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trans-Bis(ethylenediamine)bis(sulfadiazinato)-copper(II)

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Key indicators

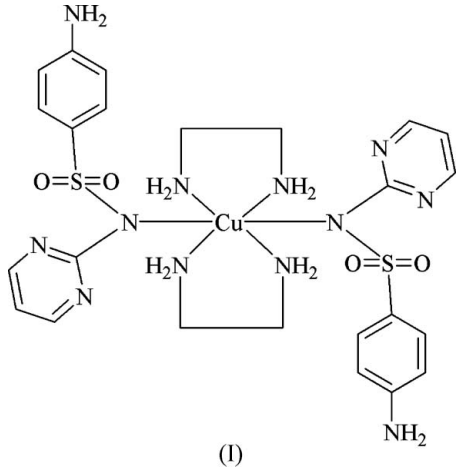
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.144
Data-to-parameter ratio = 16.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, *trans*-$[Cu(C_2H_8N_2)_2(C_{10}H_9N_4O_2S)_2]$, consists of neutral molecules. The Cu^{2+} ion occupies an inversion centre and exhibits an elongated distorted octahedral geometry, with two monodentate sulfadiazinate (sdz) anions and two bidentate ethylenediamine ligands. Both sdz ligands are *N*-coordinated *via* an N atom of the sulfonamide group. The crystal structure is stabilized by hydrogen bonds and weak van der Waals interactions.

Comment

In the structure of the title compound, (I), $[Cu(sdz)_2(en)_2]$, the Cu^{II} ion occupies an inversion centre and is octahedrally coordinated by two en and two sdz ligands, forming a CuN_6 coordination environment. The en molecules act as bidentate ligands, forming two five-membered chelate rings with a *trans* arrangement. The structure has a Jahn–Teller-distorted octahedral geometry around the Cu^{II} atom with four N atoms of the two chelating ethylenediamine molecules and two sulfonamide N atoms from sulfadiazine molecules completing the coordination of the elongated octahedral structure.



(I)

The two $Cu—N_{en}$ bond distances are almost equivalent, but significantly shorter than the $Cu—N_{sdz}$ bond distances, resulting in the formation of a distorted octahedral geometry elongated along the $Cu—N_{sdz}$ bonds. Thus, the en N atoms form the equatorial plane of the coordination octahedron, while the sulfonamide N atoms of sdz occupy the axial positions.

The Cu1—N1 bond distances of 2.672 (2) Å are elongated as a result of the Jahn–Teller effect. The bond lengths within the sulfadiazine and ethylenediamine are as expected. The Cu—N distances of 2.005 (3) and 2.013 (3) Å, involving the

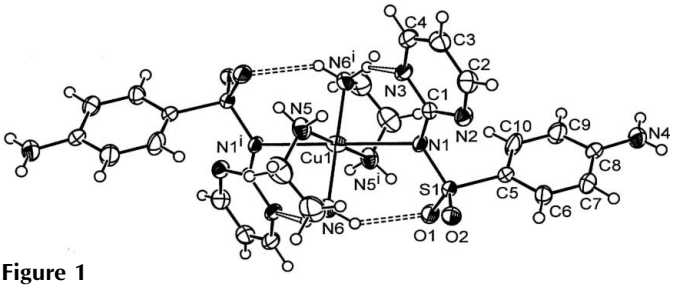


Figure 1
The molecular structure, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity. Symmetry code as in Table 1. Dashed lines indicate hydrogen bonds.

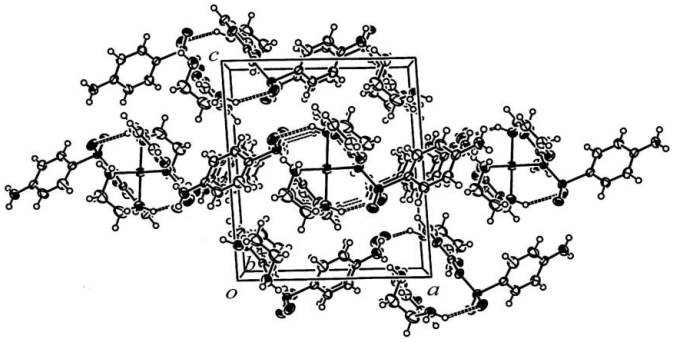


Figure 2
The molecular packing of (I) viewed along the *b* axis. Dashed lines indicate the hydrogen-bonding interactions.

ethylenediamine molecules, are comparable to the corresponding values 1.997 (3) and 2.001 (3) Å (Lokaj *et al.*, 1991), 2.033 (3) and 2.042 (3) Å (Anacona *et al.*, 2002), 1.996 (2) and 2.022 (3) Å (Kovbasyuk *et al.*, 1997), 2.007 (3)–2.024 (3) Å (Kovbasyuk *et al.*, 1997), 2.016 (2) and 2.019 (2) Å (Fun *et al.*, 2002), and 2.007 (3) and 2.010 (3) Å (Kazak *et al.*, 2004). The S1—O bond distances of 1.458 (3) and 1.449 (3) Å are longer than the corresponding bonds in the pure sulfadiazine with values of 1.429 (2) and 1.437 (2) Å.

The crystal structure of the complex exhibits numerous hydrogen bonds (Table 2). The amino H atoms form intramolecular hydrogen bonds with the sulfonyl O atoms, as illustrated in Fig. 1. The amine H atoms of the en ligands and terminal amino H are also involved in intermolecular hydrogen bonding with the sulfonyl O atoms of neighbouring sdz ligands (Fig. 2).

Experimental

The sodium salt of sulfadiazine (Nasdz) (0.545 g, 2 mmol) was dissolved in 50 ml of hot methanol and a methanol solution (10 ml) of $CuCl_2{\cdot}2H_2O$ (0.171 g, 1 mmol) was added slowly with constant stirring on a hot-plate at 333 K; a red precipitate was formed and the mixture was stirred for 6 h. The precipitate was filtered off and dried over silica gel. The precipitate was dissolved in a 1:10 mixture of ethylenediamine/water (10 ml), stirred for 30 minutes. The solution was then filtered and left for crystallization; a week later, blue block crystals were obtained, which were filtered off and dried over silica gel.

Crystal data

$[Cu(C_2H_8N_2)_2(C_{10}H_9N_4O_2S)_2]$
M_r = 682.29
Monoclinic, $P2_1/n$
a = 10.8610 (5) Å
b = 10.6329 (4) Å
c = 12.5227 (6) Å
β = 93.302 (2)°
V = 1443.77 (11) Å^3
Z = 2
D_x = 1.569 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 150 (2) K
Block, blue
0.15 × 0.12 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.870, T_{max} = 0.910
9385 measured reflections
3290 independent reflections
2428 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.144
S = 1.03
3290 reflections
196 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 1.6363P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.672 (2)	Cu1—N6	2.005 (3)
Cu1—N5	2.013 (3)		
N1^i—Cu1—N1	180	N1—Cu1—N6	89.68 (10)
N5^i—Cu1—N5	180	N5^i—Cu1—N6	95.10 (12)
N6^i—Cu1—N6	180	N5—Cu1—N6	84.90 (12)
N1—Cu1—N5	94.80 (10)	N1^i—Cu1—N5	85.20 (10)
N1^i—Cu1—N6	90.32 (10)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6B···O1	0.92	2.29	3.068 (4)	142
N6—H6A···N3^i	0.92	2.25	3.021 (4)	141
N5—H5B···O1^i	0.92	2.15	2.958 (4)	146

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

H atoms were placed in calculated positions (C—H = 0.95 and 0.99 Å; N—H = 0.88 and 0.92 Å, respectively, for H atoms on amino N4 (sulfadiazine), and N5 and N6 (ethylenediamine) atoms) and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 times U_{eq} of their parent atoms.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); soft-

ware used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

Acta Cryst. (2006). E**62**, m2727–m2729 [https://doi.org/10.1107/S1600536806038797]

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$b = 10.6329\ (4)$ Å
$c = 12.5227\ (6)$ Å
$\beta = 93.302\ (2)°$
$V = 1443.77\ (11)$ Å^3
$Z = 2$
$F(000) = 710$
$D_x = 1.569$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3290 reflections
$\theta = 2.9–27.5°$
$\mu = 0.96$ mm^{-1}
$T = 150$ K
Block, blue
0.15 × 0.12 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.870$, $T_{max} = 0.910$
9385 measured reflections
3290 independent reflections
2428 reflections with $I > 2\sigma(I)$
$R_{int} = 0.089$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -14\rightarrow13$
$k = -13\rightarrow13$
$l = -14\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.144$
$S = 1.03$
3290 reflections
196 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
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 1.6363P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.5000	0.5000	0.0300 (2)
S1	0.74294 (7)	0.28794 (8)	0.40827 (6)	0.0270 (2)
O1	0.7552 (2)	0.4133 (2)	0.3629 (2)	0.0394 (6)
O2	0.7047 (2)	0.1936 (2)	0.32966 (18)	0.0379 (6)
N1	0.6557 (2)	0.3053 (2)	0.5048 (2)	0.0243 (6)
N2	0.6659 (3)	0.0859 (2)	0.5436 (2)	0.0290 (6)
N3	0.5561 (3)	0.2321 (3)	0.6484 (2)	0.0299 (6)
N4	1.2330 (3)	0.1285 (3)	0.5971 (2)	0.0392 (8)
H4A	1.2742	0.0678	0.5674	0.047*
H4B	1.2629	0.1641	0.6565	0.047*
C1	0.6261 (3)	0.2035 (3)	0.5656 (2)	0.0234 (7)
C2	0.6220 (3)	−0.0065 (3)	0.6034 (3)	0.0340 (8)
H2	0.6466	−0.0903	0.5890	0.041*
C3	0.5442 (3)	0.0124 (3)	0.6836 (3)	0.0334 (8)
H3	0.5116	−0.0556	0.7224	0.040*
C4	0.5158 (3)	0.1349 (3)	0.7050 (3)	0.0334 (8)
H4	0.4652	0.1519	0.7627	0.040*
C5	0.8905 (3)	0.2446 (3)	0.4622 (2)	0.0253 (7)
C6	0.9564 (3)	0.1499 (3)	0.4142 (3)	0.0295 (7)
H6	0.9223	0.1098	0.3515	0.035*
C7	1.0713 (3)	0.1139 (3)	0.4571 (3)	0.0308 (8)
H7	1.1167	0.0513	0.4222	0.037*
C8	1.1206 (3)	0.1680 (3)	0.5503 (3)	0.0288 (7)
C9	1.0573 (4)	0.2663 (4)	0.5950 (3)	0.0463 (10)
H9	1.0927	0.3087	0.6561	0.056*
C10	0.9428 (4)	0.3031 (4)	0.5512 (3)	0.0459 (10)
H10	0.8999	0.3698	0.5833	0.055*
N5	0.3469 (3)	0.3931 (3)	0.4975 (2)	0.0337 (7)
H5A	0.3668	0.3132	0.5208	0.040*
H5B	0.2917	0.4267	0.5426	0.040*
N6	0.4818 (3)	0.4869 (3)	0.3402 (2)	0.0327 (7)
H6A	0.4539	0.5618	0.3111	0.039*
H6B	0.5565	0.4681	0.3130	0.039*
C11	0.2911 (4)	0.3878 (4)	0.3888 (4)	0.0514 (11)
H11A	0.2388	0.4629	0.3743	0.062*
H11B	0.2385	0.3120	0.3799	0.062*
C12	0.3900 (4)	0.3834 (4)	0.3138 (4)	0.0543 (12)
H12A	0.3547	0.3939	0.2397	0.065*
H12B	0.4319	0.3007	0.3189	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0355 (4)	0.0300 (3)	0.0244 (3)	−0.0055 (2)	0.0015 (2)	0.0009 (2)
S1	0.0243 (4)	0.0329 (4)	0.0241 (4)	0.0095 (3)	0.0058 (3)	0.0050 (3)
O1	0.0382 (15)	0.0408 (14)	0.0409 (15)	0.0138 (11)	0.0163 (11)	0.0189 (12)
O2	0.0363 (14)	0.0540 (16)	0.0226 (12)	0.0115 (12)	−0.0042 (10)	−0.0080 (11)
N1	0.0229 (14)	0.0223 (13)	0.0285 (15)	0.0066 (10)	0.0089 (11)	0.0042 (11)
N2	0.0320 (16)	0.0225 (13)	0.0329 (16)	0.0046 (11)	0.0059 (12)	0.0002 (12)
N3	0.0303 (15)	0.0311 (15)	0.0294 (15)	0.0068 (12)	0.0118 (12)	0.0050 (12)
N4	0.0280 (16)	0.053 (2)	0.0366 (17)	0.0071 (14)	−0.0023 (13)	−0.0027 (15)
C1	0.0195 (16)	0.0266 (16)	0.0241 (16)	0.0036 (12)	0.0008 (12)	0.0023 (13)
C2	0.039 (2)	0.0224 (17)	0.041 (2)	0.0024 (14)	0.0022 (16)	−0.0004 (15)
C3	0.032 (2)	0.0307 (18)	0.037 (2)	−0.0051 (14)	0.0020 (15)	0.0086 (15)
C4	0.0324 (19)	0.0367 (19)	0.0323 (18)	0.0054 (15)	0.0110 (15)	0.0063 (15)
C5	0.0244 (16)	0.0297 (17)	0.0224 (16)	0.0044 (13)	0.0060 (13)	0.0029 (13)
C6	0.0275 (18)	0.0293 (17)	0.0317 (18)	0.0045 (13)	0.0003 (14)	−0.0022 (14)
C7	0.0292 (18)	0.0257 (17)	0.038 (2)	0.0038 (13)	0.0062 (15)	−0.0026 (15)
C8	0.0239 (17)	0.0360 (18)	0.0273 (17)	0.0015 (14)	0.0081 (13)	0.0038 (15)
C9	0.034 (2)	0.070 (3)	0.034 (2)	0.0128 (19)	−0.0041 (16)	−0.019 (2)
C10	0.035 (2)	0.062 (3)	0.041 (2)	0.0196 (19)	0.0022 (17)	−0.0236 (19)
N5	0.0321 (16)	0.0248 (14)	0.0441 (18)	0.0021 (12)	−0.0002 (14)	0.0052 (13)
N6	0.0339 (17)	0.0356 (16)	0.0284 (15)	0.0109 (12)	−0.0006 (13)	0.0002 (12)
C11	0.053 (3)	0.043 (2)	0.056 (3)	−0.0060 (19)	−0.014 (2)	0.001 (2)
C12	0.059 (3)	0.057 (3)	0.045 (2)	0.004 (2)	−0.014 (2)	−0.015 (2)

Geometric parameters (Å, º)

Cu1—N1	2.672 (2)	C4—H4	0.9500
Cu1—N1^{i}	2.672 (2)	C5—C6	1.392 (4)
Cu1—N5	2.013 (3)	C5—C10	1.370 (5)
Cu1—N5^{i}	2.013 (3)	C6—C7	1.384 (5)
Cu1—N6	2.005 (3)	C6—H6	0.9500
Cu1—N6^{i}	2.005 (3)	C7—C8	1.381 (5)
S1—O1	1.458 (3)	C7—H7	0.9500
S1—O2	1.449 (3)	C8—C9	1.386 (5)
S1—N1	1.589 (3)	C9—C10	1.387 (5)
S1—C5	1.764 (3)	C9—H9	0.9500
N1—C1	1.372 (4)	C10—H10	0.9500
N2—C1	1.356 (4)	N5—C11	1.459 (5)
N2—C2	1.339 (4)	N5—H5A	0.9200
N3—C1	1.355 (4)	N5—H5B	0.9200
N3—C4	1.342 (4)	N6—C12	1.508 (5)
N4—C8	1.388 (4)	N6—H6A	0.9200
N4—H4A	0.8800	N6—H6B	0.9200
N4—H4B	0.8800	C11—C12	1.468 (6)
C2—C3	1.365 (5)	C11—H11A	0.9900
C2—H2	0.9500	C11—H11B	0.9900

C3—C4	1.368 (5)	C12—H12A	0.9900
C3—H3	0.9500	C12—H12B	0.9900
N1^{i}—Cu1—N1	180.000 (1)	C10—C5—S1	121.1 (3)
N5^{i}—Cu1—N5	180.000 (1)	C6—C5—S1	120.1 (2)
N6^{i}—Cu1—N6	180.000 (1)	C5—C6—C7	120.4 (3)
N1^{i}—Cu1—N5	85.20 (10)	C7—C6—H6	119.8
N1—Cu1—N5	94.80 (10)	C5—C6—H6	119.8
N1^{i}—Cu1—N5^{i}	94.80 (10)	C6—C7—C8	120.7 (3)
N1—Cu1—N5^{i}	85.20 (10)	C8—C7—H7	119.7
N1^{i}—Cu1—N6	90.32 (10)	C6—C7—H7	119.7
N1—Cu1—N6	89.68 (10)	C7—C8—C9	118.5 (3)
N1^{i}—Cu1—N6^{i}	89.68 (10)	C7—C8—N4	121.3 (3)
N1—Cu1—N6^{i}	90.32 (10)	C9—C8—N4	120.1 (3)
N5^{i}—Cu1—N6^{i}	84.90 (12)	C8—C9—C10	120.5 (3)
N5—Cu1—N6^{i}	95.10 (12)	C8—C9—H9	119.7
N5^{i}—Cu1—N6	95.10 (12)	C10—C9—H9	119.7
N5—Cu1—N6	84.90 (12)	C5—C10—C9	120.9 (3)
O1—S1—O2	113.38 (15)	C5—C10—H10	119.6
O1—S1—N1	105.22 (14)	C9—C10—H10	119.6
O2—S1—N1	115.90 (15)	C11—N5—Cu1	109.6 (2)
O2—S1—C5	107.32 (15)	C11—N5—H5A	109.8
O1—S1—C5	106.65 (16)	Cu1—N5—H5A	109.8
N1—S1—C5	107.91 (14)	C11—N5—H5B	109.8
C1—N1—S1	120.0 (2)	Cu1—N5—H5B	109.8
C1—N1—Cu1	117.11 (19)	H5A—N5—H5B	108.2
S1—N1—Cu1	118.50 (13)	C12—N6—Cu1	107.2 (2)
C1—N2—C2	115.8 (3)	C12—N6—H6A	110.3
C1—N3—C4	116.5 (3)	Cu1—N6—H6A	110.3
C8—N4—H4A	120.0	C12—N6—H6B	110.3
C8—N4—H4B	120.0	Cu1—N6—H6B	110.3
H4A—N4—H4B	120.0	H6A—N6—H6B	108.5
N2—C1—N3	124.2 (3)	N5—C11—C12	108.5 (3)
N1—C1—N3	114.0 (3)	N5—C11—H11A	110.0
N1—C1—N2	121.8 (3)	C12—C11—H11A	110.0
N2—C2—C3	123.9 (3)	N5—C11—H11B	110.0
N2—C2—H2	118.0	C12—C11—H11B	110.0
C3—C2—H2	118.0	H11A—C11—H11B	108.4
C2—C3—C4	116.1 (3)	C11—C12—N6	109.6 (3)
C2—C3—H3	121.9	C11—C12—H12A	109.7
C4—C3—H3	121.9	N6—C12—H12A	109.7
N3—C4—C3	123.1 (3)	C11—C12—H12B	109.7
N3—C4—H4	118.5	N6—C12—H12B	109.7
C3—C4—H4	118.5	H12A—C12—H12B	108.2
C6—C5—C10	118.7 (3)		
O2—S1—N1—C1	54.3 (3)	O1—S1—C5—C10	69.3 (3)
O1—S1—N1—C1	−179.5 (2)	N1—S1—C5—C10	−43.3 (3)

C5—S1—N1—C1	−66.0 (3)	O2—S1—C5—C6	11.5 (3)
O2—S1—N1—Cu1	−101.41 (16)	O1—S1—C5—C6	−110.3 (3)
O1—S1—N1—Cu1	24.70 (19)	N1—S1—C5—C6	137.0 (3)
C5—S1—N1—Cu1	138.27 (15)	C10—C5—C6—C7	1.4 (5)
N6^{i}—Cu1—N1—C1	56.7 (2)	S1—C5—C6—C7	−178.9 (3)
N6—Cu1—N1—C1	−123.3 (2)	C5—C6—C7—C8	2.3 (5)
N5^{i}—Cu1—N1—C1	141.5 (2)	C6—C7—C8—C9	−5.2 (5)
N5—Cu1—N1—C1	−38.5 (2)	C6—C7—C8—N4	176.8 (3)
N6^{i}—Cu1—N1—S1	−146.87 (17)	C7—C8—C9—C10	4.6 (6)
N6—Cu1—N1—S1	33.13 (17)	N4—C8—C9—C10	−177.4 (4)
N5^{i}—Cu1—N1—S1	−62.01 (17)	C6—C5—C10—C9	−2.1 (6)
N5—Cu1—N1—S1	117.99 (17)	S1—C5—C10—C9	178.2 (3)
C4—N3—C1—N2	−6.2 (5)	C8—C9—C10—C5	−0.9 (7)
C4—N3—C1—N1	174.6 (3)	N6^{i}—Cu1—N5—C11	167.5 (3)
C2—N2—C1—N3	6.3 (5)	N6—Cu1—N5—C11	−12.5 (3)
C2—N2—C1—N1	−174.6 (3)	N1^{i}—Cu1—N5—C11	78.2 (3)
S1—N1—C1—N3	176.9 (2)	N1—Cu1—N5—C11	−101.8 (3)
Cu1—N1—C1—N3	−27.0 (3)	N5^{i}—Cu1—N6—C12	166.2 (2)
S1—N1—C1—N2	−2.3 (4)	N5—Cu1—N6—C12	−13.8 (2)
Cu1—N1—C1—N2	153.7 (2)	N1^{i}—Cu1—N6—C12	−99.0 (2)
C1—N2—C2—C3	−1.4 (5)	N1—Cu1—N6—C12	81.0 (2)
N2—C2—C3—C4	−3.0 (6)	Cu1—N5—C11—C12	37.1 (4)
C1—N3—C4—C3	1.2 (5)	N5—C11—C12—N6	−50.1 (4)
C2—C3—C4—N3	3.1 (6)	Cu1—N6—C12—C11	38.3 (4)
O2—S1—C5—C10	−168.8 (3)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*B*···O1	0.92	2.29	3.068 (4)	142
N6—H6*A*···N3^{i}	0.92	2.25	3.021 (4)	141
N5—H5*B*···O1^{i}	0.92	2.15	2.958 (4)	146

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.