atom parameters constrained |
| $wR(F^2)$ = 0.101 | $w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 1.7815P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.06 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 2422 reflections | $\Delta\rho_{max}$ = 0.53 e Å$^{-3}$ |
| 154 parameters | $\Delta\rho_{min}$ = −0.32 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 | 0.67661 (3) | 0.25183 (3) | 0.56808 (3) | 0.04173 (17) |
| S1 | 0.71478 (8) | 0.24875 (6) | 0.77139 (6) | 0.0457 (2) |
| Cl1 | 0.63766 (7) | 0.19728 (7) | 0.42107 (5) | 0.0492 (3) |
| N1 | 0.6667 (2) | 0.12565 (17) | 0.64085 (16) | 0.0339 (6) |
| C4 | 0.6342 (3) | 0.0371 (2) | 0.6037 (2) | 0.0403 (8) |
| H4 | 0.6262 | 0.0313 | 0.5433 | 0.048* |
| S2 | 0.57245 (7) | 0.22466 (6) | 0.91426 (6) | 0.0427 (2) |
| C3 | 0.6125 (3) | −0.0448 (2) | 0.6519 (2) | 0.0462 (9) |
| H3 | 0.5881 | −0.1055 | 0.6256 | 0.055* |
| N2 | 0.6603 (2) | 0.0539 (2) | 0.78057 (18) | 0.0431 (7) |
| C2 | 0.6283 (3) | −0.0331 (2) | 0.7404 (2) | 0.0487 (9) |
| H2 | 0.6163 | −0.0883 | 0.7747 | 0.058* |
| N3 | 0.6021 (2) | 0.4215 (2) | 0.8873 (2) | 0.0495 (7) |
| N4 | 0.4249 (2) | 0.36602 (19) | 0.90977 (16) | 0.0347 (6) |
| C1 | 0.6763 (2) | 0.1290 (2) | 0.7280 (2) | 0.0335 (7) |
| C5 | 0.7080 (3) | 0.2308 (3) | 0.8853 (2) | 0.0419 (8) |
| H5B | 0.7473 | 0.2857 | 0.9177 | 0.050* |
| H5A | 0.7463 | 0.1688 | 0.9042 | 0.050* |
| C6 | 0.5306 (3) | 0.3511 (2) | 0.9025 (2) | 0.0372 (7) |
| C7 | 0.3891 (3) | 0.4610 (2) | 0.8990 (2) | 0.0440 (8) |
| H7 | 0.3165 | 0.4750 | 0.9040 | 0.053* |
| C8 | 0.4552 (3) | 0.5384 (3) | 0.8808 (3) | 0.0555 (10) |
| H8 | 0.4286 | 0.6037 | 0.8716 | 0.067* |
| C9 | 0.5628 (3) | 0.5152 (3) | 0.8768 (3) | 0.0580 (10) |
| H9 | 0.6101 | 0.5668 | 0.8665 | 0.070* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0473 (3) | 0.0431 (3) | 0.0374 (3) | −0.00333 (17) | 0.0148 (2) | 0.00048 (16) |
| S1 | 0.0600 (6) | 0.0452 (5) | 0.0334 (5) | −0.0081 (4) | 0.0119 (4) | −0.0025 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl1 | 0.0425 (5) | 0.0745 (6) | 0.0324 (4) | −0.0175 (4) | 0.0111 (4) | −0.0133 (4) |
| N1 | 0.0332 (14) | 0.0363 (13) | 0.0333 (14) | −0.0018 (10) | 0.0089 (11) | 0.0012 (11) |
| C4 | 0.0369 (18) | 0.0428 (18) | 0.0419 (19) | 0.0027 (14) | 0.0082 (15) | −0.0042 (14) |
| S2 | 0.0347 (5) | 0.0452 (5) | 0.0500 (5) | 0.0051 (3) | 0.0119 (4) | 0.0040 (4) |
| C3 | 0.048 (2) | 0.0329 (17) | 0.058 (2) | −0.0022 (14) | 0.0113 (18) | −0.0005 (15) |
| N2 | 0.0436 (16) | 0.0449 (15) | 0.0419 (16) | 0.0064 (12) | 0.0099 (13) | 0.0107 (12) |
| C2 | 0.049 (2) | 0.0370 (18) | 0.062 (3) | 0.0052 (15) | 0.0137 (18) | 0.0173 (16) |
| N3 | 0.0385 (16) | 0.0484 (17) | 0.065 (2) | −0.0026 (13) | 0.0179 (15) | −0.0011 (14) |
| N4 | 0.0308 (14) | 0.0413 (14) | 0.0326 (14) | 0.0009 (11) | 0.0064 (11) | −0.0012 (11) |
| C1 | 0.0253 (15) | 0.0404 (16) | 0.0357 (18) | 0.0039 (12) | 0.0077 (13) | 0.0033 (13) |
| C5 | 0.0334 (18) | 0.057 (2) | 0.0353 (18) | 0.0070 (14) | 0.0064 (14) | −0.0054 (15) |
| C6 | 0.0362 (18) | 0.0459 (18) | 0.0303 (16) | −0.0006 (14) | 0.0074 (14) | −0.0042 (13) |
| C7 | 0.0339 (18) | 0.051 (2) | 0.049 (2) | 0.0063 (15) | 0.0096 (16) | 0.0011 (16) |
| C8 | 0.054 (2) | 0.0432 (19) | 0.070 (3) | 0.0049 (17) | 0.0126 (19) | 0.0068 (18) |
| C9 | 0.051 (2) | 0.051 (2) | 0.075 (3) | −0.0079 (17) | 0.020 (2) | 0.0051 (19) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—N4$^{i}$ | 2.029 (3) | N2—C1 | 1.322 (4) |
| Cu1—N1 | 2.033 (2) | N2—C2 | 1.341 (4) |
| Cu1—Cl1 | 2.3698 (9) | C2—H2 | 0.9300 |
| Cu1—Cl1$^{ii}$ | 2.3704 (10) | N3—C6 | 1.331 (4) |
| Cu1—Cu1$^{ii}$ | 2.9909 (9) | N3—C9 | 1.334 (4) |
| S1—C1 | 1.760 (3) | N4—C7 | 1.337 (4) |
| S1—C5 | 1.799 (3) | N4—C6 | 1.343 (4) |
| Cl1—Cu1$^{ii}$ | 2.3704 (10) | N4—Cu1$^{i}$ | 2.029 (3) |
| N1—C1 | 1.339 (4) | C5—H5B | 0.9700 |
| N1—C4 | 1.341 (4) | C5—H5A | 0.9700 |
| C4—C3 | 1.369 (4) | C7—C8 | 1.368 (5) |
| C4—H4 | 0.9300 | C7—H7 | 0.9300 |
| S2—C6 | 1.755 (3) | C8—C9 | 1.373 (5) |
| S2—C5 | 1.801 (3) | C8—H8 | 0.9300 |
| C3—C2 | 1.367 (5) | C9—H9 | 0.9300 |
| C3—H3 | 0.9300 | | |
| N4$^{i}$—Cu1—N1 | 115.34 (10) | C6—N3—C9 | 115.9 (3) |
| N4$^{i}$—Cu1—Cl1 | 110.69 (7) | C7—N4—C6 | 115.8 (3) |
| N1—Cu1—Cl1 | 105.24 (7) | C7—N4—Cu1$^{i}$ | 121.6 (2) |
| N4$^{i}$—Cu1—Cl1$^{ii}$ | 113.04 (7) | C6—N4—Cu1$^{i}$ | 122.6 (2) |
| N1—Cu1—Cl1$^{ii}$ | 109.65 (7) | N2—C1—N1 | 126.9 (3) |
| Cl1—Cu1—Cl1$^{ii}$ | 101.76 (3) | N2—C1—S1 | 120.0 (2) |
| N4$^{i}$—Cu1—Cu1$^{ii}$ | 126.16 (7) | N1—C1—S1 | 113.1 (2) |
| N1—Cu1—Cu1$^{ii}$ | 118.34 (7) | S1—C5—S2 | 116.02 (18) |
| Cl1—Cu1—Cu1$^{ii}$ | 50.89 (2) | S1—C5—H5B | 108.3 |
| Cl1$^{ii}$—Cu1—Cu1$^{ii}$ | 50.87 (2) | S2—C5—H5B | 108.3 |
| C1—S1—C5 | 101.88 (15) | S1—C5—H5A | 108.3 |
| Cu1—Cl1—Cu1$^{ii}$ | 78.24 (3) | S2—C5—H5A | 108.3 |

| | | | |
|---|---|---|---|
| C1—N1—C4 | 115.9 (3) | H5B—C5—H5A | 107.4 |
| C1—N1—Cu1 | 121.97 (19) | N3—C6—N4 | 126.3 (3) |
| C4—N1—Cu1 | 121.4 (2) | N3—C6—S2 | 119.8 (2) |
| N1—C4—C3 | 122.1 (3) | N4—C6—S2 | 114.0 (2) |
| N1—C4—H4 | 118.9 | N4—C7—C8 | 122.5 (3) |
| C3—C4—H4 | 118.9 | N4—C7—H7 | 118.8 |
| C6—S2—C5 | 101.55 (15) | C8—C7—H7 | 118.8 |
| C2—C3—C4 | 116.6 (3) | C7—C8—C9 | 117.0 (3) |
| C2—C3—H3 | 121.7 | C7—C8—H8 | 121.5 |
| C4—C3—H3 | 121.7 | C9—C8—H8 | 121.5 |
| C1—N2—C2 | 115.0 (3) | N3—C9—C8 | 122.6 (3) |
| N2—C2—C3 | 123.4 (3) | N3—C9—H9 | 118.7 |
| N2—C2—H2 | 118.3 | C8—C9—H9 | 118.7 |
| C3—C2—H2 | 118.3 | | |
| $N4^{i}$—Cu1—Cl1—$Cu1^{ii}$ | 120.39 (8) | C4—N1—C1—S1 | −178.0 (2) |
| N1—Cu1—Cl1—$Cu1^{ii}$ | −114.37 (8) | Cu1—N1—C1—S1 | −7.5 (3) |
| $Cl1^{ii}$—Cu1—Cl1—$Cu1^{ii}$ | 0.0 | C5—S1—C1—N2 | −5.1 (3) |
| $N4^{i}$—Cu1—N1—C1 | −52.8 (2) | C5—S1—C1—N1 | 175.0 (2) |
| Cl1—Cu1—N1—C1 | −175.1 (2) | C1—S1—C5—S2 | −74.1 (2) |
| $Cl1^{ii}$—Cu1—N1—C1 | 76.1 (2) | C6—S2—C5—S1 | −72.9 (2) |
| $Cu1^{ii}$—Cu1—N1—C1 | 131.5 (2) | C9—N3—C6—N4 | −1.3 (5) |
| $N4^{i}$—Cu1—N1—C4 | 117.2 (2) | C9—N3—C6—S2 | 178.2 (3) |
| Cl1—Cu1—N1—C4 | −5.1 (2) | C7—N4—C6—N3 | 1.2 (5) |
| $Cl1^{ii}$—Cu1—N1—C4 | −113.9 (2) | $Cu1^{i}$—N4—C6—N3 | 179.4 (3) |
| $Cu1^{ii}$—Cu1—N1—C4 | −58.5 (2) | C7—N4—C6—S2 | −178.4 (2) |
| C1—N1—C4—C3 | −0.2 (4) | $Cu1^{i}$—N4—C6—S2 | −0.2 (3) |
| Cu1—N1—C4—C3 | −170.7 (2) | C5—S2—C6—N3 | −7.6 (3) |
| N1—C4—C3—C2 | −1.7 (5) | C5—S2—C6—N4 | 172.0 (2) |
| C1—N2—C2—C3 | −0.3 (5) | C6—N4—C7—C8 | 0.6 (5) |
| C4—C3—C2—N2 | 2.0 (5) | $Cu1^{i}$—N4—C7—C8 | −177.5 (3) |
| C2—N2—C1—N1 | −1.9 (5) | N4—C7—C8—C9 | −2.2 (6) |
| C2—N2—C1—S1 | 178.2 (2) | C6—N3—C9—C8 | −0.4 (6) |
| C4—N1—C1—N2 | 2.1 (4) | C7—C8—C9—N3 | 2.1 (6) |
| Cu1—N1—C1—N2 | 172.6 (2) | | |

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+3/2, −*y*+1/2, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···$Cl1^{iii}$ | 0.93 | 2.67 | 3.537 (4) | 155 |

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

**Fig. 1**

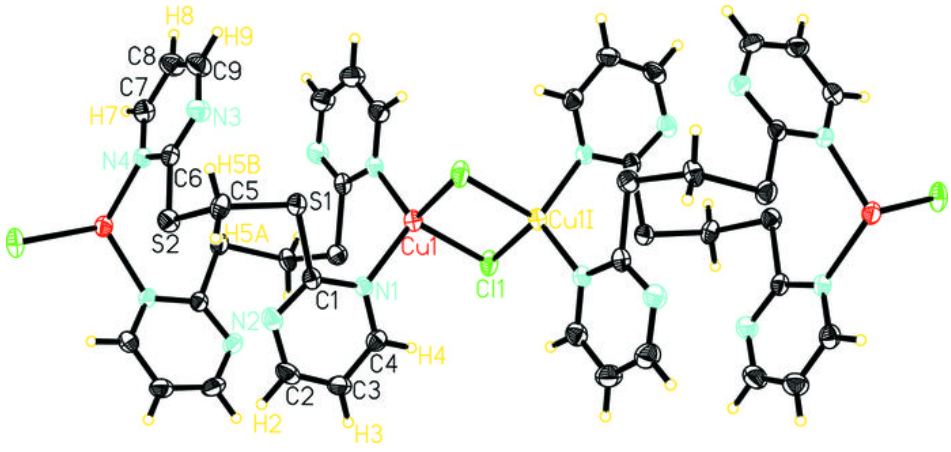
H8
H9
C8
C9
C7
H7
N3
N4
C6
H5B
C5
S1
S2
H5A
Cu1
Cu1I
Cl1
C1
N1
N2
C4
H4
C2
C3
H2
H3

**Fig. 2**