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catena-Poly[[(5-phenyl-2,2′-bipyridine-κ^2N,N')copper(I)]-μ-thiocyanido-κ^2N:*S*]

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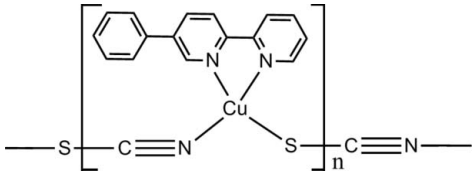
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 14.7.

The title compound, $[Cu(NCS)(C_{16}H_{12}N_2)]_n$, was synthesised under hydrothermal conditions. The Cu^I ion shows distorted tetrahedral geometry being coordinated by two N atoms from a 5-phenyl-2,2′-bipyridine ligand and by the N and S atoms from two different thiocyanate anions. The Cu^I ions are bridged by thiocyanide groups, forming a one-dimensional coordination polymer along the *b* axis. The crystal packing is through van der Waals contacts and C—H$\cdots\pi$ interactions.

Related literature

For applications of coordination metal complexes, see: Kong *et al.* (2008); Ohba *et al.* (2008). For related compounds, see Chen *et al.* (2009); Cui *et al.* (2011); Zhang *et al.* (2008).



Experimental

Crystal data

$[Cu(NCS)(C_{16}H_{12}N_2)]$
M_r = 353.90
Orthorhombic, *Pbca*
a = 7.7978 (9) Å
b = 10.7744 (12) Å
c = 35.325 (4) Å
V = 2967.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 153 K
0.42 × 0.09 × 0.06 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.840, T_{max} = 0.914
15488 measured reflections
2932 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.03
2932 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.917 (2)	Cu1—N3	2.121 (2)
Cu1—N2	2.079 (2)	Cu1—S1	2.3313 (9)

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

Cg is the centroid of the C12–C17 ring.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C17—H17$\cdots$*Cg*^{i}	0.93	2.92	3.757 (3)	150

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); 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: KP2379).

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Acta Cryst. (2012). E**68**, m165 [doi:10.1107/S1600536812000682]

catena-Poly[[(5-phenyl-2,2′-bipyridine-κ^2N,N')copper(I)]-μ-thiocyanido-κ^2N:*S*]

Shuxin Cui, Minghui Zuo, Jingping Zhang, Yulong Zhao and Hui Wang

S1. Comment

The title compound $[Cu(SCN)(5\text{-ph-}2,2'\text{-bpy})]_n$(I), was synthesised under hydrothermal conditions. In the complex, the Cu^I ion shows distorted tetrahedral geometry coordinated by two N atoms from a 5-ph-2,2,-bpy ligand, N and S atoms from the different thiocyanate anions (Fig.1 and Table 1). The Cu^Iions are bridged by thiocyanide groups to form a one-dimensional coordination polymeric along the *b* axis (Fig. 2). Crystal packing is through van der Waals contacts and C-H···π interaction [C17-H···Cg(C12→C17)symmetry operation: 1/2+x,3/2-y,1-z with geometric parameters H···Cg of 2.92 Å, C17···Cg of 3.757 (3) Å, and C17-H···Cg of 150 °].

S2. Experimental

A mixture of $Cu(Ac)_2$ (0.086 g, 0.64 mmol), 5-ph-2,2′-bpy (0.0231 g, 0.1 mmol), KSCN (0.059 g, 0.6 mmol), and water (8 mL) was added to a 15-mL Teflon-lined autoclave and heated at 443 K for 3 d. The autoclave was then cooled to room temperature. Red block crystals of (I) deposited on the wall of container were collected and air-dried.

S3. Refinement

Hydrogen atoms bound to carbon were placed in calculated positions and refined using a riding model with an isotropic displacement parameter fixed at 1.2 times U_{eq} for the atom to which they are attached.

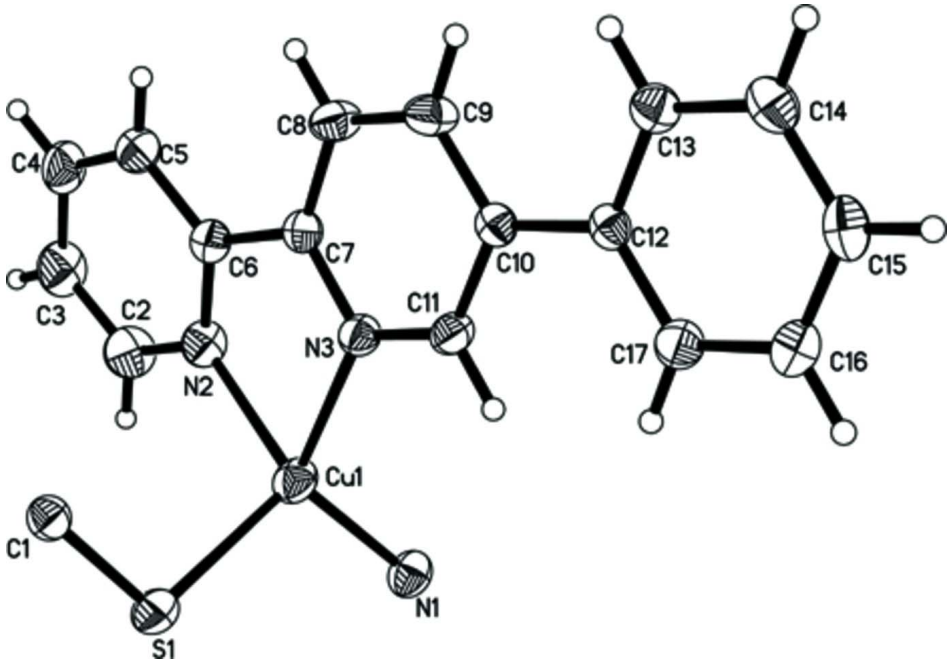

Figure 1

Complex (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small of arbitrary radii.

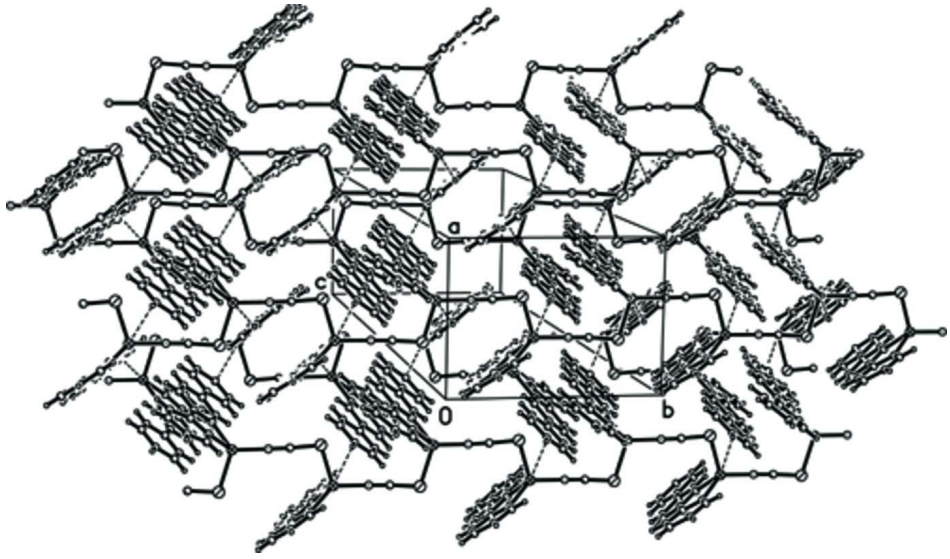

Figure 2

A perspective view of polymer chain of complex (I).

***catena*-Poly[[(5-phenyl-2,2′-bipyridine-κ^2N,N')copper(I)]-μ-thiocyanido-κ^2N:*S*]**

Crystal data

$[Cu(NCS)(C_{16}H_{12}N_2)]$
M_r = 353.90
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 7.7978 (9) Å
b = 10.7744 (12) Å

c = 35.325 (4) Å
V = 2967.8 (6) Å^3
Z = 8
F(000) = 1440
D_x = 1.584 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 15488 reflections
θ = 2.3–26.0°
μ = 1.61 mm^{-1}
T = 153 K
Block, red
0.42 × 0.09 × 0.06 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.840, T_{max} = 0.914

15488 measured reflections
2932 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.0°, θ_{min} = 2.3°
h = −9→9
k = −13→10
l = −43→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.03
2932 reflections
199 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.9913P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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	1.11691 (4)	0.67597 (3)	0.345104 (9)	0.04739 (14)
S1	1.40271 (9)	0.61263 (7)	0.34368 (3)	0.0578 (2)
N1	1.1156 (3)	0.8538 (2)	0.34377 (6)	0.0470 (6)
C1	1.3879 (3)	0.4601 (3)	0.34412 (7)	0.0402 (6)
N3	0.9620 (3)	0.59247 (18)	0.38739 (6)	0.0373 (5)
C12	0.8393 (3)	0.6026 (2)	0.49059 (6)	0.0325 (5)
C7	0.8656 (3)	0.4982 (2)	0.37430 (7)	0.0351 (5)
C10	0.8445 (3)	0.5642 (2)	0.45016 (6)	0.0327 (5)
N2	0.9760 (3)	0.5504 (2)	0.31300 (6)	0.0460 (5)
C6	0.8833 (3)	0.4689 (2)	0.33359 (7)	0.0378 (6)

C8	0.7568 (3)	0.4343 (3)	0.39843 (7)	0.0457 (6)
H8	0.6907	0.3691	0.3893	0.055*
C15	0.8303 (4)	0.6706 (3)	0.56739 (7)	0.0461 (7)
H15	0.8272	0.6938	0.5927	0.055*
C11	0.9497 (3)	0.6232 (2)	0.42376 (7)	0.0381 (6)
H11	1.0163	0.6891	0.4323	0.046*
C17	0.9373 (3)	0.7005 (2)	0.50432 (7)	0.0423 (6)
H17	1.0077	0.7444	0.4878	0.051*
C16	0.9318 (3)	0.7338 (3)	0.54203 (8)	0.0471 (7)
H16	0.9979	0.8002	0.5504	0.057*
C14	0.7336 (3)	0.5726 (3)	0.55461 (7)	0.0465 (6)
H14	0.6649	0.5287	0.5714	0.056*
C9	0.7469 (3)	0.4675 (2)	0.43580 (7)	0.0451 (6)
H9	0.6733	0.4244	0.4518	0.054*
C5	0.8093 (4)	0.3650 (3)	0.31698 (8)	0.0490 (7)
H5	0.7476	0.3088	0.3316	0.059*
C13	0.7381 (3)	0.5388 (2)	0.51663 (7)	0.0426 (6)
H13	0.6720	0.4722	0.5084	0.051*
C3	0.9202 (4)	0.4297 (3)	0.25767 (9)	0.0643 (9)
H3	0.9332	0.4194	0.2317	0.077*
C4	0.8281 (4)	0.3458 (3)	0.27870 (9)	0.0621 (9)
H4	0.7789	0.2768	0.2672	0.074*
C2	0.9924 (4)	0.5287 (3)	0.27587 (8)	0.0607 (8)
H2	1.0568	0.5844	0.2616	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0601 (2)	0.0344 (2)	0.0477 (2)	−0.00445 (15)	0.00674 (16)	0.00251 (14)
S1	0.0532 (4)	0.0325 (4)	0.0878 (6)	−0.0041 (3)	0.0084 (4)	−0.0025 (4)
N1	0.0582 (15)	0.0369 (13)	0.0459 (14)	0.0008 (11)	−0.0004 (11)	0.0028 (10)
C1	0.0414 (14)	0.0413 (16)	0.0378 (14)	−0.0003 (11)	0.0025 (11)	−0.0002 (11)
N3	0.0432 (11)	0.0341 (11)	0.0346 (11)	−0.0032 (9)	0.0032 (9)	0.0012 (9)
C12	0.0312 (12)	0.0312 (12)	0.0349 (13)	0.0072 (10)	0.0011 (10)	0.0035 (10)
C7	0.0361 (12)	0.0336 (13)	0.0357 (13)	0.0044 (11)	−0.0020 (10)	0.0018 (10)
C10	0.0323 (12)	0.0324 (12)	0.0334 (13)	0.0048 (10)	−0.0004 (10)	0.0035 (10)
N2	0.0554 (13)	0.0483 (13)	0.0344 (12)	−0.0005 (11)	−0.0003 (10)	0.0018 (10)
C6	0.0387 (13)	0.0382 (14)	0.0365 (13)	0.0040 (11)	−0.0043 (11)	−0.0002 (11)
C8	0.0485 (15)	0.0470 (15)	0.0415 (14)	−0.0155 (13)	−0.0023 (12)	−0.0002 (12)
C15	0.0520 (15)	0.0526 (17)	0.0337 (14)	0.0146 (14)	0.0011 (12)	−0.0028 (12)
C11	0.0446 (14)	0.0335 (13)	0.0364 (14)	−0.0058 (11)	0.0010 (11)	−0.0011 (11)
C17	0.0482 (14)	0.0396 (15)	0.0392 (14)	−0.0019 (12)	0.0032 (11)	0.0023 (12)
C16	0.0535 (16)	0.0406 (15)	0.0473 (16)	0.0018 (13)	−0.0021 (12)	−0.0062 (12)
C14	0.0467 (15)	0.0547 (17)	0.0381 (14)	0.0032 (14)	0.0070 (12)	0.0049 (13)
C9	0.0443 (14)	0.0525 (16)	0.0386 (14)	−0.0143 (13)	0.0010 (12)	0.0051 (12)
C5	0.0486 (15)	0.0484 (16)	0.0501 (17)	−0.0032 (13)	−0.0006 (13)	−0.0068 (13)
C13	0.0436 (14)	0.0425 (15)	0.0416 (14)	−0.0008 (12)	0.0026 (12)	0.0012 (11)
C3	0.076 (2)	0.080 (2)	0.0370 (16)	0.0006 (19)	−0.0013 (15)	−0.0126 (16)

C4	0.0609 (18)	0.066 (2)	0.059 (2)	0.0003 (16)	−0.0046 (16)	−0.0277 (16)
C2	0.074 (2)	0.071 (2)	0.0367 (16)	−0.0054 (17)	0.0034 (14)	0.0021 (14)

Geometric parameters (Å, º)

Cu1—N1	1.917 (2)	C8—H8	0.9300
Cu1—N2	2.079 (2)	C15—C14	1.374 (4)
Cu1—N3	2.121 (2)	C15—C16	1.376 (4)
Cu1—S1	2.3313 (9)	C15—H15	0.9300
S1—C1	1.648 (3)	C11—H11	0.9300
N1—C1^{i}	1.145 (4)	C17—C16	1.380 (4)
C1—N1^{ii}	1.145 (4)	C17—H17	0.9300
N3—C11	1.330 (3)	C16—H16	0.9300
N3—C7	1.346 (3)	C14—C13	1.390 (3)
C12—C17	1.390 (3)	C14—H14	0.9300
C12—C13	1.393 (3)	C9—H9	0.9300
C12—C10	1.487 (3)	C5—C4	1.376 (4)
C7—C8	1.385 (3)	C5—H5	0.9300
C7—C6	1.479 (3)	C13—H13	0.9300
C10—C9	1.386 (3)	C3—C2	1.367 (4)
C10—C11	1.395 (3)	C3—C4	1.373 (5)
N2—C2	1.339 (3)	C3—H3	0.9300
N2—C6	1.350 (3)	C4—H4	0.9300
C6—C5	1.390 (4)	C2—H2	0.9300
C8—C9	1.370 (4)		
N1—Cu1—N2	129.35 (9)	C16—C15—H15	120.6
N1—Cu1—N3	115.99 (9)	N3—C11—C10	125.1 (2)
N2—Cu1—N3	78.88 (8)	N3—C11—H11	117.5
N1—Cu1—S1	107.29 (7)	C10—C11—H11	117.5
N2—Cu1—S1	107.64 (7)	C16—C17—C12	121.1 (2)
N3—Cu1—S1	115.82 (6)	C16—C17—H17	119.4
C1—S1—Cu1	102.99 (9)	C12—C17—H17	119.4
C1^{i}—N1—Cu1	177.7 (2)	C15—C16—C17	121.2 (3)
N1^{ii}—C1—S1	177.1 (2)	C15—C16—H16	119.4
C11—N3—C7	118.7 (2)	C17—C16—H16	119.4
C11—N3—Cu1	127.99 (17)	C15—C14—C13	120.3 (2)
C7—N3—Cu1	113.34 (15)	C15—C14—H14	119.8
C17—C12—C13	117.1 (2)	C13—C14—H14	119.8
C17—C12—C10	122.1 (2)	C8—C9—C10	121.2 (2)
C13—C12—C10	120.8 (2)	C8—C9—H9	119.4
N3—C7—C8	120.3 (2)	C10—C9—H9	119.4
N3—C7—C6	116.3 (2)	C4—C5—C6	119.4 (3)
C8—C7—C6	123.3 (2)	C4—C5—H5	120.3
C9—C10—C11	114.9 (2)	C6—C5—H5	120.3
C9—C10—C12	123.0 (2)	C14—C13—C12	121.5 (2)
C11—C10—C12	122.1 (2)	C14—C13—H13	119.3
C2—N2—C6	117.8 (2)	C12—C13—H13	119.3

C2—N2—Cu1	126.7 (2)	C2—C3—C4	118.3 (3)
C6—N2—Cu1	114.36 (17)	C2—C3—H3	120.8
N2—C6—C5	121.3 (2)	C4—C3—H3	120.8
N2—C6—C7	115.8 (2)	C3—C4—C5	119.3 (3)
C5—C6—C7	122.9 (2)	C3—C4—H4	120.4
C9—C8—C7	119.9 (2)	C5—C4—H4	120.4
C9—C8—H8	120.1	N2—C2—C3	123.9 (3)
C7—C8—H8	120.1	N2—C2—H2	118.1
C14—C15—C16	118.8 (2)	C3—C2—H2	118.1
C14—C15—H15	120.6		

N1—Cu1—S1—C1	−178.99 (11)	C8—C7—C6—N2	171.1 (2)
N2—Cu1—S1—C1	−36.25 (11)	N3—C7—C6—C5	171.7 (2)
N3—Cu1—S1—C1	49.68 (11)	C8—C7—C6—C5	−8.5 (4)
N1—Cu1—N3—C11	−45.7 (2)	N3—C7—C8—C9	0.2 (4)
N2—Cu1—N3—C11	−174.2 (2)	C6—C7—C8—C9	−179.6 (2)
S1—Cu1—N3—C11	81.5 (2)	C7—N3—C11—C10	0.6 (4)
N1—Cu1—N3—C7	133.67 (16)	Cu1—N3—C11—C10	179.92 (18)
N2—Cu1—N3—C7	5.13 (16)	C9—C10—C11—N3	−0.7 (4)
S1—Cu1—N3—C7	−99.22 (16)	C12—C10—C11—N3	179.1 (2)
C11—N3—C7—C8	−0.3 (3)	C13—C12—C17—C16	−1.0 (4)
Cu1—N3—C7—C8	−179.74 (18)	C10—C12—C17—C16	−179.3 (2)
C11—N3—C7—C6	179.4 (2)	C14—C15—C16—C17	0.2 (4)
Cu1—N3—C7—C6	0.0 (3)	C12—C17—C16—C15	0.5 (4)
C17—C12—C10—C9	−179.4 (2)	C16—C15—C14—C13	−0.4 (4)
C13—C12—C10—C9	2.2 (3)	C7—C8—C9—C10	−0.2 (4)
C17—C12—C10—C11	0.9 (3)	C11—C10—C9—C8	0.4 (4)
C13—C12—C10—C11	−177.5 (2)	C12—C10—C9—C8	−179.3 (2)
N1—Cu1—N2—C2	68.4 (3)	N2—C6—C5—C4	−1.2 (4)
N3—Cu1—N2—C2	−176.9 (3)	C7—C6—C5—C4	178.4 (3)
S1—Cu1—N2—C2	−63.2 (2)	C15—C14—C13—C12	−0.1 (4)
N1—Cu1—N2—C6	−124.53 (18)	C17—C12—C13—C14	0.7 (4)
N3—Cu1—N2—C6	−9.93 (18)	C10—C12—C13—C14	179.2 (2)
S1—Cu1—N2—C6	103.86 (17)	C2—C3—C4—C5	1.0 (5)
C2—N2—C6—C5	0.9 (4)	C6—C5—C4—C3	0.2 (5)
Cu1—N2—C6—C5	−167.4 (2)	C6—N2—C2—C3	0.4 (5)
C2—N2—C6—C7	−178.8 (2)	Cu1—N2—C2—C3	167.1 (2)
Cu1—N2—C6—C7	13.0 (3)	C4—C3—C2—N2	−1.4 (5)
N3—C7—C6—N2	−8.7 (3)		

Symmetry codes: (i) −*x*+5/2, *y*+1/2, *z*; (ii) −*x*+5/2, *y*−1/2, *z*.

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···*Cg*^{iii}	0.93	2.92	3.757 (3)	150

Symmetry code: (iii) *x*+1/2, −*y*+3/2, −*z*+1.