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catena-Poly[[di-μ-iodido-dicopper(I)-(*Cu—Cu*)]bis(μ-4,4′-di-3-pyridyl-2,2′-disulfanediyldipyrimidine)]

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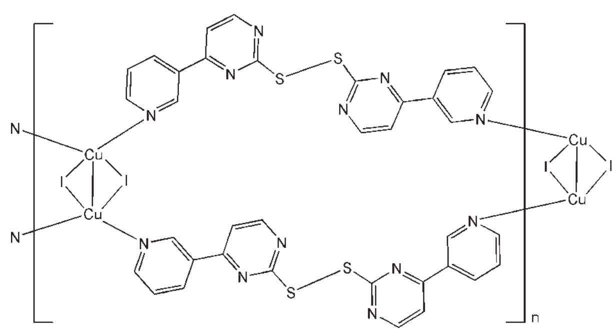
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 14.1.

The title complex, $[Cu_2I_2(C_{18}H_{12}N_6S_2)_2]_n$, contains a Cu_2I_2 core with a Cu—Cu distance of 2.6935 (14) Å. The Cu^I atom is coordinated by two bridging 4,4′-di-3-pyridyl-2,2′-disulfanediyldipyrimidine ligands and two bridging I atoms, forming a double chain.

Related literature

For coordination polymers with 4,4′-dipyridinedisulfide, see: Horikoshi & Mochida (2006). For coordination polymers with 2,2′-dithiobis(4-pyridin-4-yl-pyrimidine), see: Zhu *et al.* (2009). For the structure of free 2,2′-dithiobis(3-pyridin-4-yl-pyrimidine), see: Ji *et al.* (2009).



Experimental

Crystal data

$[Cu_2I_2(C_{18}H_{12}N_6S_2)_2]$
M_r = 1133.86
Triclinic, $P\overline{1}$
a = 8.5561 (6) Å
b = 10.7702 (8) Å
c = 11.9045 (8) Å
α = 98.110 (1)°
β = 107.193 (1)°
γ = 96.449 (1)°
V = 1023.66 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.80 mm^{-1}
T = 298 K
0.19 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001) T_{min} = 0.611, T_{max} = 0.715
5395 measured reflections
3568 independent reflections
2956 reflections with $I > 2\sigma(I)$
R_{int} = 0.097

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 0.99
3568 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—I1	2.6550 (7)	Cu1—N1	2.037 (4)
Cu1—I1^{i}	2.6579 (8)	Cu1—N6^{ii}	2.060 (4)

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x, y+1, z-1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); 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: HY2260).

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Acta Cryst. (2010). E**66**, m41   [doi:10.1107/S1600536809052325]

catena-Poly[[di-μ-iodido-dicopper(I)(*Cu*—*Cu*)]bis(μ-4,4′-di-3-pyridyl-2,2′-disulfanediyldipyrimidine)]

Hai-Bin Zhu

S1. Comment

In recent years, heterocyclic disulfide ligands have received increasing attention because of their conformationally defined dihedral angle (Horikoshi & Mochida, 2006). As continuation of our previous research (Zhu *et al.*, 2009), we report here a copper(I) coordination polymer with a 2,2′-dithiobis(3-pyridin-4-ylpyrimidine) (*L*) ligand.

The Cu^I atom in the title complex has a tetrahedral coordination geometry completed by two N atoms from two different *L* ligands and two bridging I atoms (Fig. 1 and Table 1). The C—S—S—C torsion angle of 81.2 (2)° in *L* is almost identical with the free molecule (Ji *et al.*, 2009). Alternative linkings of one Cu_2I_2 core and two bridging *L* ligands generate a one-dimensional double chain (Fig. 2).

S2. Experimental

A CH_2Cl_2 solution (5 ml) of ligand *L* (0.1 mmol) was slowly added into a CuI (0.1 mmol) solution in acetonitrile (10 ml). The mixture was kept on standing for 3 d to give single crystals suitable for X-ray diffraction analysis.

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The highest residual electron density was found 0.98 Å from I1 and the deepest hole 0.92 Å from I1.

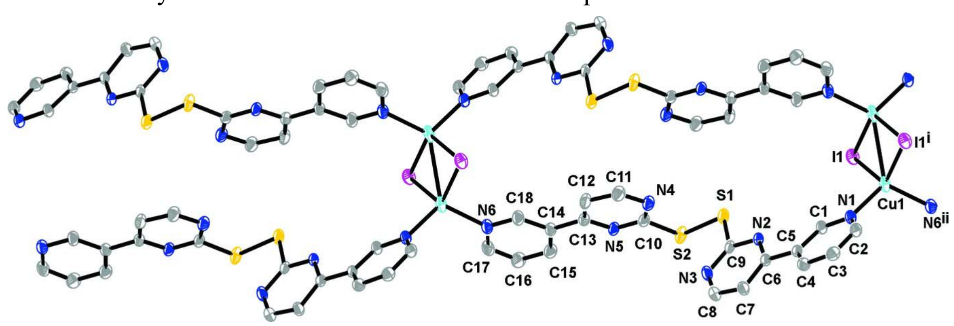

Figure 1

The structure of the title compound with 30% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry codes: (i) -*x* + 1, -*y* + 2, -*z*; (ii) *x*, *y* + 1, *z* - 1.]

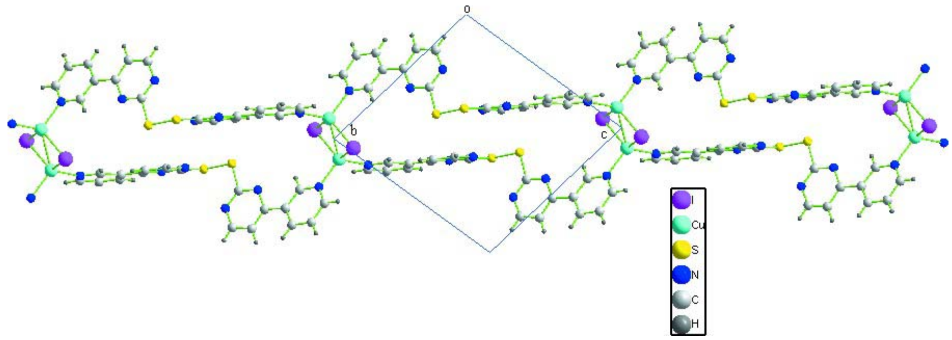

Figure 2

The one-dimensional double chain viewed along the *a* axis.

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c = 11.9045 (8) Å
α = 98.110 (1)°
β = 107.193 (1)°
γ = 96.449 (1)°
V = 1023.66 (13) Å^3
Z = 1
F(000) = 552
D_x = 1.839 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3568 reflections
θ = 2.3–25.5°
μ = 2.80 mm^{-1}
T = 298 K
Block, yellow
0.19 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.611, T_{max} = 0.715
5395 measured reflections
3568 independent reflections
2956 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −7→10
k = −12→12
l = −14→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 0.99
3568 reflections
253 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
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.28 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
I1	0.31696 (4)	0.97725 (3)	0.10525 (3)	0.04697 (15)
Cu1	0.38873 (9)	0.92391 (6)	−0.09670 (6)	0.0503 (2)
S1	0.13540 (17)	0.55124 (12)	0.27577 (10)	0.0447 (3)
S2	0.02067 (16)	0.43336 (14)	0.35509 (12)	0.0498 (3)
N2	0.2094 (5)	0.5182 (3)	0.0809 (3)	0.0340 (8)
C5	0.3021 (5)	0.5258 (4)	−0.0900 (4)	0.0328 (10)
N3	0.0948 (5)	0.3267 (4)	0.1271 (4)	0.0426 (10)
N1	0.3815 (5)	0.7322 (4)	−0.1296 (3)	0.0387 (9)
C9	0.1455 (5)	0.4513 (4)	0.1466 (4)	0.0340 (10)
N5	0.1235 (5)	0.2820 (4)	0.4999 (3)	0.0381 (9)
C1	0.3142 (6)	0.6574 (4)	−0.0705 (4)	0.0356 (10)
H1A	0.2728	0.6955	−0.0127	0.043*
C6	0.2284 (5)	0.4523 (4)	−0.0183 (4)	0.0330 (10)
C10	0.1797 (6)	0.3566 (5)	0.4357 (4)	0.0392 (11)
C3	0.4346 (6)	0.5483 (5)	−0.2380 (4)	0.0436 (11)
H3B	0.4772	0.5130	−0.2963	0.052*
C13	0.2302 (6)	0.2187 (4)	0.5638 (4)	0.0381 (10)
C12	0.3936 (6)	0.2331 (5)	0.5625 (4)	0.0480 (13)
H12A	0.4704	0.1894	0.6067	0.058*
C4	0.3639 (6)	0.4719 (5)	−0.1776 (4)	0.0411 (11)
H4A	0.3572	0.3842	−0.1951	0.049*
N4	0.3312 (5)	0.3777 (4)	0.4277 (3)	0.0453 (10)
C11	0.4371 (6)	0.3147 (5)	0.4933 (5)	0.0515 (13)
H11A	0.5461	0.3261	0.4925	0.062*
C2	0.4419 (6)	0.6772 (5)	−0.2117 (4)	0.0418 (11)
H2B	0.4909	0.7284	−0.2528	0.050*
C8	0.1115 (6)	0.2636 (5)	0.0281 (5)	0.0457 (12)
H8A	0.0766	0.1761	0.0087	0.055*
C7	0.1775 (6)	0.3213 (4)	−0.0466 (4)	0.0416 (11)
H7A	0.1883	0.2739	−0.1148	0.050*
C14	0.1671 (6)	0.1341 (4)	0.6336 (4)	0.0380 (10)
C15	−0.0011 (6)	0.1112 (5)	0.6209 (4)	0.0475 (12)
H15A	−0.0761	0.1500	0.5691	0.057*
C16	−0.0545 (7)	0.0301 (5)	0.6864 (5)	0.0532 (14)
H16A	−0.1663	0.0141	0.6796	0.064*
C18	0.2701 (7)	0.0733 (5)	0.7125 (4)	0.0456 (12)
H18A	0.3827	0.0880	0.7217	0.055*
C17	0.0554 (7)	−0.0264 (5)	0.7604 (4)	0.0503 (13)
H17A	0.0161	−0.0825	0.8023	0.060*
N6	0.2191 (5)	−0.0053 (4)	0.7765 (3)	0.0442 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0504 (2)	0.0489 (2)	0.0526 (2)	0.00536 (15)	0.02987 (17)	0.01773 (16)

Cu1	0.0647 (4)	0.0437 (4)	0.0576 (4)	0.0113 (3)	0.0319 (3)	0.0285 (3)
S1	0.0595 (8)	0.0464 (7)	0.0346 (6)	0.0117 (6)	0.0179 (6)	0.0187 (5)
S2	0.0478 (7)	0.0725 (9)	0.0424 (7)	0.0181 (7)	0.0204 (6)	0.0338 (7)
N2	0.039 (2)	0.034 (2)	0.0308 (19)	0.0039 (16)	0.0112 (16)	0.0143 (16)
C5	0.031 (2)	0.036 (2)	0.031 (2)	0.0029 (19)	0.0078 (18)	0.0140 (19)
N3	0.045 (2)	0.040 (2)	0.049 (2)	0.0049 (18)	0.0167 (19)	0.0225 (19)
N1	0.044 (2)	0.038 (2)	0.038 (2)	0.0031 (17)	0.0182 (18)	0.0159 (17)
C9	0.035 (2)	0.040 (3)	0.028 (2)	0.008 (2)	0.0081 (19)	0.0147 (19)
N5	0.042 (2)	0.046 (2)	0.0293 (19)	0.0054 (18)	0.0114 (17)	0.0156 (17)
C1	0.042 (3)	0.035 (2)	0.036 (2)	0.007 (2)	0.018 (2)	0.012 (2)
C6	0.033 (2)	0.034 (2)	0.033 (2)	0.0050 (19)	0.0091 (19)	0.0131 (19)
C10	0.044 (3)	0.045 (3)	0.030 (2)	0.004 (2)	0.012 (2)	0.012 (2)
C3	0.046 (3)	0.053 (3)	0.036 (2)	0.008 (2)	0.018 (2)	0.008 (2)
C13	0.046 (3)	0.040 (3)	0.029 (2)	0.004 (2)	0.011 (2)	0.012 (2)
C12	0.041 (3)	0.060 (3)	0.047 (3)	0.012 (2)	0.010 (2)	0.030 (3)
C4	0.046 (3)	0.039 (3)	0.039 (3)	0.005 (2)	0.015 (2)	0.008 (2)
N4	0.043 (2)	0.057 (3)	0.039 (2)	0.006 (2)	0.0127 (18)	0.021 (2)
C11	0.038 (3)	0.069 (4)	0.051 (3)	0.001 (3)	0.013 (2)	0.027 (3)
C2	0.046 (3)	0.048 (3)	0.036 (3)	0.000 (2)	0.018 (2)	0.016 (2)
C8	0.051 (3)	0.034 (3)	0.052 (3)	0.004 (2)	0.015 (2)	0.014 (2)
C7	0.056 (3)	0.031 (2)	0.039 (3)	0.006 (2)	0.017 (2)	0.010 (2)
C14	0.046 (3)	0.037 (2)	0.033 (2)	0.005 (2)	0.016 (2)	0.010 (2)
C15	0.046 (3)	0.059 (3)	0.040 (3)	0.004 (2)	0.014 (2)	0.017 (2)
C16	0.050 (3)	0.070 (4)	0.045 (3)	0.001 (3)	0.022 (2)	0.018 (3)
C18	0.049 (3)	0.048 (3)	0.045 (3)	0.004 (2)	0.018 (2)	0.021 (2)
C17	0.064 (3)	0.048 (3)	0.047 (3)	−0.002 (3)	0.029 (3)	0.018 (2)
N6	0.054 (3)	0.042 (2)	0.041 (2)	0.0064 (19)	0.0178 (19)	0.0175 (18)

Geometric parameters (Å, º)

Cu1—I1	2.6550 (7)	C3—H3B	0.9300
Cu1—I1^{i}	2.6579 (8)	C13—C12	1.394 (7)
Cu1—N1	2.037 (4)	C13—C14	1.477 (6)
Cu1—N6^{ii}	2.060 (4)	C12—C11	1.379 (7)
Cu1—Cu1^{i}	2.6935 (14)	C12—H12A	0.9300
S1—C9	1.779 (5)	C4—H4A	0.9300
S1—S2	2.0183 (17)	N4—C11	1.327 (6)
S2—C10	1.778 (5)	C11—H11A	0.9300
N2—C9	1.323 (5)	C2—H2B	0.9300
N2—C6	1.352 (6)	C8—C7	1.367 (6)
C5—C1	1.390 (6)	C8—H8A	0.9300
C5—C4	1.389 (6)	C7—H7A	0.9300
C5—C6	1.466 (6)	C14—C18	1.379 (7)
N3—C9	1.329 (6)	C14—C15	1.392 (7)
N3—C8	1.329 (6)	C15—C16	1.376 (7)
N1—C2	1.333 (6)	C15—H15A	0.9300
N1—C1	1.330 (5)	C16—C17	1.349 (7)
N5—C13	1.324 (6)	C16—H16A	0.9300

N5—C10	1.328 (6)	C18—N6	1.336 (6)
C1—H1A	0.9300	C18—H18A	0.9300
C6—C7	1.391 (6)	C17—N6	1.344 (7)
C10—N4	1.325 (6)	C17—H17A	0.9300
C3—C2	1.370 (7)	N6—Cu1^{iii}	2.060 (4)
C3—C4	1.368 (6)		

Cu1—I1—Cu1^{i}	60.92 (3)	C12—C13—C14	123.0 (4)
N1—Cu1—N6^{ii}	115.68 (16)	C11—C12—C13	117.4 (4)
N1—Cu1—I1	106.36 (10)	C11—C12—H12A	121.3
N6^{ii}—Cu1—I1	106.25 (12)	C13—C12—H12A	121.3
N1—Cu1—I1^{i}	105.02 (11)	C3—C4—C5	119.8 (4)
N6^{ii}—Cu1—I1^{i}	104.97 (12)	C3—C4—H4A	120.1
I1—Cu1—I1^{i}	119.08 (3)	C5—C4—H4A	120.1
N1—Cu1—Cu1^{i}	122.23 (11)	C10—N4—C11	113.9 (4)
N6^{ii}—Cu1—Cu1^{i}	122.06 (12)	N4—C11—C12	123.3 (5)
I1—Cu1—Cu1^{i}	59.59 (2)	N4—C11—H11A	118.3
I1^{i}—Cu1—Cu1^{i}	59.49 (3)	C12—C11—H11A	118.3
C9—S1—S2	104.18 (16)	N1—C2—C3	122.6 (4)
C10—S2—S1	104.60 (17)	N1—C2—H2B	118.7
C9—N2—C6	116.6 (4)	C3—C2—H2B	118.7
C1—C5—C4	116.6 (4)	C7—C8—N3	123.1 (4)
C1—C5—C6	119.6 (4)	C7—C8—H8A	118.5
C4—C5—C6	123.8 (4)	N3—C8—H8A	118.5
C9—N3—C8	114.2 (4)	C8—C7—C6	118.6 (4)
C2—N1—C1	117.8 (4)	C8—C7—H7A	120.7
C2—N1—Cu1	121.4 (3)	C6—C7—H7A	120.7
C1—N1—Cu1	120.8 (3)	C18—C14—C15	117.0 (4)
N2—C9—N3	128.4 (4)	C18—C14—C13	122.1 (4)
N2—C9—S1	110.9 (3)	C15—C14—C13	120.8 (4)
N3—C9—S1	120.7 (3)	C14—C15—C16	118.8 (5)
C13—N5—C10	116.9 (4)	C14—C15—H15A	120.6
N1—C1—C5	123.9 (4)	C16—C15—H15A	120.6
N1—C1—H1A	118.0	C17—C16—C15	120.0 (5)
C5—C1—H1A	118.0	C17—C16—H16A	120.0
N2—C6—C7	119.1 (4)	C15—C16—H16A	120.0
N2—C6—C5	116.7 (4)	N6—C18—C14	124.5 (5)
C7—C6—C5	124.2 (4)	N6—C18—H18A	117.8
N4—C10—N5	128.4 (4)	C14—C18—H18A	117.8
N4—C10—S2	120.6 (3)	C16—C17—N6	123.1 (5)
N5—C10—S2	111.1 (3)	C16—C17—H17A	118.5
C2—C3—C4	119.3 (4)	N6—C17—H17A	118.5
C2—C3—H3B	120.4	C18—N6—C17	116.6 (4)
C4—C3—H3B	120.4	C18—N6—Cu1^{iii}	120.4 (4)
N5—C13—C12	120.0 (4)	C17—N6—Cu1^{iii}	122.7 (3)
N5—C13—C14	117.0 (4)		

Cu1^{i}—I1—Cu1—N1	118.18 (12)	C10—N5—C13—C12	0.7 (7)

Cu1^{i}—I1—Cu1—N6^{ii}	−118.04 (12)	C10—N5—C13—C14	−179.0 (4)
Cu1^{i}—I1—Cu1—I1^{i}	0.0	N5—C13—C12—C11	0.1 (7)
C9—S1—S2—C10	81.1 (2)	C14—C13—C12—C11	179.7 (4)
N6^{ii}—Cu1—N1—C2	75.1 (4)	C2—C3—C4—C5	−0.6 (7)
I1—Cu1—N1—C2	−167.2 (3)	C1—C5—C4—C3	1.1 (6)
I1^{i}—Cu1—N1—C2	−40.1 (4)	C6—C5—C4—C3	−178.3 (4)
Cu1^{i}—Cu1—N1—C2	−103.2 (3)	N5—C10—N4—C11	0.0 (8)
N6^{ii}—Cu1—N1—C1	−104.0 (4)	S2—C10—N4—C11	179.6 (4)
I1—Cu1—N1—C1	13.7 (4)	C10—N4—C11—C12	0.8 (8)
I1^{i}—Cu1—N1—C1	140.8 (3)	C13—C12—C11—N4	−0.9 (8)
Cu1^{i}—Cu1—N1—C1	77.7 (4)	C1—N1—C2—C3	1.0 (7)
C6—N2—C9—N3	−1.0 (7)	Cu1—N1—C2—C3	−178.1 (4)
C6—N2—C9—S1	178.0 (3)	C4—C3—C2—N1	−0.5 (7)
C8—N3—C9—N2	−0.2 (7)	C9—N3—C8—C7	1.0 (7)
C8—N3—C9—S1	−179.1 (3)	N3—C8—C7—C6	−0.6 (8)
S2—S1—C9—N2	176.0 (3)	N2—C6—C7—C8	−0.7 (7)
S2—S1—C9—N3	−4.8 (4)	C5—C6—C7—C8	179.6 (4)
C2—N1—C1—C5	−0.5 (7)	N5—C13—C14—C18	−173.4 (4)
Cu1—N1—C1—C5	178.7 (3)	C12—C13—C14—C18	6.9 (7)
C4—C5—C1—N1	−0.5 (7)	N5—C13—C14—C15	7.5 (7)
C6—C5—C1—N1	178.9 (4)	C12—C13—C14—C15	−172.2 (5)
C9—N2—C6—C7	1.4 (6)	C18—C14—C15—C16	−0.2 (7)
C9—N2—C6—C5	−178.8 (4)	C13—C14—C15—C16	178.9 (4)
C1—C5—C6—N2	−14.3 (6)	C14—C15—C16—C17	−0.6 (8)
C4—C5—C6—N2	165.0 (4)	C15—C14—C18—N6	0.0 (7)
C1—C5—C6—C7	165.5 (4)	C13—C14—C18—N6	−179.1 (4)
C4—C5—C6—C7	−15.2 (7)	C15—C16—C17—N6	1.6 (8)
C13—N5—C10—N4	−0.8 (7)	C14—C18—N6—C17	0.9 (7)
C13—N5—C10—S2	179.6 (3)	C14—C18—N6—Cu1^{iii}	−174.0 (4)
S1—S2—C10—N4	−4.1 (4)	C16—C17—N6—C18	−1.7 (8)
S1—S2—C10—N5	175.5 (3)	C16—C17—N6—Cu1^{iii}	173.0 (4)

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x, y+1, z-1$; (iii) $x, y-1, z+1$.