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trans-{1,8-Bis[(*S*)-1-phenylethyl]-1,3,6,8,10,13-hexaazacyclotetradecane}-bis(thiocyanato-κN)copper(II)

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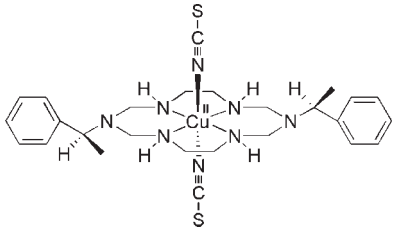
Key indicators: single-crystal X-ray study; T = 195 K; mean σ(C–C) = 0.009 Å; R factor = 0.048; wR factor = 0.115; data-to-parameter ratio = 18.7.

In the title thiocyanate-coordinated aza-macrocyclic copper(II) complex, $[Cu(NCS)_2(C_{24}H_{38}N_6)]$, the Cu^{II} atom is coordinated by the four secondary N atoms of the aza-macrocyclic ligand and by the two N atoms of the thiocyanate ions in a tetragonally distorted octahedral geometry. The average equatorial Cu—N bond length is shorter than the average axial Cu—N bond length [2.010 (2) and 2.528 (4) Å, respectively]. An N—H···N hydrogen-bonding interaction between the secondary amine N atom and the adjacent thiocyanate ion leads to a polymeric chain along the *a* axis.

Related literature

For the potential applications of chiral metal complexes in chiral recognition and chiral catalysis, see: Katsuki *et al.* (2000); Lehn (1995) and as chiral building blocks, see: Du *et al.* (2003); Gao *et al.* (2005). It has been reported that the enantiomers of $[Ru(1,10\text{-phenanthroline})_3]^{2+}$ induce chiral aggregation of various achiral anionic porphyrins, see: Randazzo *et al.* (2008). For typical C—S bond lengths, see: Banerjee & Zubieta (2004); Stølevik & Postmyr (1997). For the preparation, see: Han *et al.* (2008).



Experimental

Crystal data

$[Cu(NCS)_2(C_{24}H_{38}N_6)]$
M_r = 590.30
Monoclinic, $P2_1$
a = 6.5976 (5) Å
b = 14.7609 (11) Å
c = 15.2847 (12) Å
β = 99.952 (2)°
V = 1466.13 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 195 K
0.38 × 0.26 × 0.15 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.751, T_{max} = 0.871
10954 measured reflections
6272 independent reflections
4364 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.115
S = 1.11
6272 reflections
336 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Absolute structure: Flack (1983), 2485 Friedel pairs
Flack parameter: −0.01 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N7^{i}	0.93	2.54	3.258 (7)	135
N4—H4···N8^{ii}	0.93	2.46	3.202 (7)	137

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); 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: JH2175).

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supporting information

Acta Cryst. (2010). E**66**, m919–m920 [https://doi.org/10.1107/S1600536810026632]

trans-{1,8-Bis[(*S*)-1-phenylethyl]-1,3,6,8,10,13-hexaazacyclotetradecane}bis-(thiocyanato-κN)copper(II)

Jong Won Shin, Sankara Rao Rowthu, Jae Jeong Ryoo and Kil Sik Min

S1. Comment

Chiral metal complexes have attracted considerable attention in chemistry and material science because of their potential applications for chiral recognition and chiral catalysis (Lehn, 1995; Katsuki *et al.*, 2000). Very recently, it has reported the enantiomers of $[Ru(1,10\text{-phenanthroline})_3]^{2+}$ induce chiral aggregation of various achiral anionic porphyrins and that the complexes can transfer molecular information, *i.e.* energy and chirality (Randazzo *et al.*, 2008). However, the study of chiral macrocyclic metal complexes has been limited due to the difficult of preparation, although these complexes are ve ry useful for chiral building blocks (Du *et al.*, 2003; Gao *et al.*, 2005). Here, we report the synthesis and crystal structure of copper(II) azamacrocyclic chiral complex, *trans*-Dithiocyanato(1,8-di(*S*-α-methylbenzyl)- 1,3,6,8,10,13-hexaazacyclo-tetradecane)copper(II), with two thiocyanate ions axially.

In the title compound, the coordination geometry around copper(II) ion is a tetragonally distorted octahedron in which copper(II) ion is coordinated to the four secondary N atoms of the azamacrocyclic ligand in the square-planar fashion and two N atoms from the thiocyanate ions at the axial positions as shown in Figure 1. The average Ni—N_{eq} and Ni—N_{ax} bond distances are 2.010 (2) and 2.528 (4) Å, respectively. The former is much less than the latter, which can be attributed to a rather large Jahn-Teller distortion of the copper(II) ion and/or the ring contraction of the azamacrocyclic ligand. In the coordinated thiocyanate ions, the average N—C and C—S bond distances are 1.160 (6) and 1.638 (5) Å, respectively. The former is very similar to CN triple bond length, while the latter is slightly shorter than the normal CS single bond distance (Stølevik & Postmyr, 1997; Banerjee & Zubieta, 2004). The pendant arms of azamacrocyclic ligand have chiral carbon atoms (S type). All thiocyanate ions binding copper(II) ions axially are involved in an N—H···N(of NCS) hydrogen bonding interactions (Table 1), which gives rise to a one-dimensional polymeric chain propagating along the *a* axis (Figure 2). The shortest Cu···Cu intrachain separation within the hydrogen-bonded one-dimensional polymer is 6.598 (1) Å and is about 37% shorter than the shortest interchain Cu···Cu distance of 10.448 (1) Å.

S2. Experimental

The title compound is prepared as follows. $[Cu(C_{24}H_{38}N_6)](ClO_4)_2$ was prepared by a slightly modified literature procedure: as $CuCl_2.2H_2O$ and *S*-(-)-1-Phenylethylamine were used instead of $NiCl_2.6H_2O$ and *R*-(+)-1-Phenylethylamine (Han *et al.*, 2008). To an MeCN solution (10 ml) of $[Cu(C_{24}H_{38}N_6)](ClO_4)_2$ (90 mg, 0.15 mmol) was added dropwise an aqueous solution (10 ml) containing NaSCN (24 mg, 0.30 mmol) at ambient temperature. The color of the solution changed to pale pink. The mixture was stirred for 30 min during which time a pink precipitate of formed which was collected by filtration, washed with MeCN and water, and dried in air. Single crystals of the title compound suitable for X-ray crystallography were grown by layering of the MeCN solution of $[Cu(C_{24}H_{38}N_6)](ClO_4)_2$ on the aqueous solution of NaSCN within one week.

S3. Refinement

All H atoms in the title compound were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (ring H atoms) or 0.99–1.00 (open chain H atoms) Å and N—H distance of 0.93 Å, and with U_{iso}(H) values of 1.2 times the equivalent anisotropic displacement parameters of the parent C and N atoms.

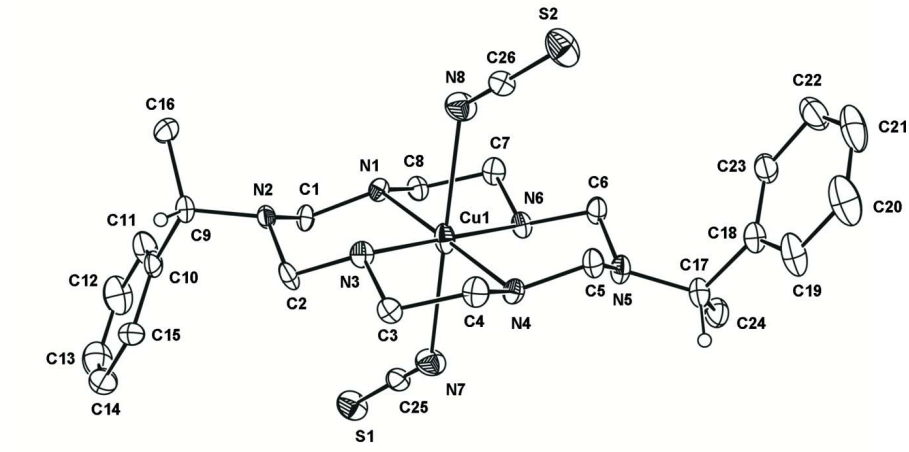

Figure 1

ORTEP drawing of the molecular title compound with atomic numbering scheme at 30% probability.

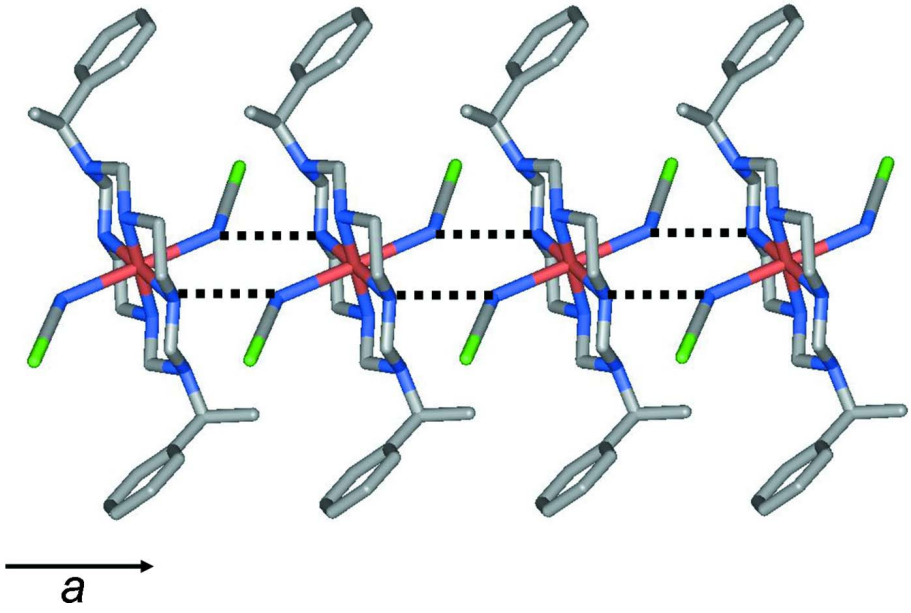

Figure 2

Perspective view of the title compound showing a one-dimensional chain formed by N—H···N (of NCS) hydrogen bonding interactions.

trans-{1,8-Bis[(*S*)-1-phenylethyl]- 1,3,6,8,10,13-hexaazacyclotetradecane}bis(thiocyanato-κ*N*)copper(II)

Crystal data

$[Cu(NCS)_2(C_{24}H_{38}N_6)]$
$M_r = 590.30$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 6.5976$ (5) Å
$b = 14.7609$ (11) Å
$c = 15.2847$ (12) Å
$\beta = 99.952$ (2)°
$V = 1466.13$ (19) Å^3
$Z = 2$
$F(000) = 622$
$D_x = 1.337$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4491 reflections
$\theta = 2.7$–$27.9°$
$\mu = 0.92$ mm^{-1}
$T = 195$ K
Block, purple
0.38 × 0.26 × 0.15 mm

Data collection

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.751$, $T_{max} = 0.871$
10954 measured reflections
6272 independent reflections
4364 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.4°$
$h = -6 \rightarrow 8$
$k = -19 \rightarrow 19$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.115$
$S = 1.11$
6272 reflections
336 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0195P)^2 + 1.3207P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}
Absolute structure: Flack (1983), 2485 Friedel pairs
Absolute structure parameter: −0.01 (2)

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	0.50430 (12)	0.54334 (8)	0.25843 (4)	0.03442 (15)
S1	0.7793 (3)	0.26210 (11)	0.15869 (12)	0.0543 (5)
S2	0.2363 (3)	0.82615 (11)	0.34351 (12)	0.0583 (5)

N1	0.2789 (7)	0.4510 (3)	0.2305 (2)	0.0254 (9)
H1	0.1630	0.4766	0.2476	0.030*
N2	0.3528 (7)	0.3783 (3)	0.3734 (3)	0.0274 (10)
N3	0.5658 (7)	0.5102 (3)	0.3877 (2)	0.0303 (11)
H3	0.4650	0.5373	0.4146	0.036*
N4	0.7316 (7)	0.6346 (3)	0.2878 (2)	0.0273 (10)
H4	0.8493	0.6078	0.2736	0.033*
N5	0.6763 (8)	0.7003 (3)	0.1436 (3)	0.0342 (11)
N6	0.4452 (7)	0.5748 (3)	0.1283 (2)	0.0294 (11)
H6	0.5388	0.5424	0.1015	0.035*
N7	0.7810 (9)	0.4420 (4)	0.2165 (3)	0.0486 (14)
N8	0.2189 (8)	0.6434 (4)	0.2945 (3)	0.0484 (14)
C1	0.3104 (9)	0.3626 (4)	0.2767 (3)	0.0297 (12)
H1A	0.1858	0.3246	0.2609	0.036*
H1B	0.4275	0.3303	0.2582	0.036*
C2	0.5574 (9)	0.4111 (4)	0.4052 (3)	0.0339 (13)
H2A	0.6567	0.3789	0.3746	0.041*
H2B	0.5953	0.3994	0.4697	0.041*
C3	0.7627 (7)	0.5530 (5)	0.4258 (3)	0.0288 (12)
H3A	0.8787	0.5158	0.4127	0.035*
H3B	0.7747	0.5582	0.4910	0.035*
C4	0.7689 (9)	0.6463 (4)	0.3847 (3)	0.0359 (14)
H4A	0.6618	0.6857	0.4027	0.043*
H4B	0.9049	0.6748	0.4047	0.043*
C5	0.7015 (10)	0.7205 (4)	0.2374 (3)	0.0341 (13)
H5A	0.5780	0.7522	0.2505	0.041*
H5B	0.8222	0.7605	0.2549	0.041*
C6	0.4694 (9)	0.6717 (4)	0.1056 (3)	0.0345 (13)
H6A	0.4461	0.6794	0.0403	0.041*
H6B	0.3674	0.7091	0.1298	0.041*
C7	0.2393 (8)	0.5371 (5)	0.0934 (3)	0.0348 (12)
H7A	0.2174	0.5339	0.0278	0.042*
H7B	0.1307	0.5758	0.1111	0.042*
C8	0.2317 (9)	0.4425 (4)	0.1326 (3)	0.0311 (12)
H8A	0.0933	0.4158	0.1142	0.037*
H8B	0.3339	0.4027	0.1115	0.037*
C9	0.2883 (9)	0.3009 (4)	0.4249 (3)	0.0361 (13)
H9	0.3499	0.3132	0.4883	0.043*
C10	0.3729 (9)	0.2099 (3)	0.4034 (3)	0.0331 (13)
C11	0.2610 (11)	0.1501 (5)	0.3414 (4)	0.0534 (18)
H11	0.1285	0.1674	0.3112	0.064*
C12	0.3396 (14)	0.0674 (5)	0.3239 (4)	0.066 (2)
H12	0.2606	0.0278	0.2824	0.079*
C13	0.5321 (13)	0.0415 (7)	0.3659 (4)	0.0688 (19)
H13	0.5858	−0.0158	0.3530	0.083*
C14	0.6468 (11)	0.0979 (5)	0.4265 (4)	0.0541 (18)
H14	0.7794	0.0797	0.4558	0.065*
C15	0.5689 (9)	0.1810 (4)	0.4445 (4)	0.0402 (14)

H15	0.6501	0.2199	0.4860	0.048*
C16	0.0579 (8)	0.3032 (4)	0.4214 (4)	0.0473 (15)
H16A	−0.0116	0.3002	0.3594	0.071*
H16B	0.0197	0.3595	0.4483	0.071*
H16C	0.0163	0.2513	0.4542	0.071*
C17	0.7789 (9)	0.7675 (4)	0.0932 (3)	0.0380 (14)
H17	0.9250	0.7709	0.1244	0.046*
C18	0.6930 (9)	0.8627 (4)	0.0969 (3)	0.0390 (14)
C19	0.8066 (12)	0.9284 (5)	0.1483 (4)	0.059 (2)
H19	0.9418	0.9143	0.1778	0.071*
C20	0.7286 (15)	1.0139 (5)	0.1579 (4)	0.074 (3)
H20	0.8100	1.0583	0.1928	0.089*
C21	0.5318 (14)	1.0343 (6)	0.1165 (4)	0.070 (2)
H21	0.4761	1.0925	0.1243	0.084*
C22	0.4137 (12)	0.9710 (5)	0.0634 (4)	0.060 (2)
H22	0.2793	0.9855	0.0334	0.072*
C23	0.4972 (10)	0.8857 (4)	0.0553 (4)	0.0453 (16)
H23	0.4166	0.8415	0.0198	0.054*
C24	0.7881 (9)	0.7340 (4)	0.0004 (3)	0.0456 (14)
H24A	0.8273	0.6699	0.0028	0.068*
H24B	0.8902	0.7693	−0.0246	0.068*
H24C	0.6527	0.7411	−0.0371	0.068*
C25	0.7772 (9)	0.3680 (5)	0.1908 (4)	0.0360 (14)
C26	0.2274 (9)	0.7192 (4)	0.3148 (4)	0.0368 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0461 (3)	0.0263 (2)	0.0280 (3)	−0.0102 (3)	−0.0019 (2)	0.0032 (3)
S1	0.0567 (12)	0.0369 (10)	0.0655 (11)	−0.0006 (9)	−0.0005 (9)	−0.0091 (8)
S2	0.0683 (13)	0.0330 (10)	0.0674 (11)	−0.0024 (9)	−0.0058 (9)	−0.0068 (8)
N1	0.029 (2)	0.020 (2)	0.028 (2)	−0.0074 (19)	0.0044 (17)	−0.0053 (16)
N2	0.027 (2)	0.024 (2)	0.031 (2)	−0.0027 (19)	0.0019 (18)	0.0087 (17)
N3	0.035 (3)	0.027 (2)	0.029 (2)	−0.004 (2)	0.0039 (18)	−0.0033 (16)
N4	0.029 (2)	0.023 (2)	0.029 (2)	−0.008 (2)	0.0031 (17)	−0.0032 (18)
N5	0.041 (3)	0.033 (3)	0.028 (2)	−0.008 (2)	0.004 (2)	0.0076 (19)
N6	0.040 (3)	0.023 (2)	0.0237 (19)	−0.003 (2)	0.0022 (18)	−0.0013 (15)
N7	0.048 (4)	0.036 (3)	0.062 (3)	0.007 (3)	0.012 (3)	−0.007 (3)
N8	0.047 (4)	0.034 (3)	0.063 (3)	0.001 (3)	0.009 (3)	−0.009 (3)
C1	0.039 (3)	0.020 (3)	0.031 (3)	−0.008 (2)	0.008 (2)	0.002 (2)
C2	0.041 (3)	0.023 (3)	0.033 (3)	0.003 (3)	−0.005 (2)	0.011 (2)
C3	0.031 (3)	0.028 (3)	0.026 (2)	−0.001 (3)	−0.0013 (18)	−0.003 (2)
C4	0.043 (4)	0.039 (3)	0.024 (2)	−0.004 (3)	0.002 (2)	−0.002 (2)
C5	0.042 (4)	0.025 (3)	0.033 (3)	−0.006 (3)	0.002 (2)	0.004 (2)
C6	0.039 (3)	0.033 (3)	0.031 (3)	−0.006 (3)	0.004 (2)	0.008 (2)
C7	0.041 (3)	0.039 (3)	0.0217 (19)	−0.007 (3)	−0.0029 (18)	−0.001 (3)
C8	0.040 (3)	0.026 (3)	0.027 (2)	0.001 (3)	0.006 (2)	−0.001 (2)
C9	0.041 (3)	0.036 (3)	0.033 (3)	0.002 (3)	0.010 (2)	0.015 (2)

C10	0.041 (3)	0.021 (3)	0.038 (3)	−0.004 (2)	0.009 (2)	0.008 (2)
C11	0.064 (5)	0.040 (4)	0.050 (4)	−0.008 (3)	−0.006 (3)	0.011 (3)
C12	0.097 (6)	0.041 (4)	0.056 (4)	−0.009 (4)	0.005 (4)	−0.005 (3)
C13	0.099 (6)	0.045 (4)	0.068 (4)	0.008 (5)	0.029 (4)	0.000 (5)
C14	0.051 (4)	0.043 (4)	0.073 (4)	0.014 (3)	0.023 (3)	0.011 (3)
C15	0.029 (3)	0.041 (3)	0.050 (3)	0.003 (3)	0.007 (3)	0.007 (3)
C16	0.027 (3)	0.059 (4)	0.056 (4)	−0.003 (3)	0.009 (3)	0.021 (3)
C17	0.050 (4)	0.025 (3)	0.040 (3)	−0.003 (3)	0.010 (3)	0.005 (2)
C18	0.050 (4)	0.032 (3)	0.035 (3)	−0.003 (3)	0.007 (3)	0.008 (2)
C19	0.091 (6)	0.031 (3)	0.048 (4)	−0.009 (4)	−0.007 (4)	0.007 (3)
C20	0.123 (8)	0.042 (4)	0.050 (4)	−0.005 (4)	−0.009 (4)	0.001 (3)
C21	0.131 (7)	0.026 (3)	0.058 (4)	0.002 (5)	0.029 (4)	0.000 (4)
C22	0.077 (5)	0.046 (4)	0.059 (4)	0.021 (4)	0.021 (4)	0.018 (3)
C23	0.056 (4)	0.032 (3)	0.051 (3)	0.004 (3)	0.018 (3)	0.009 (3)
C24	0.058 (4)	0.040 (3)	0.044 (3)	0.002 (3)	0.022 (3)	0.007 (3)
C25	0.032 (3)	0.042 (4)	0.033 (3)	0.004 (3)	0.003 (2)	0.005 (3)
C26	0.033 (3)	0.037 (4)	0.040 (3)	0.005 (3)	0.005 (3)	0.004 (3)

Geometric parameters (Å, º)

Cu1—N3	2.008 (4)	C6—H6B	0.9900
Cu1—N4	2.008 (4)	C7—C8	1.523 (9)
Cu1—N1	2.008 (4)	C7—H7A	0.9900
Cu1—N6	2.014 (4)	C7—H7B	0.9900
Cu1—N7	2.527 (6)	C8—H8A	0.9900
Cu1—N8	2.528 (6)	C8—H8B	0.9900
S1—C25	1.639 (7)	C9—C16	1.512 (7)
S2—C26	1.636 (7)	C9—C10	1.513 (8)
N1—C8	1.480 (6)	C9—H9	1.0000
N1—C1	1.482 (6)	C10—C15	1.403 (7)
N1—H1	0.9300	C10—C11	1.406 (8)
N2—C2	1.437 (7)	C11—C12	1.372 (10)
N2—C1	1.474 (6)	C11—H11	0.9500
N2—C9	1.490 (6)	C12—C13	1.375 (10)
N3—C3	1.470 (7)	C12—H12	0.9500
N3—C2	1.490 (6)	C13—C14	1.372 (10)
N3—H3	0.9300	C13—H13	0.9500
N4—C4	1.469 (6)	C14—C15	1.376 (8)
N4—C5	1.479 (7)	C14—H14	0.9500
N4—H4	0.9300	C15—H15	0.9500
N5—C5	1.445 (6)	C16—H16A	0.9800
N5—C6	1.450 (7)	C16—H16B	0.9800
N5—C17	1.490 (7)	C16—H16C	0.9800
N6—C7	1.480 (7)	C17—C24	1.514 (7)
N6—C6	1.487 (7)	C17—C18	1.520 (8)
N6—H6	0.9300	C17—H17	1.0000
N7—C25	1.160 (8)	C18—C23	1.379 (8)
N8—C26	1.160 (8)	C18—C19	1.384 (9)

C1—H1A	0.9900	C19—C20	1.381 (10)
C1—H1B	0.9900	C19—H19	0.9500
C2—H2A	0.9900	C20—C21	1.376 (11)
C2—H2B	0.9900	C20—H20	0.9500
C3—C4	1.518 (8)	C21—C22	1.385 (11)
C3—H3A	0.9900	C21—H21	0.9500
C3—H3B	0.9900	C22—C23	1.389 (9)
C4—H4A	0.9900	C22—H22	0.9500
C4—H4B	0.9900	C23—H23	0.9500
C5—H5A	0.9900	C24—H24A	0.9800
C5—H5B	0.9900	C24—H24B	0.9800
C6—H6A	0.9900	C24—H24C	0.9800

N3—Cu1—N4	85.80 (17)	N6—C7—H7A	110.3
N3—Cu1—N1	93.45 (17)	C8—C7—H7A	110.3
N4—Cu1—N1	179.2 (2)	N6—C7—H7B	110.3
N3—Cu1—N6	179.1 (2)	C8—C7—H7B	110.3
N4—Cu1—N6	94.36 (17)	H7A—C7—H7B	108.6
N1—Cu1—N6	86.38 (17)	N1—C8—C7	107.8 (4)
C8—N1—C1	113.3 (4)	N1—C8—H8A	110.2
C8—N1—Cu1	106.9 (3)	C7—C8—H8A	110.2
C1—N1—Cu1	117.3 (3)	N1—C8—H8B	110.2
C8—N1—H1	106.2	C7—C8—H8B	110.2
C1—N1—H1	106.2	H8A—C8—H8B	108.5
Cu1—N1—H1	106.2	N2—C9—C16	110.0 (4)
C2—N2—C1	113.3 (4)	N2—C9—C10	114.6 (4)
C2—N2—C9	114.7 (4)	C16—C9—C10	114.7 (5)
C1—N2—C9	112.7 (4)	N2—C9—H9	105.6
C3—N3—C2	114.1 (4)	C16—C9—H9	105.6
C3—N3—Cu1	107.4 (3)	C10—C9—H9	105.6
C2—N3—Cu1	114.1 (3)	C15—C10—C11	116.6 (6)
C3—N3—H3	106.9	C15—C10—C9	121.2 (5)
C2—N3—H3	106.9	C11—C10—C9	122.2 (5)
Cu1—N3—H3	106.9	C12—C11—C10	121.2 (7)
C4—N4—C5	114.1 (4)	C12—C11—H11	119.4
C4—N4—Cu1	107.1 (3)	C10—C11—H11	119.4
C5—N4—Cu1	115.5 (3)	C11—C12—C13	120.5 (7)
C4—N4—H4	106.5	C11—C12—H12	119.8
C5—N4—H4	106.5	C13—C12—H12	119.8
Cu1—N4—H4	106.5	C14—C13—C12	120.2 (8)
C5—N5—C6	113.4 (5)	C14—C13—H13	119.9
C5—N5—C17	113.0 (4)	C12—C13—H13	119.9
C6—N5—C17	117.8 (4)	C13—C14—C15	119.7 (7)
C7—N6—C6	114.0 (5)	C13—C14—H14	120.2
C7—N6—Cu1	106.2 (3)	C15—C14—H14	120.2
C6—N6—Cu1	116.2 (3)	C14—C15—C10	121.9 (6)
C7—N6—H6	106.6	C14—C15—H15	119.0
C6—N6—H6	106.6	C10—C15—H15	119.0

Cu1—N6—H6	106.6	C9—C16—H16A	109.5
N2—C1—N1	109.0 (4)	C9—C16—H16B	109.5
N2—C1—H1A	109.9	H16A—C16—H16B	109.5
N1—C1—H1A	109.9	C9—C16—H16C	109.5
N2—C1—H1B	109.9	H16A—C16—H16C	109.5
N1—C1—H1B	109.9	H16B—C16—H16C	109.5
H1A—C1—H1B	108.3	N5—C17—C24	111.2 (4)
N2—C2—N3	109.4 (4)	N5—C17—C18	113.0 (5)
N2—C2—H2A	109.8	C24—C17—C18	114.4 (4)
N3—C2—H2A	109.8	N5—C17—H17	105.8
N2—C2—H2B	109.8	C24—C17—H17	105.8
N3—C2—H2B	109.8	C18—C17—H17	105.8
H2A—C2—H2B	108.2	C23—C18—C19	117.5 (6)
N3—C3—C4	108.1 (4)	C23—C18—C17	122.4 (6)
N3—C3—H3A	110.1	C19—C18—C17	120.0 (6)
C4—C3—H3A	110.1	C20—C19—C18	121.7 (7)
N3—C3—H3B	110.1	C20—C19—H19	119.2
C4—C3—H3B	110.1	C18—C19—H19	119.2
H3A—C3—H3B	108.4	C21—C20—C19	119.4 (7)
N4—C4—C3	107.3 (4)	C21—C20—H20	120.3
N4—C4—H4A	110.2	C19—C20—H20	120.3
C3—C4—H4A	110.2	C20—C21—C22	120.8 (7)
N4—C4—H4B	110.2	C20—C21—H21	119.6
C3—C4—H4B	110.2	C22—C21—H21	119.6
H4A—C4—H4B	108.5	C21—C22—C23	118.2 (7)
N5—C5—N4	108.8 (4)	C21—C22—H22	120.9
N5—C5—H5A	109.9	C23—C22—H22	120.9
N4—C5—H5A	109.9	C18—C23—C22	122.4 (7)
N5—C5—H5B	109.9	C18—C23—H23	118.8
N4—C5—H5B	109.9	C22—C23—H23	118.8
H5A—C5—H5B	108.3	C17—C24—H24A	109.5
N5—C6—N6	108.5 (4)	C17—C24—H24B	109.5
N5—C6—H6A	110.0	H24A—C24—H24B	109.5
N6—C6—H6A	110.0	C17—C24—H24C	109.5
N5—C6—H6B	110.0	H24A—C24—H24C	109.5
N6—C6—H6B	110.0	H24B—C24—H24C	109.5
H6A—C6—H6B	108.4	N7—C25—S1	177.3 (6)
N6—C7—C8	107.1 (4)	N8—C26—S2	179.3 (6)

N3—Cu1—N1—C8	−166.4 (3)	C6—N6—C7—C8	−172.6 (4)
N6—Cu1—N1—C8	12.7 (3)	Cu1—N6—C7—C8	−43.4 (5)
N3—Cu1—N1—C1	−38.0 (4)	C1—N1—C8—C7	−170.5 (4)
N6—Cu1—N1—C1	141.1 (4)	Cu1—N1—C8—C7	−39.7 (5)
N4—Cu1—N3—C3	−12.5 (4)	N6—C7—C8—N1	56.3 (6)
N1—Cu1—N3—C3	167.1 (4)	C2—N2—C9—C16	150.3 (5)
N4—Cu1—N3—C2	−140.0 (4)	C1—N2—C9—C16	−78.0 (6)
N1—Cu1—N3—C2	39.6 (4)	C2—N2—C9—C10	−78.8 (6)
N3—Cu1—N4—C4	−16.9 (4)	C1—N2—C9—C10	52.9 (6)

N6—Cu1—N4—C4	164.0 (4)	N2—C9—C10—C15	84.8 (6)
N3—Cu1—N4—C5	−145.2 (4)	C16—C9—C10—C15	−146.6 (5)
N6—Cu1—N4—C5	35.7 (4)	N2—C9—C10—C11	−95.1 (6)
N4—Cu1—N6—C7	−162.9 (4)	C16—C9—C10—C11	33.5 (7)
N1—Cu1—N6—C7	17.4 (4)	C15—C10—C11—C12	1.1 (9)
N4—Cu1—N6—C6	−35.0 (4)	C9—C10—C11—C12	−179.1 (6)
N1—Cu1—N6—C6	145.4 (4)	C10—C11—C12—C13	−0.9 (11)
C2—N2—C1—N1	−75.4 (6)	C11—C12—C13—C14	0.5 (11)
C9—N2—C1—N1	152.3 (4)	C12—C13—C14—C15	−0.5 (11)
C8—N1—C1—N2	−179.1 (4)	C13—C14—C15—C10	0.7 (10)
Cu1—N1—C1—N2	55.6 (5)	C11—C10—C15—C14	−1.0 (9)
C1—N2—C2—N3	80.1 (5)	C9—C10—C15—C14	179.1 (5)
C9—N2—C2—N3	−148.6 (4)	C5—N5—C17—C24	168.0 (5)
C3—N3—C2—N2	174.0 (4)	C6—N5—C17—C24	−56.7 (7)
Cu1—N3—C2—N2	−62.0 (5)	C5—N5—C17—C18	−61.8 (6)
C2—N3—C3—C4	166.4 (4)	C6—N5—C17—C18	73.6 (6)
Cu1—N3—C3—C4	38.9 (5)	N5—C17—C18—C23	−68.8 (7)
C5—N4—C4—C3	171.2 (4)	C24—C17—C18—C23	59.8 (7)
Cu1—N4—C4—C3	42.1 (5)	N5—C17—C18—C19	106.6 (6)
N3—C3—C4—N4	−54.6 (6)	C24—C17—C18—C19	−124.8 (6)
C6—N5—C5—N4	81.0 (6)	C23—C18—C19—C20	−0.1 (10)
C17—N5—C5—N4	−141.6 (5)	C17—C18—C19—C20	−175.8 (6)
C4—N4—C5—N5	177.3 (5)	C18—C19—C20—C21	1.0 (11)
Cu1—N4—C5—N5	−58.0 (6)	C19—C20—C21—C22	−1.8 (11)
C5—N5—C6—N6	−79.4 (5)	C20—C21—C22—C23	1.8 (10)
C17—N5—C6—N6	145.4 (5)	C19—C18—C23—C22	0.2 (9)
C7—N6—C6—N5	179.9 (4)	C17—C18—C23—C22	175.7 (5)
Cu1—N6—C6—N5	55.9 (6)	C21—C22—C23—C18	−1.0 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N7^{i}	0.93	2.54	3.258 (7)	135
N4—H4···N8^{ii}	0.93	2.46	3.202 (7)	137

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