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# *catena*-Poly[[[2-(pyridin-2-yldisulfanyl)-pyridine-$\kappa^2N,S$]copper(I)]-$\mu_{1,5}$-dicyanamido]

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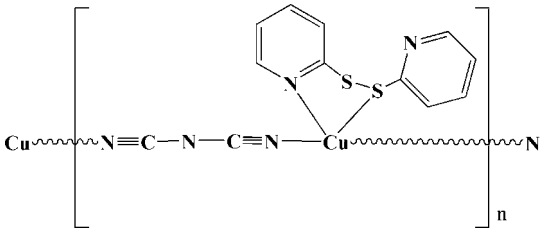
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.028; $wR$ factor = 0.081; data-to-parameter ratio = 14.7.

In the title compound, $[Cu(C_2N_3)(C_{10}H_8N_2S_2)]_n$, the $Cu^I$ atoms are connected by bridging dicyanamide ligands, forming chains parallel to [100]. Each $Cu^I$ atom displays a tetrahedral coordination environment, formed by one S atom and three N atoms from one 2-(pyridin-2-yldisulfanyl)pyridine and two dicyanamide ligands. The crystal structure is stabilized by C—H···N hydrogen bonds, forming a three-dimensional network.

## Related literature

For potential applications of metal-organic frameworks, see: Eddaoudi *et al.* (2001). For metal-organic frameworks constructed from flexible ligands, see: Xu *et al.* (2009). For related structures, see: Mal *et al.* (2006); Schlueter *et al.* (2007); Sen *et al.* (2007).




## Experimental

### *Crystal data*

$[Cu(C_2N_3)(C_{10}H_8N_2S_2)]$
$M_r$ = 349.92
Triclinic, $P\overline{1}$
$a$ = 7.6294 (15) Å
$b$ = 9.5964 (19) Å
$c$ = 10.202 (2) Å
$\alpha$ = 84.19 (3)°
$\beta$ = 80.63 (3)°
$\gamma$ = 70.93 (3)°
$V$ = 695.6 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.87 mm$^{-1}$
$T$ = 293 K
0.20 × 0.16 × 0.12 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.893, $T_{max}$ = 1.000
6615 measured reflections
2669 independent reflections
2301 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.081
$S$ = 1.07
2669 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9···N3$^{i}$ | 0.93 | 2.53 | 3.453 (3) | 171 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: ZQ2085).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m285 [ **doi:10.1107/S1600536811002728** ]

# *catena*-Poly[[[2-(pyridin-2-yldisulfanyl)pyridine-$\kappa^2N,S$]copper(I)]-$\mu_{1,5}$-dicyanamido]

**S. Wu, W. Jiang, F. Li and L. Liu**

## Comment

Metal-organic compounds have attracted much attention because of their diverse structures (Eddaoudi *et al.*, 2001). Flexible ligands can play different roles in constructing metal-organic frameworks (Xu *et al.*, 2009). The title compound, $\{C_{12}H_8CuN_5S_2\}_n$, is constructed by two kinds of flexible ligands: briding dicyanamide ligands and chelate 2-(pyridin-2-yldisulfanyl)pyridine ligands. In this paper, the crystal structure of the title compound is presented. As illustrated in Fig. 1, the Cu atoms are connected by briding dicyanamide ligands, forming a serrate chain. Each Cu atom displays a tetrahedral coordination environment, formed by one S atom and three N atoms from one 2-(pyridin-2-yldisulfanyl)pyridine and two dicyanamide ligands, where the Cu—S and average Cu—N bonds are 2.472 (1) and 1.969 Å, respectively. The crystal structure is stabilized by C—H···N hydrogen bonds [H9···N3$^{iii}$ = 2.53 Å, C9···N3$^{iii}$ = 3.453 (3) Å, and C9—H9···N3$^{iii}$ = 171°] between the central N atom of the dicyanamide and one H atom of a pyridine ring, forming a three-dimensional network [symmetry code: (iii) $x + 1, y - 1, z$].

## Experimental

$CuN(CN)_2$ (0.4 mmol) and $NaN(CN)_2$ (1.2 mmol) were added into 2 ml DMF with thorough stir for 6 minutes. After filtration, the colorless filtrate was carefully laid on the surface with the solution of bis(2-pyridyl)disulfide (0.5 mmol) in 5 ml *i*-PrOH. Colorless crystals were obtained after 3 weeks.

## Refinement

The H atoms were positioned geometrically and refined with a riding model, with C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}$(C).

## Figures

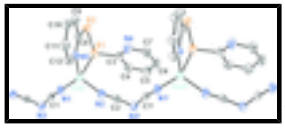


Fig. 1. The molecular structure of a portion of the title compound, with atom labels and 30% probability displacement ellipsoids. All H atoms have been omitted [symmetry code: (i) $x+1, y, z$].

## *catena*-Poly[[[2-(pyridin-2-yldisulfanyl)pyridine- $\kappa^2N,S$]copper(I)]-$\mu_{1,5}$-dicyanamido]

*Crystal data*

| | |
|---|---|
| $[Cu(C_2N_3)(C_{10}H_8N_2S_2)]$ | $Z = 2$ |
| $M_r = 349.92$ | $F(000) = 352$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.671$ Mg m$^{-3}$ |

| | |
|---|---|
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.6294$ (15) Å | Cell parameters from 3088 reflections |
| $b = 9.5964$ (19) Å | $\theta = 3.0$–$28.9°$ |
| $c = 10.202$ (2) Å | $\mu = 1.87$ mm$^{-1}$ |
| $\alpha = 84.19$ (3)° | $T = 293$ K |
| $\beta = 80.63$ (3)° | Block, colourless |
| $\gamma = 70.93$ (3)° | 0.20 × 0.16 × 0.12 mm |
| $V = 695.6$ (2) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 2669 independent reflections |
| Radiation source: fine-focus sealed tube | 2301 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.018$ |
| ω scans | $\theta_{max} = 26.0°$, $\theta_{min} = 3.1°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -8 \rightarrow 9$ |
| $T_{min} = 0.893$, $T_{max} = 1.000$ | $k = -11 \rightarrow 11$ |
| 6615 measured reflections | $l = -12 \rightarrow 12$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.081$ | H-atom parameters constrained |
| $S = 1.07$ | $w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.0204P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2669 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 181 parameters | $\Delta\rho_{max} = 0.39$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.29$ e Å$^{-3}$ |

*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 | −0.03943 (3) | 0.83530 (3) | 0.16964 (3) | 0.05693 (13) |
| S1 | −0.00326 (7) | 0.67390 (7) | 0.37486 (5) | 0.05609 (17) |
| S2 | 0.11161 (9) | 0.47767 (7) | 0.28919 (5) | 0.06255 (18) |
| N1 | −0.3026 (2) | 0.9293 (2) | 0.16879 (19) | 0.0580 (5) |
| N2 | 0.1131 (2) | 0.9633 (2) | 0.17961 (19) | 0.0599 (5) |
| N3 | −0.6377 (2) | 1.0592 (2) | 0.2077 (2) | 0.0694 (6) |
| N4 | 0.3589 (3) | 0.6469 (2) | 0.38308 (18) | 0.0610 (5) |
| N5 | 0.1249 (2) | 0.65814 (18) | 0.06703 (15) | 0.0464 (4) |
| C1 | −0.4605 (3) | 0.9840 (2) | 0.1839 (2) | 0.0489 (5) |
| C2 | 0.2361 (3) | 1.0016 (2) | 0.1905 (2) | 0.0480 (5) |
| C3 | 0.1841 (3) | 0.7106 (2) | 0.43562 (18) | 0.0452 (4) |
| C4 | 0.1311 (3) | 0.8103 (3) | 0.5330 (2) | 0.0612 (6) |
| H4 | 0.0059 | 0.8499 | 0.5684 | 0.073* |
| C5 | 0.2682 (4) | 0.8504 (3) | 0.5770 (2) | 0.0709 (7) |
| H5 | 0.2372 | 0.9197 | 0.6414 | 0.085* |
| C6 | 0.4516 (4) | 0.7863 (3) | 0.5242 (2) | 0.0692 (7) |
| H6 | 0.5475 | 0.8109 | 0.5519 | 0.083* |
| C7 | 0.4889 (3) | 0.6858 (3) | 0.4302 (2) | 0.0695 (7) |
| H7 | 0.6136 | 0.6409 | 0.3963 | 0.083* |
| C8 | 0.1811 (3) | 0.5212 (2) | 0.11824 (18) | 0.0462 (5) |
| C9 | 0.2919 (4) | 0.4027 (2) | 0.0454 (2) | 0.0627 (6) |
| H9 | 0.3245 | 0.3078 | 0.0850 | 0.075* |
| C10 | 0.3528 (4) | 0.4264 (3) | −0.0852 (2) | 0.0681 (7) |
| H10 | 0.4289 | 0.3484 | −0.1362 | 0.082* |
| C11 | 0.2996 (4) | 0.5682 (3) | −0.1403 (2) | 0.0660 (6) |
| H11 | 0.3402 | 0.5877 | −0.2292 | 0.079* |
| C12 | 0.1868 (3) | 0.6795 (2) | −0.0633 (2) | 0.0568 (5) |
| H12 | 0.1505 | 0.7748 | −0.1019 | 0.068* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.03597 (17) | 0.0595 (2) | 0.0745 (2) | −0.01273 (13) | −0.00278 (13) | −0.01572 (14) |
| S1 | 0.0434 (3) | 0.0798 (4) | 0.0469 (3) | −0.0244 (3) | 0.0007 (2) | −0.0063 (3) |
| S2 | 0.0847 (4) | 0.0645 (4) | 0.0502 (3) | −0.0423 (3) | −0.0082 (3) | 0.0048 (3) |
| N1 | 0.0393 (10) | 0.0623 (11) | 0.0748 (12) | −0.0157 (9) | −0.0099 (8) | −0.0125 (9) |
| N2 | 0.0394 (10) | 0.0572 (11) | 0.0836 (13) | −0.0155 (9) | −0.0067 (9) | −0.0086 (10) |
| N3 | 0.0382 (10) | 0.0433 (10) | 0.1278 (17) | −0.0077 (8) | −0.0184 (10) | −0.0154 (11) |
| N4 | 0.0464 (10) | 0.0763 (13) | 0.0606 (10) | −0.0187 (9) | 0.0016 (8) | −0.0213 (10) |
| N5 | 0.0448 (9) | 0.0463 (9) | 0.0459 (9) | −0.0120 (7) | −0.0051 (7) | −0.0025 (7) |
| C1 | 0.0433 (12) | 0.0430 (10) | 0.0654 (12) | −0.0170 (9) | −0.0154 (10) | −0.0011 (9) |
| C2 | 0.0353 (10) | 0.0381 (10) | 0.0647 (12) | −0.0040 (8) | −0.0064 (9) | −0.0028 (9) |
| C3 | 0.0450 (11) | 0.0532 (11) | 0.0357 (9) | −0.0147 (9) | −0.0049 (8) | 0.0008 (9) |
| C4 | 0.0542 (13) | 0.0674 (14) | 0.0528 (11) | −0.0058 (11) | −0.0028 (10) | −0.0145 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0843 (18) | 0.0700 (15) | 0.0601 (13) | −0.0197 (14) | −0.0148 (12) | −0.0186 (12) |
| C6 | 0.0719 (16) | 0.0802 (17) | 0.0667 (14) | −0.0325 (14) | −0.0237 (13) | −0.0036 (13) |
| C7 | 0.0453 (12) | 0.0879 (18) | 0.0762 (15) | −0.0188 (12) | −0.0066 (11) | −0.0184 (14) |
| C8 | 0.0496 (11) | 0.0484 (11) | 0.0467 (10) | −0.0227 (9) | −0.0093 (9) | −0.0022 (9) |
| C9 | 0.0802 (17) | 0.0417 (11) | 0.0665 (14) | −0.0190 (11) | −0.0118 (12) | −0.0030 (11) |
| C10 | 0.0834 (18) | 0.0525 (13) | 0.0635 (14) | −0.0162 (12) | 0.0008 (12) | −0.0167 (11) |
| C11 | 0.0817 (17) | 0.0652 (15) | 0.0466 (11) | −0.0200 (13) | 0.0006 (11) | −0.0081 (11) |
| C12 | 0.0596 (13) | 0.0518 (12) | 0.0520 (11) | −0.0108 (10) | −0.0056 (10) | 0.0024 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.9143 (18) | C3—C4 | 1.369 (3) |
| Cu1—N2 | 1.967 (2) | C4—C5 | 1.377 (4) |
| Cu1—N5 | 2.0244 (18) | C4—H4 | 0.9300 |
| Cu1—S1 | 2.4720 (10) | C5—C6 | 1.373 (4) |
| S1—C3 | 1.792 (2) | C5—H5 | 0.9300 |
| S1—S2 | 2.0207 (11) | C6—C7 | 1.361 (4) |
| S2—C8 | 1.787 (2) | C6—H6 | 0.9300 |
| N1—C1 | 1.138 (3) | C7—H7 | 0.9300 |
| N2—C2 | 1.138 (3) | C8—C9 | 1.378 (3) |
| N3—C2$^{i}$ | 1.298 (3) | C9—C10 | 1.360 (3) |
| N3—C1 | 1.303 (3) | C9—H9 | 0.9300 |
| N4—C3 | 1.319 (3) | C10—C11 | 1.375 (3) |
| N4—C7 | 1.337 (3) | C10—H10 | 0.9300 |
| N5—C8 | 1.322 (3) | C11—C12 | 1.359 (3) |
| N5—C12 | 1.356 (3) | C11—H11 | 0.9300 |
| C2—N3$^{ii}$ | 1.298 (3) | C12—H12 | 0.9300 |
| N1—Cu1—N2 | 117.16 (8) | C6—C5—C4 | 118.9 (2) |
| N1—Cu1—N5 | 126.58 (8) | C6—C5—H5 | 120.6 |
| N2—Cu1—N5 | 107.60 (7) | C4—C5—H5 | 120.6 |
| N1—Cu1—S1 | 106.75 (7) | C7—C6—C5 | 118.1 (2) |
| N2—Cu1—S1 | 104.29 (6) | C7—C6—H6 | 121.0 |
| N5—Cu1—S1 | 87.90 (5) | C5—C6—H6 | 121.0 |
| C3—S1—S2 | 105.95 (8) | N4—C7—C6 | 124.6 (2) |
| C3—S1—Cu1 | 102.35 (7) | N4—C7—H7 | 117.7 |
| S2—S1—Cu1 | 98.20 (4) | C6—C7—H7 | 117.7 |
| C8—S2—S1 | 105.52 (8) | N5—C8—C9 | 123.48 (18) |
| C1—N1—Cu1 | 172.06 (19) | N5—C8—S2 | 121.22 (16) |
| C2—N2—Cu1 | 161.63 (17) | C9—C8—S2 | 115.29 (16) |
| C2$^{i}$—N3—C1 | 120.23 (19) | C10—C9—C8 | 119.1 (2) |
| C3—N4—C7 | 115.9 (2) | C10—C9—H9 | 120.5 |
| C8—N5—C12 | 116.52 (18) | C8—C9—H9 | 120.5 |
| C8—N5—Cu1 | 124.88 (13) | C9—C10—C11 | 118.6 (2) |
| C12—N5—Cu1 | 118.59 (14) | C9—C10—H10 | 120.7 |
| N1—C1—N3 | 173.2 (2) | C11—C10—H10 | 120.7 |
| N2—C2—N3$^{ii}$ | 173.5 (2) | C12—C11—C10 | 119.2 (2) |
| N4—C3—C4 | 124.4 (2) | C12—C11—H11 | 120.4 |
| N4—C3—S1 | 119.92 (16) | C10—C11—H11 | 120.4 |

| | | | |
|---|---|---|---|
| C4—C3—S1 | 115.61 (16) | N5—C12—C11 | 123.1 (2) |
| C3—C4—C5 | 118.1 (2) | N5—C12—H12 | 118.5 |
| C3—C4—H4 | 120.9 | C11—C12—H12 | 118.5 |
| C5—C4—H4 | 120.9 | | |

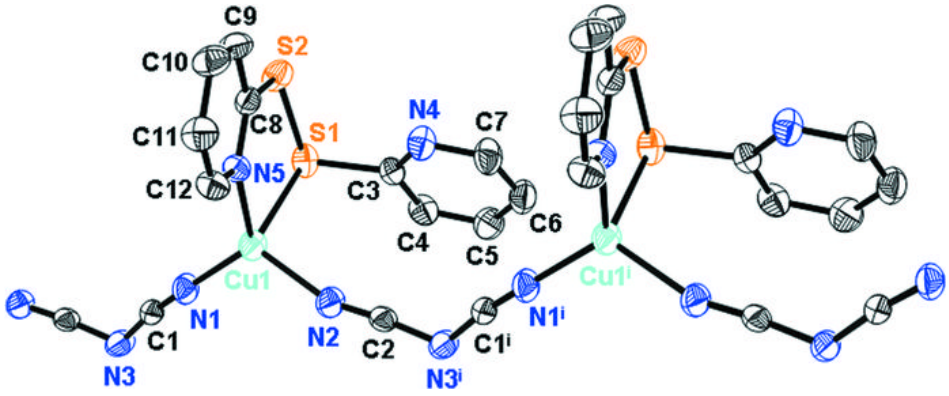
Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9···N3$^{iii}$ | 0.93 | 2.53 | 3.453 (3) | 171 |

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

**Fig. 1**


C9
S2
C10
C8
S1
N4
C7
C11
N5
C3
C12
C6
C4
C5
Cu1
Cu1i
N1
N1i
C1
N2
C2
C1i
N3
N3i