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Bis(*N*,*N*′-diphenylthiourea)iodidocopper(I) monohydrate

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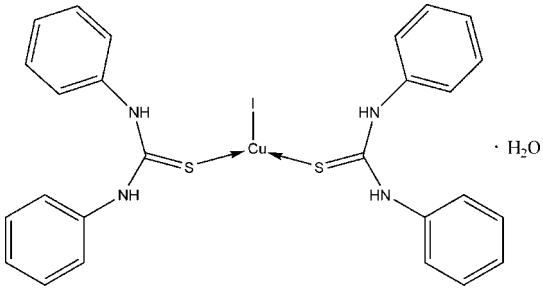
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.041; wR factor = 0.085; data-to-parameter ratio = 15.2.

In the title compound, $[CuI(C_{13}H_{12}N_2S)_2]\cdot H_2O$, each Cu(I) ion is coordinated by two S atoms [Cu—S 2.2282 (16), 2.2377 (15) Å] from two *N*,*N*′-diphenylthiourea ligands and one iodide ion [Cu—I 2.5170 (11) Å] in a trigonal planar geometry. The uncoordinated water molecules are involved in N—H···O hydrogen-bonding [N···O 2.947 (5), 3.055 (5) Å], which link the molecules into chains extended in the [101] direction. These chains are further paired by weak intermolecular O—H···S hydrogen bonds [O···S 3.490 (4) Å].

Related literature

For geometrical parameters in related crystal structures, see: Lobana *et al.* (2006).



Experimental

Crystal data

$[CuI(C_{13}H_{12}N_2S)_2]\cdot H_2O$
M_r = 665.07
Triclinic, $P\overline{1}$
a = 9.700 (4) Å
b = 12.490 (5) Å
c = 12.935 (5) Å
α = 91.489 (5)°
β = 108.110 (5)°
γ = 110.950 (5)°
V = 1374.4 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.10 mm^{-1}
T = 298 (2) K
0.28 × 0.19 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.592, T_{max} = 0.704
7290 measured reflections
4804 independent reflections
2999 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.085
S = 0.87
4804 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···I1	0.86	2.87	3.706 (4)	166
N2—H2···O1^{i}	0.86	2.14	2.947 (5)	156
N3—H3···I1	0.86	2.82	3.666 (4)	168
N4—H4···O1^{ii}	0.86	2.38	3.055 (5)	136
O1—H1*B*···S2^{iii}	0.85	2.64	3.490 (4)	179

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We thank the Natural Science Foundation of Liaocheng University (X051002) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2394).

References

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supporting information

Acta Cryst. (2008). E**64**, m763 [doi:10.1107/S1600536808007861]

Bis(*N*,*N*′-diphenylthiourea)iodidocopper(I) monohydrate

Li Jia, Lingqian Kong and Dacheng Li

S1. Comment

In this paper, we report the synthesis and the crystal structure of the title compound (I).

In (I) (Fig. 1), the Cu(I) ion is in a trigonal coordination environment formed by to two S atoms of two monodentate diphenylthiourea ligands and one iodine ion. The Cu-S [2.2282 (16), 2.2377 (15) Å] and Cu-I [2.5170 (11) Å] bond lengths agree well with those reported for the related compounds (Lobana *et al.*, 2006).

The crystalline water molecules are involved in N—H···O hydrogen-bonding (Table 1), which link the molecules into chains extended in direction [101]. These chains are further paired (Fig. 2) by the weak intermolecular O—H···S hydrogen bonds (Table 1).

S2. Experimental

CuI (0.19 g 1 mmol) and diphenylthiourea (0.46 g 2 mmol) in 10 ml acetonitrile,refluxed for 24 h, then a colourless solution formed. After filtration, the solution was allowed to evaporate slowly. Crystals suitable for X-ray diffraction were obtained after several days.

S3. Refinement

All H atoms were placed in calculated positions (O-H 0.85 Å, N-H 0.86 Å, C-H 0.93 Å), and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq} of the parent atoms.

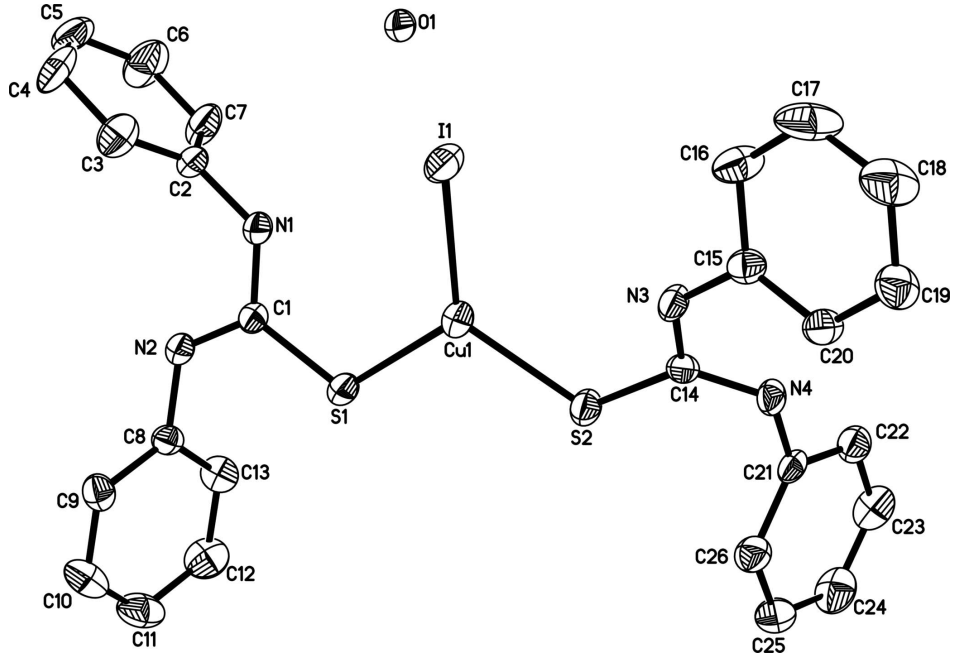

Figure 1

The molecular structure of (I), showing the atomic numbering and 40% probability displacement ellipsoids. H atoms omitted for clarity.

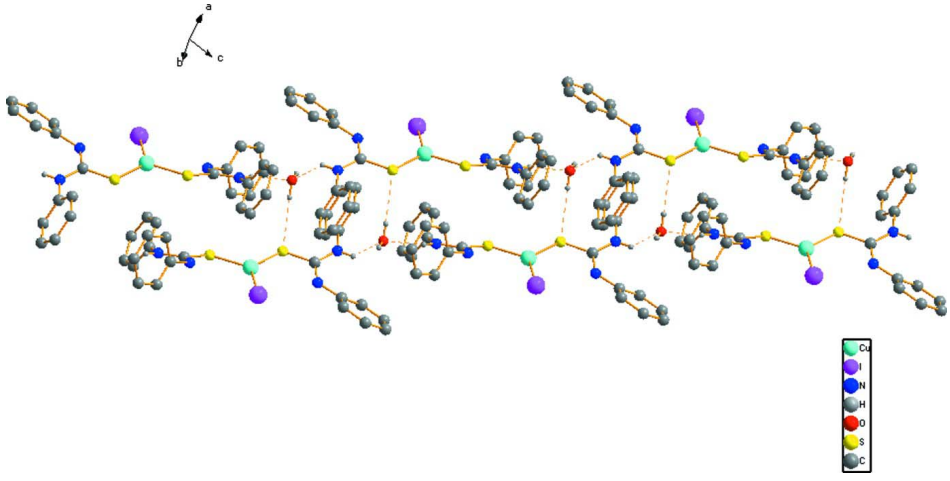

Figure 2

A portion of the crystal packing showing the paired hydrogen-bonded (dashed lines) chains. H atoms not involved in hydrogen-bonding are omitted for clarity.

Bis(*N*,*N*′-diphenylthiourea)iodidocopper(I) monohydrate

Crystal data

$[CuI(C_{13}H_{12}N_2S)_2]\cdot H_2O$
$M_r = 665.07$
Triclinic, $P\overline{1}$
$a = 9.700\ (4)$ Å
$b = 12.490\ (5)$ Å
$c = 12.935\ (5)$ Å
$\alpha = 91.489\ (5)°$
$\beta = 108.110\ (5)°$
$\gamma = 110.950\ (5)°$
$V = 1374.4\ (9)$ Å^3

$Z = 2$
$F(000) = 664$
$D_x = 1.607$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1949 reflections
$\theta = 2.4$–$22.1°$
$\mu = 2.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.28 × 0.19 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.592$, $T_{max} = 0.704$
7290 measured reflections
4804 independent reflections
2999 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.085$
$S = 0.87$
4804 reflections
316 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
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ 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	0.05943 (7)	0.11385 (5)	0.77393 (5)	0.04630 (19)
I1	0.17712 (4)	0.33136 (3)	0.82406 (3)	0.05399 (14)
N1	−0.0381 (4)	0.2061 (3)	0.5295 (3)	0.0443 (11)
H1	0.0273	0.2349	0.5952	0.053*
N2	−0.2538 (4)	0.0540 (3)	0.4163 (3)	0.0436 (11)
H2	−0.2571	0.0987	0.3669	0.052*
N3	0.2680 (4)	0.1602 (3)	1.0425 (3)	0.0405 (10)
H3	0.2322	0.1966	0.9921	0.049*
N4	0.3157 (4)	−0.0053 (3)	1.0771 (3)	0.0406 (10)
H4	0.3845	0.0350	1.1385	0.049*
O1	0.6610 (4)	0.1414 (3)	0.2058 (3)	0.0619 (11)

H1A	0.6840	0.2105	0.1920	0.074*
H1B	0.7159	0.1107	0.1858	0.074*
S1	−0.12503 (15)	0.01325 (10)	0.61534 (11)	0.0466 (4)
S2	0.11547 (15)	−0.01538 (10)	0.87828 (11)	0.0474 (4)
C1	−0.1409 (5)	0.0964 (4)	0.5129 (4)	0.0347 (12)
C2	−0.0288 (6)	0.2790 (4)	0.4464 (4)	0.0423 (13)
C3	−0.1082 (7)	0.3512 (4)	0.4296 (5)	0.0613 (16)
H3A	−0.1706	0.3526	0.4711	0.074*
C4	−0.0948 (8)	0.4228 (5)	0.3497 (5)	0.073 (2)
H4A	−0.1478	0.4729	0.3384	0.088*
C5	−0.0044 (7)	0.4203 (5)	0.2876 (5)	0.0701 (19)
H5	0.0043	0.4687	0.2345	0.084*
C6	0.0738 (8)	0.3459 (6)	0.3040 (6)	0.085 (2)
H6	0.1342	0.3424	0.2615	0.102*
C7	0.0606 (6)	0.2770 (5)	0.3844 (5)	0.0645 (17)
H7	0.1145	0.2275	0.3966	0.077*
C8	−0.3704 (5)	−0.0610 (4)	0.3884 (4)	0.0379 (12)
C9	−0.5254 (6)	−0.0777 (4)	0.3680 (4)	0.0470 (14)
H9	−0.5529	−0.0142	0.3729	0.056*
C10	−0.6383 (6)	−0.1869 (5)	0.3406 (5)	0.0624 (17)
H10	−0.7425	−0.1977	0.3278	0.075*
C11	−0.5994 (7)	−0.2808 (5)	0.3318 (5)	0.0687 (18)
H11	−0.6772	−0.3553	0.3124	0.082*
C12	−0.4450 (8)	−0.2653 (5)	0.3517 (5)	0.0665 (18)
H12	−0.4180	−0.3290	0.3465	0.080*
C13	−0.3309 (6)	−0.1546 (4)	0.3791 (5)	0.0512 (14)
H13	−0.2267	−0.1435	0.3914	0.061*
C14	0.2398 (5)	0.0499 (4)	1.0080 (4)	0.0342 (12)
C15	0.3482 (5)	0.2268 (4)	1.1501 (5)	0.0412 (13)
C16	0.4300 (7)	0.3453 (4)	1.1573 (5)	0.0581 (16)
H16	0.4354	0.3778	1.0941	0.070*
C17	0.5030 (8)	0.4140 (5)	1.2591 (6)	0.081 (2)
H17	0.5568	0.4935	1.2646	0.097*
C18	0.4967 (7)	0.3661 (5)	1.3517 (6)	0.0724 (19)
H18	0.5469	0.4131	1.4201	0.087*
C19	0.4175 (6)	0.2495 (5)	1.3452 (5)	0.0553 (15)
H19	0.4151	0.2173	1.4090	0.066*
C20	0.3410 (6)	0.1801 (4)	1.2436 (4)	0.0444 (13)
H20	0.2844	0.1012	1.2388	0.053*
C21	0.2935 (6)	−0.1242 (4)	1.0585 (4)	0.0371 (12)
C22	0.4230 (6)	−0.1510 (4)	1.0756 (4)	0.0492 (14)
H22	0.5229	−0.0927	1.0974	0.059*
C23	0.4029 (7)	−0.2666 (5)	1.0598 (5)	0.0631 (17)
H23	0.4903	−0.2856	1.0711	0.076*
C24	0.2569 (8)	−0.3529 (5)	1.0281 (5)	0.0699 (18)
H24	0.2448	−0.4300	1.0170	0.084*
C25	0.1277 (7)	−0.3252 (5)	1.0125 (5)	0.0673 (18)
H25	0.0279	−0.3838	0.9910	0.081*

C26	0.1456 (6)	−0.2107 (4)	1.0286 (5)	0.0498 (14)
H26	0.0583	−0.1920	1.0193	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0492 (4)	0.0489 (4)	0.0387 (4)	0.0194 (3)	0.0111 (3)	0.0147 (3)
I1	0.0693 (3)	0.0439 (2)	0.0507 (3)	0.02398 (19)	0.0197 (2)	0.01702 (19)
N1	0.044 (2)	0.041 (2)	0.033 (3)	0.010 (2)	0.001 (2)	0.011 (2)
N2	0.043 (2)	0.040 (2)	0.039 (3)	0.013 (2)	0.005 (2)	0.013 (2)
N3	0.053 (3)	0.037 (2)	0.030 (3)	0.019 (2)	0.008 (2)	0.010 (2)
N4	0.048 (2)	0.035 (2)	0.028 (2)	0.015 (2)	0.001 (2)	0.001 (2)
O1	0.065 (2)	0.056 (2)	0.050 (3)	0.017 (2)	0.008 (2)	0.010 (2)
S1	0.0489 (8)	0.0414 (8)	0.0394 (8)	0.0117 (6)	0.0077 (7)	0.0152 (7)
S2	0.0557 (8)	0.0400 (7)	0.0360 (8)	0.0166 (7)	0.0037 (7)	0.0076 (7)
C1	0.037 (3)	0.035 (3)	0.033 (3)	0.015 (2)	0.012 (3)	0.008 (2)
C2	0.046 (3)	0.037 (3)	0.041 (3)	0.015 (3)	0.011 (3)	0.014 (3)
C3	0.080 (4)	0.057 (4)	0.058 (4)	0.036 (3)	0.028 (4)	0.014 (3)
C4	0.112 (5)	0.057 (4)	0.066 (5)	0.052 (4)	0.025 (4)	0.032 (4)
C5	0.092 (5)	0.050 (4)	0.058 (4)	0.018 (3)	0.021 (4)	0.029 (3)
C6	0.103 (5)	0.104 (5)	0.086 (6)	0.054 (5)	0.062 (5)	0.057 (5)
C7	0.074 (4)	0.077 (4)	0.070 (5)	0.046 (4)	0.039 (4)	0.044 (4)
C8	0.039 (3)	0.041 (3)	0.029 (3)	0.009 (2)	0.012 (3)	0.006 (2)
C9	0.042 (3)	0.056 (3)	0.041 (4)	0.020 (3)	0.011 (3)	0.007 (3)
C10	0.041 (3)	0.071 (4)	0.062 (4)	0.007 (3)	0.020 (3)	−0.006 (4)
C11	0.064 (4)	0.057 (4)	0.059 (4)	−0.005 (3)	0.020 (4)	−0.007 (3)
C12	0.086 (5)	0.044 (4)	0.070 (5)	0.026 (4)	0.028 (4)	−0.003 (3)
C13	0.052 (3)	0.052 (4)	0.052 (4)	0.020 (3)	0.022 (3)	0.001 (3)
C14	0.034 (3)	0.032 (3)	0.032 (3)	0.007 (2)	0.012 (2)	0.004 (2)
C15	0.043 (3)	0.035 (3)	0.047 (4)	0.015 (2)	0.018 (3)	0.006 (3)
C16	0.082 (4)	0.040 (3)	0.055 (4)	0.013 (3)	0.039 (4)	0.009 (3)
C17	0.097 (5)	0.039 (3)	0.090 (6)	−0.008 (3)	0.050 (5)	−0.015 (4)
C18	0.084 (5)	0.057 (4)	0.061 (5)	0.006 (4)	0.031 (4)	−0.017 (4)
C19	0.057 (4)	0.058 (4)	0.043 (4)	0.015 (3)	0.016 (3)	0.000 (3)
C20	0.047 (3)	0.039 (3)	0.045 (4)	0.011 (3)	0.018 (3)	0.006 (3)
C21	0.050 (3)	0.037 (3)	0.026 (3)	0.018 (3)	0.013 (3)	0.012 (2)
C22	0.049 (3)	0.057 (4)	0.045 (4)	0.023 (3)	0.017 (3)	0.014 (3)
C23	0.081 (5)	0.070 (4)	0.065 (5)	0.046 (4)	0.039 (4)	0.022 (4)
C24	0.098 (5)	0.045 (4)	0.069 (5)	0.038 (4)	0.019 (4)	0.007 (3)
C25	0.064 (4)	0.043 (4)	0.077 (5)	0.009 (3)	0.013 (4)	0.017 (3)
C26	0.050 (3)	0.046 (3)	0.058 (4)	0.022 (3)	0.019 (3)	0.016 (3)

Geometric parameters (Å, º)

Cu1—S1	2.2282 (16)	C9—C10	1.360 (7)
Cu1—S2	2.2377 (15)	C9—H9	0.9300
Cu1—I1	2.5170 (11)	C10—C11	1.367 (7)
N1—C1	1.338 (5)	C10—H10	0.9300

N1—C2	1.431 (6)	C11—C12	1.377 (7)
N1—H1	0.8600	C11—H11	0.9300
N2—C1	1.320 (6)	C12—C13	1.378 (7)
N2—C8	1.425 (5)	C12—H12	0.9300
N2—H2	0.8600	C13—H13	0.9300
N3—C14	1.340 (5)	C15—C20	1.367 (7)
N3—C15	1.427 (6)	C15—C16	1.392 (7)
N3—H3	0.8600	C16—C17	1.378 (8)
N4—C14	1.343 (5)	C16—H16	0.9300
N4—C21	1.424 (5)	C17—C18	1.362 (8)
N4—H4	0.8600	C17—H17	0.9300
O1—H1A	0.8500	C18—C19	1.367 (7)
O1—H1B	0.8500	C18—H18	0.9300
S1—C1	1.708 (5)	C19—C20	1.380 (7)
S2—C14	1.703 (5)	C19—H19	0.9300
C2—C7	1.358 (7)	C20—H20	0.9300
C2—C3	1.363 (6)	C21—C22	1.368 (6)
C3—C4	1.389 (7)	C21—C26	1.379 (6)
C3—H3A	0.9300	C22—C23	1.386 (7)
C4—C5	1.368 (8)	C22—H22	0.9300
C4—H4A	0.9300	C23—C24	1.364 (7)
C5—C6	1.377 (8)	C23—H23	0.9300
C5—H5	0.9300	C24—C25	1.373 (7)
C6—C7	1.375 (7)	C24—H24	0.9300
C6—H6	0.9300	C25—C26	1.379 (7)
C7—H7	0.9300	C25—H25	0.9300
C8—C13	1.367 (6)	C26—H26	0.9300
C8—C9	1.378 (6)		

S1—Cu1—S2	106.87 (6)	C10—C11—C12	120.0 (5)
S1—Cu1—I1	125.81 (4)	C10—C11—H11	120.0
S2—Cu1—I1	127.32 (5)	C12—C11—H11	120.0
C1—N1—C2	125.0 (4)	C11—C12—C13	119.5 (5)
C1—N1—H1	117.5	C11—C12—H12	120.2
C2—N1—H1	117.5	C13—C12—H12	120.2
C1—N2—C8	124.3 (4)	C8—C13—C12	120.2 (5)
C1—N2—H2	117.8	C8—C13—H13	119.9
C8—N2—H2	117.8	C12—C13—H13	119.9
C14—N3—C15	130.0 (4)	N3—C14—N4	118.1 (4)
C14—N3—H3	115.0	N3—C14—S2	120.2 (4)
C15—N3—H3	115.0	N4—C14—S2	121.6 (3)
C14—N4—C21	126.3 (4)	C20—C15—C16	119.8 (5)
C14—N4—H4	116.8	C20—C15—N3	122.9 (4)
C21—N4—H4	116.8	C16—C15—N3	117.3 (5)
H1A—O1—H1B	110.0	C17—C16—C15	119.3 (6)
C1—S1—Cu1	112.56 (17)	C17—C16—H16	120.3
C14—S2—Cu1	111.44 (16)	C15—C16—H16	120.3
N2—C1—N1	118.9 (4)	C18—C17—C16	120.2 (5)

N2—C1—S1	120.9 (4)	C18—C17—H17	119.9
N1—C1—S1	120.3 (4)	C16—C17—H17	119.9
C7—C2—C3	119.7 (5)	C17—C18—C19	120.7 (6)
C7—C2—N1	119.9 (4)	C17—C18—H18	119.6
C3—C2—N1	120.4 (5)	C19—C18—H18	119.6
C2—C3—C4	119.3 (6)	C18—C19—C20	119.6 (6)
C2—C3—H3A	120.4	C18—C19—H19	120.2
C4—C3—H3A	120.4	C20—C19—H19	120.2
C5—C4—C3	120.7 (5)	C15—C20—C19	120.3 (5)
C5—C4—H4A	119.7	C15—C20—H20	119.9
C3—C4—H4A	119.7	C19—C20—H20	119.9
C4—C5—C6	119.8 (6)	C22—C21—C26	120.6 (5)
C4—C5—H5	120.1	C22—C21—N4	118.5 (4)
C6—C5—H5	120.1	C26—C21—N4	120.9 (4)
C7—C6—C5	118.7 (6)	C21—C22—C23	119.0 (5)
C7—C6—H6	120.7	C21—C22—H22	120.5
C5—C6—H6	120.7	C23—C22—H22	120.5
C2—C7—C6	121.9 (5)	C24—C23—C22	120.9 (5)
C2—C7—H7	119.0	C24—C23—H23	119.5
C6—C7—H7	119.0	C22—C23—H23	119.5
C13—C8—C9	119.7 (5)	C23—C24—C25	119.7 (5)
C13—C8—N2	120.8 (4)	C23—C24—H24	120.2
C9—C8—N2	119.5 (4)	C25—C24—H24	120.2
C10—C9—C8	120.2 (5)	C24—C25—C26	120.1 (5)
C10—C9—H9	119.9	C24—C25—H25	119.9
C8—C9—H9	119.9	C26—C25—H25	119.9
C9—C10—C11	120.4 (5)	C21—C26—C25	119.6 (5)
C9—C10—H10	119.8	C21—C26—H26	120.2
C11—C10—H10	119.8	C25—C26—H26	120.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···I1	0.86	2.87	3.706 (4)	166
N2—H2···O1^{i}	0.86	2.14	2.947 (5)	156
N3—H3···I1	0.86	2.82	3.666 (4)	168
N4—H4···O1^{ii}	0.86	2.38	3.055 (5)	136
O1—H1*B*···S2^{iii}	0.85	2.64	3.490 (4)	179

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