Diisopropylammonium (3,6-dichlorobenzene-1,2-dithiolato)cuprato(III) tetrahydrofuran monosolvate

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The asymmetric unit of the title compound, $(C_6H_{16}N)[Cu(C_6H_2Cl_2S_2)_2]\cdot C_4H_8O$, comprises a $[Cu(SC_6H_2Cl_2S)_2]^-$ anion, an $[^iPr_2NH_2]^+$ cation and a solvent tetrahydrofuran molecule. The Cu^{III} atom has an almost square-planar CuS_4 coordination environment. In the crystal, the anion and the solvent molecule are linked via N—H···O and N—H···S hydrogen bonds involving the diisopropylammonium cation. There are no other significant intermolecular interactions present.

3D view
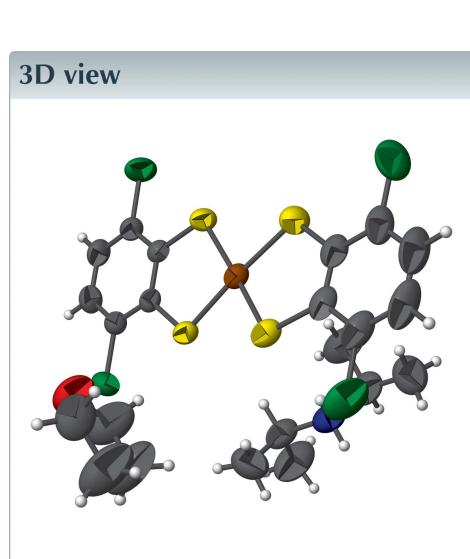
Chemical scheme
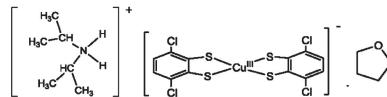
Structure description

In the title compound, Fig. 1, the anion presents a planar geometry with the copper(III) atom located at its center in a almost square planar CuS_4 coordination environment. The S—Cu—S bond angles [S4—Cu1—S2 = 87.85 (3), S4—Cu1—S3 = 92.26 (3), S2—Cu1—S1 = 92.14 (4)° and S3—Cu1—S1 = 88.45 (3) °] slightly deviate from 90°, and the Cu—S bond lengths vary from 2.1722 (9) to 2.1776 (9) Å. These geometrical parameters agree well with those observed in a similar compound containing the same anion but with the methyltriphenylphosphonium cation (Herich et al., 2015).

In the crystal, the anion and the solvent molecule are linked via N—H···O and N—H···S hydrogen bonds involving the cation (Fig. 2 and Table 1). There are no other significant intermolecular interactions present.

Synthesis and crystallization

To a solution of 1,2-$HSC_6H_2Cl_2SH$ (74 mg, 0.35 mmol) in CH_3CN (3 ml) was added $^iPr_2NH$ (99 µl, 0.70 mmol). After stirring for 5 min, $Cu(ClO_4)_2\cdot 6H_2O$ (64 mg, 0.18 mmol)

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

| $D—H \cdots A$	$D—H$	$H \cdots A$	$D \cdots A$	$D—H \cdots A$
N1—H1$A \cdots$S1	0.89	2.59	3.417 (3)	156
N1—H1$B \cdots$O1^i	0.89	1.93	2.805 (4)	170

Symmetry code: (i) $x, y + 1, z$.
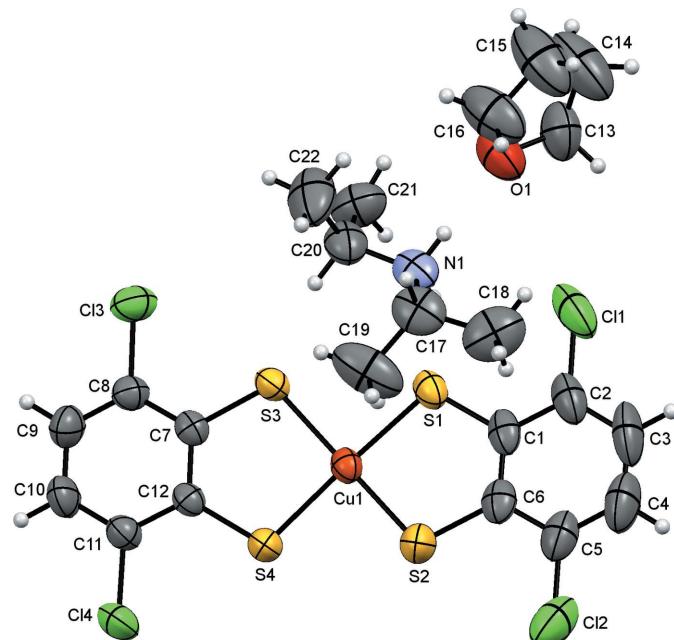
Figure 1
The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level.
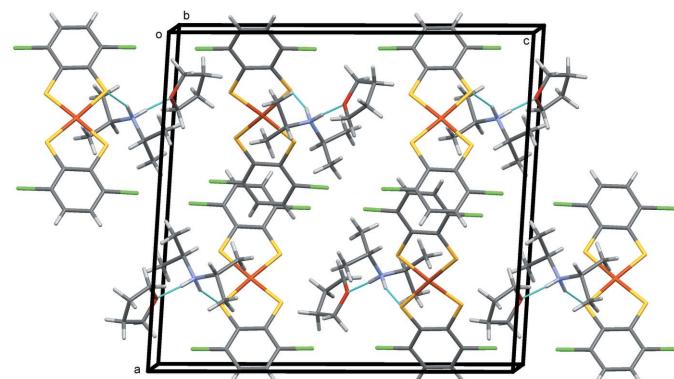

Figure 2
A view along the b axis of the crystal packing of the title compound, with the N—H$\cdots$O and N—H$\cdots$S hydrogen bonds shown as dashed lines (see Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_6H_{16}N)[Cu(C_6H_2Cl_2S_2)_2] \cdot C_4H_8O$
M_r	656.03
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	17.6487 (8), 8.8259 (3), 18.9730 (8)
β (°)	93.616 (2)
V (Å^3)	2949.5 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.40
Crystal size (mm)	$0.08 \times 0.06 \times 0.01$
Data collection	
Diffractometer	Bruker Kappa APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.90, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35036, 5305, 3766
R_{int}	0.046
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.037, 0.096, 1.01
No. of reflections	5305
No. of parameters	302
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.30, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

was added, and the reaction mixture was left for 2 h in an open atmosphere. Then the solvent was removed in vacuum, yielding a green solid. Recrystallization of this solid in THF/*n*-heptane (1:1) at room temperature produced green plate-like crystals of the title compound (yield 110 mg, 93%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

References

Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Herich, P., Fronc, M. & Kožíšek, J. (2015). *Acta Cryst.* C**71**, 159–164.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

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Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

full crystallographic data

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Crystal data

$(C_6H_{16}N)[Cu(C_6H_2Cl_2S_2)_2]\cdot C_4H_8O$	$F(000) = 1344$
$M_r = 656.03$	$D_x = 1.477$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 17.6487$ (8) Å	Cell parameters from 7896 reflections
$b = 8.8259$ (3) Å	$\theta = 2.6–22.7°$
$c = 18.9730$ (8) Å	$\mu = 1.40$ mm^{-1}
$\beta = 93.616$ (2)°	$T = 296$ K
$V = 2949.5$ (2) Å^3	Plate, green
$Z = 4$	$0.08 \times 0.06 \times 0.01$ mm

Data collection

Bruker Kappa APEXII diffractometer	35036 measured reflections
Radiation source: fine-focus sealed tube	5305 independent reflections
Graphite monochromator	3766 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.046$
Absorption correction: multi-scan (SADABS; Bruker, 2008)	$\theta_{max} = 25.3°$, $\theta_{min} = 2.6°$
	$h = -18\rightarrow21$
$T_{min} = 0.90$, $T_{max} = 0.99$	$k = -10\rightarrow10$
	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.096$	
$S = 1.01$	H-atom parameters constrained
5305 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 1.2611P]$ where $P = (F_o^2 + 2F_c^2)/3$
302 parameters	
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.30$ e Å^{-3}
	$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.89102 (17)	0.7458 (3)	0.7206 (2)	0.0564 (9)
C2	0.9492 (2)	0.8280 (4)	0.6920 (2)	0.0753 (11)
C3	1.0060 (2)	0.8945 (5)	0.7352 (3)	0.0984 (16)
H3	1.0448	0.9482	0.7155	0.118*
C4	1.0048 (3)	0.8807 (5)	0.8072 (3)	0.0986 (15)
H4	1.0431	0.9247	0.8363	0.118*
C5	0.9480 (2)	0.8031 (4)	0.8363 (2)	0.0750 (11)
C6	0.88941 (18)	0.7351 (4)	0.7939 (2)	0.0589 (9)
C7	0.59589 (16)	0.3943 (3)	0.68861 (15)	0.0420 (7)
C8	0.53460 (19)	0.3371 (3)	0.64767 (16)	0.0502 (8)
C9	0.4777 (2)	0.2576 (4)	0.67669 (19)	0.0642 (9)
H9	0.4372	0.2201	0.6481	0.077*
C10	0.4808 (2)	0.2336 (4)	0.74827 (19)	0.0621 (9)
H10	0.4422	0.1804	0.7685	0.074*
C11	0.54128 (18)	0.2887 (3)	0.78993 (16)	0.0510 (8)
C12	0.59981 (17)	0.3693 (3)	0.76139 (15)	0.0423 (7)
C13	0.8609 (2)	0.1804 (6)	0.4692 (3)	0.1000 (15)
H13A	0.8667	0.0854	0.4445	0.12*
H13B	0.9031	0.192	0.5041	0.12*
C14	0.8583 (4)	0.3070 (7)	0.4197 (4)	0.157 (3)
H14A	0.8526	0.2701	0.3715	0.188*
H14B	0.9048	0.3656	0.4252	0.188*
C15	0.7938 (4)	0.4001 (7)	0.4353 (4)	0.155 (3)
H15A	0.8108	0.4976	0.4539	0.186*
H15B	0.7613	0.4169	0.3929	0.186*
C16	0.7545 (3)	0.3222 (7)	0.4853 (3)	0.132 (2)
H16A	0.7029	0.3029	0.4669	0.158*
H16B	0.7524	0.3832	0.5277	0.158*
C18	0.7984 (3)	1.1396 (5)	0.6879 (3)	0.1110 (17)
H18A	0.7897	1.2171	0.7219	0.167*
H18B	0.8244	1.1822	0.6496	0.167*
H18C	0.8289	1.0606	0.7099	0.167*
C17	0.7231 (3)	1.0744 (4)	0.6598 (2)	0.0843 (13)
H17	0.6909	1.1586	0.6423	0.101*
C20	0.6724 (2)	0.8859 (4)	0.5608 (2)	0.0758 (11)
H20	0.6518	0.8159	0.5949	0.091*
C21	0.7039 (3)	0.7943 (6)	0.5022 (2)	0.1007 (14)
H21A	0.6656	0.7257	0.4831	0.151*
H21B	0.7472	0.7377	0.5205	0.151*

H21C	0.7187	0.8612	0.4656	0.151*
C22	0.6102 (3)	0.9937 (6)	0.5353 (3)	0.124 (2)
H22A	0.6308	1.069	0.5053	0.186*
H22B	0.5895	1.0422	0.575	0.186*
H22C	0.5709	0.9385	0.5091	0.186*
C19	0.6817 (4)	0.9914 (5)	0.7149 (3)	0.126 (2)
H19A	0.711	0.9052	0.7311	0.188*
H19B	0.6332	0.9582	0.6948	0.188*
H19C	0.6744	1.0579	0.7539	0.188*
Cl1	0.94808 (7)	0.85050 (15)	0.60108 (7)	0.1084 (4)
Cl2	0.94720 (7)	0.78663 (15)	0.92707 (7)	0.1069 (4)
Cl3	0.52868 (6)	0.36943 (11)	0.55714 (4)	0.0730 (3)
Cl4	0.54440 (6)	0.25575 (13)	0.88029 (5)	0.0835 (3)
Cu1	0.74529 (2)	0.55730 (4)	0.74061 (2)	0.04436 (13)
O1	0.79163 (18)	0.1828 (4)	0.50199 (17)	0.0995 (9)
N1	0.73755 (17)	0.9730 (3)	0.59786 (16)	0.0690 (8)
H1A	0.7725	0.9057	0.6127	0.083*
H1B	0.7581	1.0301	0.5655	0.083*
S1	0.82175 (5)	0.65214 (10)	0.66643 (5)	0.0550 (2)
S2	0.81555 (5)	0.63846 (11)	0.83102 (5)	0.0665 (3)
S3	0.66744 (5)	0.49927 (9)	0.65116 (4)	0.0492 (2)
S4	0.67634 (5)	0.44055 (10)	0.81442 (4)	0.0532 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0364 (18)	0.0413 (17)	0.092 (3)	0.0076 (15)	0.0108 (18)	0.0084 (17)
C2	0.048 (2)	0.061 (2)	0.119 (3)	−0.0013 (19)	0.021 (2)	0.018 (2)
C3	0.050 (3)	0.066 (3)	0.180 (5)	−0.019 (2)	0.017 (3)	0.010 (3)
C4	0.062 (3)	0.073 (3)	0.157 (5)	−0.019 (2)	−0.016 (3)	0.000 (3)
C5	0.055 (2)	0.058 (2)	0.110 (3)	−0.0029 (19)	−0.015 (2)	−0.002 (2)
C6	0.0426 (19)	0.0451 (18)	0.088 (3)	0.0062 (15)	−0.0024 (18)	0.0076 (18)
C7	0.0436 (18)	0.0339 (15)	0.0491 (17)	0.0028 (13)	0.0078 (14)	0.0006 (13)
C8	0.059 (2)	0.0433 (17)	0.0477 (18)	−0.0022 (16)	−0.0002 (16)	0.0007 (14)
C9	0.061 (2)	0.061 (2)	0.069 (2)	−0.0160 (19)	−0.0061 (19)	−0.0033 (18)
C10	0.060 (2)	0.057 (2)	0.070 (2)	−0.0204 (18)	0.0080 (19)	0.0032 (17)
C11	0.056 (2)	0.0490 (18)	0.0484 (18)	−0.0068 (16)	0.0085 (16)	0.0020 (14)
C12	0.0450 (18)	0.0367 (15)	0.0457 (17)	−0.0003 (14)	0.0070 (14)	0.0033 (13)
C13	0.063 (3)	0.105 (4)	0.134 (4)	−0.004 (3)	0.020 (3)	−0.003 (3)
C14	0.149 (6)	0.119 (5)	0.214 (7)	0.022 (4)	0.099 (5)	0.051 (5)
C15	0.146 (6)	0.099 (4)	0.231 (8)	0.024 (4)	0.094 (6)	0.049 (5)
C16	0.142 (5)	0.113 (4)	0.148 (5)	0.040 (4)	0.073 (4)	0.031 (4)
C18	0.135 (5)	0.084 (3)	0.112 (4)	0.030 (3)	−0.009 (3)	−0.019 (3)
C17	0.100 (3)	0.053 (2)	0.101 (3)	0.028 (2)	0.018 (3)	0.004 (2)
C20	0.069 (3)	0.064 (2)	0.094 (3)	0.005 (2)	0.002 (2)	0.024 (2)
C21	0.113 (4)	0.111 (4)	0.077 (3)	0.010 (3)	−0.008 (3)	−0.005 (3)
C22	0.076 (3)	0.106 (4)	0.187 (6)	0.011 (3)	−0.017 (3)	0.054 (4)
C19	0.187 (6)	0.080 (3)	0.118 (4)	0.036 (4)	0.079 (4)	0.011 (3)

Cl1	0.0833 (8)	0.1147 (10)	0.1327 (10)	−0.0095 (7)	0.0513 (7)	0.0343 (8)
Cl2	0.0963 (8)	0.1068 (9)	0.1116 (9)	−0.0110 (7)	−0.0393 (7)	−0.0080 (7)
Cl3	0.0935 (7)	0.0751 (6)	0.0486 (5)	−0.0089 (5)	−0.0093 (5)	0.0011 (4)
Cl4	0.0905 (7)	0.1071 (8)	0.0540 (5)	−0.0341 (6)	0.0134 (5)	0.0160 (5)
Cu1	0.0377 (2)	0.0421 (2)	0.0538 (2)	0.00205 (16)	0.00665 (17)	0.00594 (17)
O1	0.092 (2)	0.095 (2)	0.115 (2)	0.0046 (18)	0.0376 (19)	0.0226 (19)
N1	0.068 (2)	0.0602 (18)	0.080 (2)	0.0217 (16)	0.0127 (17)	0.0166 (16)
S1	0.0422 (5)	0.0579 (5)	0.0659 (5)	0.0026 (4)	0.0123 (4)	0.0120 (4)
S2	0.0565 (6)	0.0795 (7)	0.0627 (5)	−0.0151 (5)	−0.0021 (4)	0.0062 (5)
S3	0.0528 (5)	0.0506 (4)	0.0449 (4)	−0.0043 (4)	0.0097 (4)	0.0058 (4)
S4	0.0493 (5)	0.0640 (5)	0.0460 (4)	−0.0095 (4)	0.0012 (4)	0.0089 (4)

Geometric parameters (Å, º)

C1—C2	1.394 (5)	C15—H15A	0.97
C1—C6	1.397 (5)	C15—H15B	0.97
C1—S1	1.753 (4)	C16—O1	1.420 (6)
C2—C3	1.384 (6)	C16—H16A	0.97
C2—Cl1	1.736 (4)	C16—H16B	0.97
C3—C4	1.373 (7)	C18—C17	1.514 (6)
C3—H3	0.93	C18—H18A	0.96
C4—C5	1.360 (6)	C18—H18B	0.96
C4—H4	0.93	C18—H18C	0.96
C5—C6	1.404 (5)	C17—C19	1.503 (6)
C5—Cl2	1.729 (5)	C17—N1	1.512 (5)
C6—S2	1.743 (3)	C17—H17	0.98
C7—C8	1.387 (4)	C20—C22	1.509 (5)
C7—C12	1.396 (4)	C20—C21	1.509 (6)
C7—S3	1.752 (3)	C20—N1	1.518 (5)
C8—C9	1.369 (4)	C20—H20	0.98
C8—Cl3	1.738 (3)	C21—H21A	0.96
C9—C10	1.372 (5)	C21—H21B	0.96
C9—H9	0.93	C21—H21C	0.96
C10—C11	1.377 (4)	C22—H22A	0.96
C10—H10	0.93	C22—H22B	0.96
C11—C12	1.392 (4)	C22—H22C	0.96
C11—Cl4	1.736 (3)	C19—H19A	0.96
C12—S4	1.749 (3)	C19—H19B	0.96
C13—O1	1.406 (5)	C19—H19C	0.96
C13—C14	1.459 (7)	Cu1—S4	2.1722 (9)
C13—H13A	0.97	Cu1—S2	2.1736 (10)
C13—H13B	0.97	Cu1—S3	2.1763 (9)
C14—C15	1.450 (7)	Cu1—S1	2.1776 (9)
C14—H14A	0.97	N1—H1A	0.89
C14—H14B	0.97	N1—H1B	0.89
C15—C16	1.391 (7)		
C2—C1—C6	118.9 (3)	C15—C16—H16B	109.7

C2—C1—S1	121.4 (3)	O1—C16—H16B	109.7
C6—C1—S1	119.6 (2)	H16A—C16—H16B	108.2
C3—C2—C1	121.0 (4)	C17—C18—H18A	109.5
C3—C2—Cl1	120.1 (3)	C17—C18—H18B	109.5
C1—C2—Cl1	118.9 (3)	H18A—C18—H18B	109.5
C2—C3—C4	119.6 (4)	C17—C18—H18C	109.5
C2—C3—H3	120.2	H18A—C18—H18C	109.5
C4—C3—H3	120.2	H18B—C18—H18C	109.5
C5—C4—C3	120.5 (4)	C19—C17—N1	111.4 (3)
C5—C4—H4	119.8	C19—C17—C18	113.3 (5)
C3—C4—H4	119.8	N1—C17—C18	108.1 (3)
C4—C5—C6	121.2 (4)	C19—C17—H17	108.0
C4—C5—Cl2	120.0 (4)	N1—C17—H17	108.0
C6—C5—Cl2	118.9 (3)	C18—C17—H17	108.0
C5—C6—C1	118.8 (3)	C22—C20—C21	113.2 (4)
C5—C6—S2	121.3 (3)	C22—C20—N1	110.1 (3)
C1—C6—S2	119.9 (3)	C21—C20—N1	108.0 (3)
C8—C7—C12	119.0 (3)	C22—C20—H20	108.5
C8—C7—S3	121.5 (2)	C21—C20—H20	108.5
C12—C7—S3	119.5 (2)	N1—C20—H20	108.5
C9—C8—C7	121.9 (3)	C20—C21—H21A	109.5
C9—C8—Cl3	118.8 (3)	C20—C21—H21B	109.5
C7—C8—Cl3	119.3 (2)	H21A—C21—H21B	109.5
C8—C9—C10	119.5 (3)	C20—C21—H21C	109.5
C8—C9—H9	120.2	H21A—C21—H21C	109.5
C10—C9—H9	120.2	H21B—C21—H21C	109.5
C9—C10—C11	119.6 (3)	C20—C22—H22A	109.5
C9—C10—H10	120.2	C20—C22—H22B	109.5
C11—C10—H10	120.2	H22A—C22—H22B	109.5
C10—C11—C12	121.7 (3)	C20—C22—H22C	109.5
C10—C11—Cl4	118.9 (2)	H22A—C22—H22C	109.5
C12—C11—Cl4	119.4 (2)	H22B—C22—H22C	109.5
C11—C12—C7	118.3 (3)	C17—C19—H19A	109.5
C11—C12—S4	121.7 (2)	C17—C19—H19B	109.5
C7—C12—S4	120.0 (2)	H19A—C19—H19B	109.5
O1—C13—C14	106.3 (4)	C17—C19—H19C	109.5
O1—C13—H13A	110.5	H19A—C19—H19C	109.5
C14—C13—H13A	110.5	H19B—C19—H19C	109.5
O1—C13—H13B	110.5	S4—Cu1—S2	87.85 (3)
C14—C13—H13B	110.5	S4—Cu1—S3	92.26 (3)
H13A—C13—H13B	108.7	S2—Cu1—S3	173.53 (4)
C13—C14—C15	107.1 (5)	S4—Cu1—S1	173.81 (4)
C13—C14—H14A	110.3	S2—Cu1—S1	92.14 (4)
C15—C14—H14A	110.3	S3—Cu1—S1	88.45 (3)
C13—C14—H14B	110.3	C13—O1—C16	108.5 (4)
C15—C14—H14B	110.3	C17—N1—C20	120.0 (3)
H14A—C14—H14B	108.5	C17—N1—H1A	107.3
C16—C15—C14	107.0 (5)	C20—N1—H1A	107.3

C16—C15—H15A	110.3	C17—N1—H1B	107.3
C14—C15—H15A	110.3	C20—N1—H1B	107.3
C16—C15—H15B	110.3	H1A—N1—H1B	106.9
C14—C15—H15B	110.3	C1—S1—Cu1	103.90 (12)
H15A—C15—H15B	108.6	C6—S2—Cu1	104.27 (13)
C15—C16—O1	109.7 (4)	C7—S3—Cu1	104.12 (10)
C15—C16—H16A	109.7	C12—S4—Cu1	104.08 (10)
O1—C16—H16A	109.7		
C6—C1—C2—C3	2.0 (5)	C10—C11—C12—C7	0.3 (5)
S1—C1—C2—C3	−176.4 (3)	Cl4—C11—C12—C7	−179.9 (2)
C6—C1—C2—Cl1	−176.3 (3)	C10—C11—C12—S4	179.5 (3)
S1—C1—C2—Cl1	5.3 (4)	Cl4—C11—C12—S4	−0.7 (4)
C1—C2—C3—C4	−0.7 (7)	C8—C7—C12—C11	−0.6 (4)
Cl1—C2—C3—C4	177.6 (4)	S3—C7—C12—C11	178.5 (2)
C2—C3—C4—C5	−0.4 (7)	C8—C7—C12—S4	−179.9 (2)
C3—C4—C5—C6	0.2 (7)	S3—C7—C12—S4	−0.8 (3)
C3—C4—C5—Cl2	180.0 (4)	O1—C13—C14—C15	11.8 (7)
C4—C5—C6—C1	1.2 (5)	C13—C14—C15—C16	−7.2 (9)
Cl2—C5—C6—C1	−178.6 (3)	C14—C15—C16—O1	−0.1 (8)
C4—C5—C6—S2	−178.8 (3)	C14—C13—O1—C16	−11.9 (6)
Cl2—C5—C6—S2	1.3 (4)	C15—C16—O1—C13	7.7 (7)
C2—C1—C6—C5	−2.2 (5)	C19—C17—N1—C20	52.1 (5)
S1—C1—C6—C5	176.2 (2)	C18—C17—N1—C20	177.2 (3)
C2—C1—C6—S2	177.8 (2)	C22—C20—N1—C17	56.5 (5)
S1—C1—C6—S2	−3.8 (4)	C21—C20—N1—C17	−179.5 (3)
C12—C7—C8—C9	0.4 (5)	C2—C1—S1—Cu1	−177.0 (2)
S3—C7—C8—C9	−178.7 (2)	C6—C1—S1—Cu1	4.6 (3)
C12—C7—C8—Cl3	179.3 (2)	C5—C6—S2—Cu1	−179.1 (3)
S3—C7—C8—Cl3	0.2 (4)	C1—C6—S2—Cu1	0.8 (3)
C7—C8—C9—C10	0.1 (5)	C8—C7—S3—Cu1	179.6 (2)
Cl3—C8—C9—C10	−178.8 (3)	C12—C7—S3—Cu1	0.5 (2)
C8—C9—C10—C11	−0.5 (5)	C11—C12—S4—Cu1	−178.7 (2)
C9—C10—C11—C12	0.3 (5)	C7—C12—S4—Cu1	0.6 (3)
C9—C10—C11—Cl4	−179.5 (3)		

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*A*⋯S1	0.89	2.59	3.417 (3)	156
N1—H1*B*⋯O1[i]	0.89	1.93	2.805 (4)	170

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