Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chlorido(1,10-phenanthroline)[1,1,1-trifluoro-3-(2-thenoyl)acetonato]copper(II)

Shuangzhuan Gao, Jine Zhang, Yanping Li and Zhigang Zhang*

Institute of Molecular Science, Chemical Biology and Molecular Engineering Laboratory of Education Ministry, Shanxi University, Taiyuan, Shanxi 030006, People's Republic of China
Correspondence e-mail: zgzhang@sxu.edu.cn

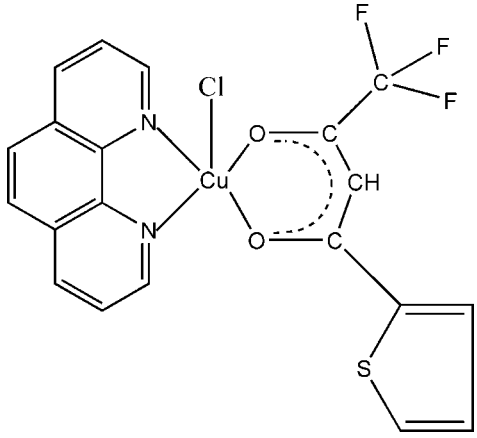
Received 15 November 2007; accepted 28 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.062; wR factor = 0.142; data-to-parameter ratio = 12.5.

In the title compound, $[Cu(C_8H_4F_3O_2S)Cl(C_{12}H_8N_2)]$, the Cu^{II} ion exhibits a distorted square-pyramidal geometry. The coordination environment of the cation comprises two N atoms from 1,10-phenanthroline and two O atoms from thenoyltrifluoroacetone in the basal plane and one Cl^- anion at the apical site. There are weak intermolecular C—H···Cl bonds.

Related literature

For related literature, see: Lenaerts *et al.* (2005); Li *et al.* (2005); Perkins *et al.* (2005, 2007).



Experimental

Crystal data

$[Cu(C_8H_4F_3O_2S)Cl(C_{12}H_8N_2)]$
M_r = 500.37
Monoclinic, $P2_1/n$
a = 12.461 (9) Å
b = 13.238 (9) Å
c = 12.932 (8) Å
β = 115.689 (10)°
V = 1922 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 298 (2) K
0.4 × 0.1 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
T_{min} = 0.60, T_{max} = 0.94
9166 measured reflections
3376 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.142
S = 1.00
3376 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O2	1.941 (4)	Cu1—N2	2.013 (5)
Cu1—O1	1.956 (4)	Cu1—Cl1	2.467 (2)
Cu1—N1	2.007 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···Cl1^{i}	0.93	2.68	3.604 (6)	177

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Natural Science Foundation of Shanxi Province for financial support (grant No. 20041012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2136).

References

Bruker (2000). *SMART* (Version 5.0), *SAINT* (Version 6.02) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Lenaerts, P., Storms, A., Mullens, J., D'Haen, J., Goerller-Walrand, C., Binnemans, K. & Driesen, K. (2005). *Chem. Mater.* **17**, 5194–5201.
Li, Z., Xu, D., Wu, J. & Chiang, M. (2005). *J. Chem. Crystallogr.* **45**, 615–619.
Perkins, W. J., Maxwell, T., Goforth, A. M., Smith, M. D., Peterson, L. R. Jr & zur Loye, H.-C. (2005). *Acta Cryst.* E**61**, m2047–m2049.
Perkins, W. J., Maxwell, T., Williams, K. B., Goforth, A. M., Smith, M. D., Peterson, L. R. Jr & zur Loye, H.-C. (2007). *Acta Cryst.* E**63**, m423–m425.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

supporting information

Acta Cryst. (2008). E**64**, m105 [https://doi.org/10.1107/S1600536807064203]

Chlorido(1,10-phenanthroline)[1,1,1-trifluoro-3-(2-thenoyl)acetonato]copper(II)

Shuangzhuan Gao, Jine Zhang, Yanping Li and Zhigang Zhang

S1. Comment

Metal complexes of 2-thenoyltrifluoroacetone are attractive due to their potential applications in new material design (Lenaerts, *et al.*, 2005; Perkins, *et al.*, 2005, 2007). In this paper, we report a novel Cu complex of 2-thenoyltrifluoro-acetone.

A displacement ellipsoid drawing of (I) is shown in Fig. 1. Selected bond lengths are listed in Table 1. The Cu^{II} ion exhibits a distorted square pyramidal geometry. The coordination environment of the cation is comprised of two N atoms from 1,10-phenanthroline and two O atoms from 2-thenoyltrifluoroacetone at the basal positions, and one Cl anion at the apical site (Cu1—Cl1: 2.467 (2) Å. There are weak intermolecular bonds (C18—H18···$Cl1^{i}$; i: 3/2 - *x*, -1/2 + *y*, 3/2 - *z*) linking adjacent molecules (Table 2 and Fig. 2).

S2. Experimental

All chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification.

The title compound was synthesized by modified procedures already reportred in the literature (Li, *et al.*, 2005). When an ethanol solution (10 ml) of 1,10-phenanthroline (0.196 g) was slowly added to an aqueous solution (10 ml) of $CuCl_2.2H_2O$ (0.171 g), a great amount of precipitate appeared after refluxing. Then an ethanol solution (15 ml) of 2-thenoyltrifluoroactone (0.222 g) was added, and the reaction mixture was kept refluxing until the precipitate was completely dissolved. After filtering, the solution was evaporated slowly at room temperature, and green crystals suitable for X-ray analysis were collected.

S3. Refinement

H atoms attached to C atoms were placed in geometrically idealized positions,with Csp^2—H = 0.930 Å, constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

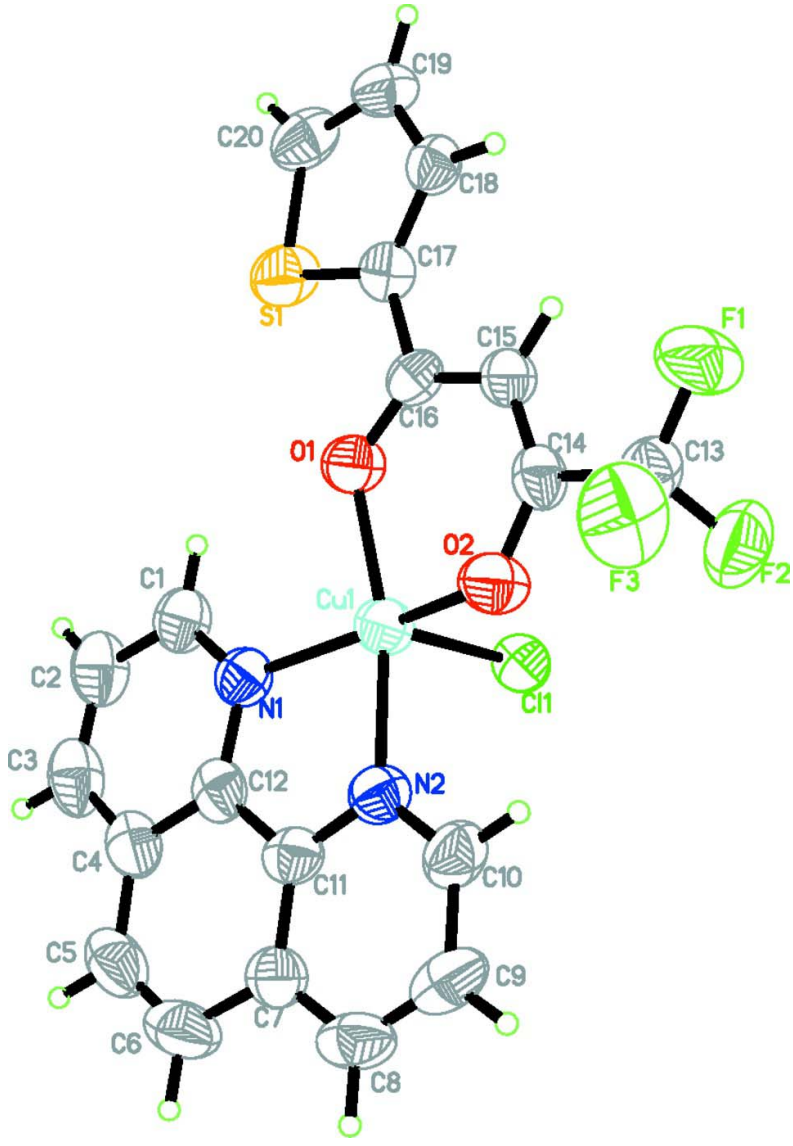


Figure 1

The structure of the title compound in 30% probability ellipsoids.

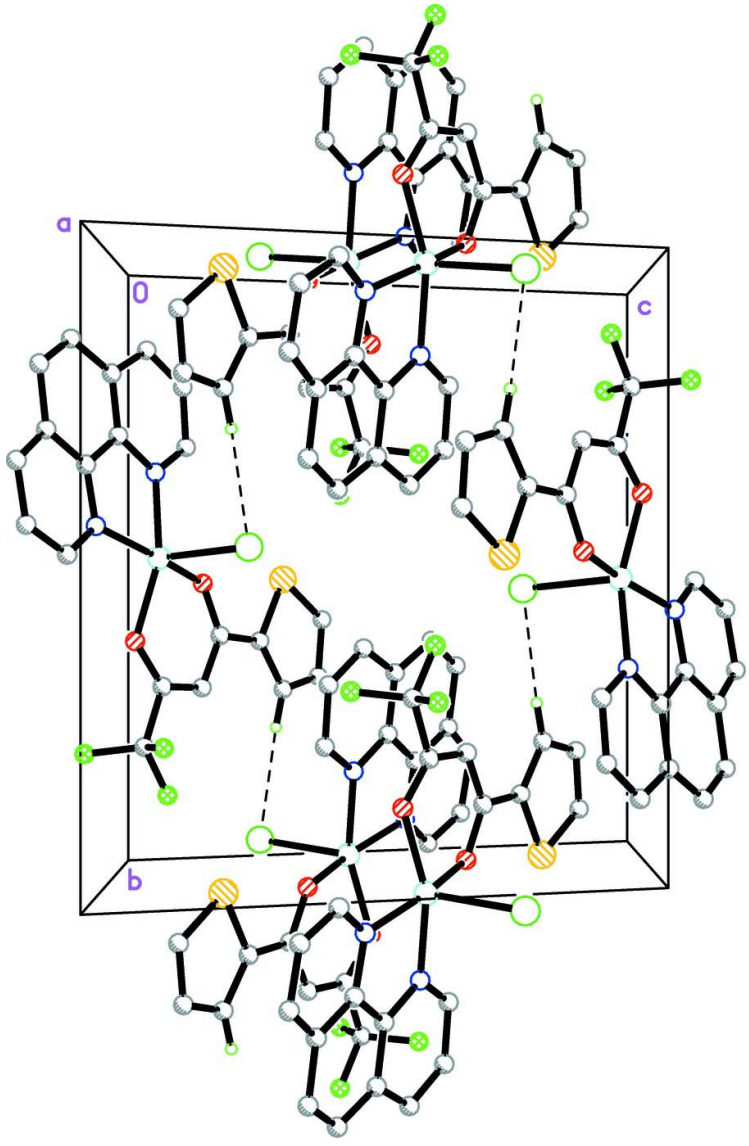


Figure 2

A packing diagram viewed down the *a* axis. H atoms not taking part in H-bonding not shown.

Chlorido(1,10-phenanthroline)[1,1,1-trifluoro-3-(2-thenoyl)acetonato]copper(II)

Crystal data

$[Cu(C_8H_4F_3O_2S)Cl(C_{12}H_8N_2)]$
$M_r = 500.37$
Monoclinic, $P2_1/n$
Hall symbol: -p 2yn
$a = 12.461\ (9)$ Å
$b = 13.238\ (9)$ Å
$c = 12.932\ (8)$ Å
$\beta = 115.689\ (10)°$
$V = 1922\ (2)$ Å^3
$Z = 4$

$F(000) = 1004$
$D_x = 1.729$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 814 reflections
$\theta = 2.3–18.8°$
$\mu = 1.43$ mm^{-1}
$T = 298$ K
Block, green
0.4 × 0.1 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
T_{min} = 0.60, T_{max} = 0.94
9166 measured reflections
3376 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 25.0°, θ_{min} = 1.9°
$h = -7 \rightarrow 14$
$k = -14 \rightarrow 15$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.142
S = 1.00
3376 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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	0.71468 (6)	0.01669 (5)	0.57227 (6)	0.0501 (3)
N1	0.6585 (4)	0.1601 (3)	0.5616 (4)	0.0478 (11)
N2	0.7777 (4)	0.0686 (3)	0.4629 (4)	0.0494 (12)
O1	0.6154 (3)	−0.0264 (3)	0.6471 (3)	0.0544 (10)
O2	0.7311 (3)	−0.1210 (3)	0.5297 (3)	0.0590 (11)
Cl1	0.90480 (13)	0.03410 (10)	0.74564 (12)	0.0541 (4)
C1	0.6010 (5)	0.2048 (4)	0.6148 (5)	0.0535 (15)
H1	0.5748	0.1654	0.6589	0.064*
C2	0.5784 (5)	0.3075 (4)	0.6072 (5)	0.0606 (17)
H2	0.5386	0.3360	0.6465	0.073*
C3	0.6144 (5)	0.3664 (4)	0.5425 (5)	0.0642 (19)
H3	0.5996	0.4355	0.5377	0.077*
C4	0.6738 (5)	0.3234 (4)	0.4829 (5)	0.0548 (16)
C5	0.7162 (6)	0.3764 (5)	0.4130 (6)	0.0684 (19)
H5	0.7002	0.4452	0.4008	0.082*
C6	0.7791 (6)	0.3311 (5)	0.3632 (6)	0.0720 (19)

H6	0.8067	0.3691	0.3192	0.086*
C7	0.8040 (5)	0.2238 (5)	0.3778 (5)	0.0542 (15)
C8	0.8706 (5)	0.1718 (5)	0.3331 (5)	0.0641 (17)
H8	0.9029	0.2059	0.2904	0.077*
C9	0.8890 (5)	0.0690 (5)	0.3517 (5)	0.0664 (18)
H9	0.9325	0.0327	0.3213	0.080*
C10	0.8400 (5)	0.0217 (5)	0.4178 (5)	0.0571 (16)
H10	0.8523	−0.0474	0.4307	0.069*
C11	0.7609 (4)	0.1693 (4)	0.4442 (4)	0.0466 (14)
C12	0.6948 (5)	0.2193 (4)	0.4964 (4)	0.0475 (14)
C13	0.7552 (6)	−0.2949 (4)	0.5483 (6)	0.0580 (16)
C14	0.7086 (5)	−0.1973 (4)	0.5779 (5)	0.0453 (14)
C15	0.6530 (4)	−0.2017 (4)	0.6474 (4)	0.0445 (13)
H15	0.6439	−0.2644	0.6752	0.053*
C16	0.6080 (4)	−0.1150 (4)	0.6796 (4)	0.0429 (13)
C17	0.5462 (5)	−0.1259 (4)	0.7522 (4)	0.0449 (13)
C18	0.5205 (4)	−0.2110 (4)	0.7965 (4)	0.0466 (14)
H18	0.5408	−0.2757	0.7833	0.056*
C19	0.4607 (5)	−0.1909 (4)	0.8637 (5)	0.0557 (15)
H19	0.4366	−0.2408	0.8997	0.067*
C20	0.4413 (5)	−0.0913 (5)	0.8711 (5)	0.0644 (17)
H20	0.4027	−0.0649	0.9125	0.077*
F1	0.7280 (4)	−0.3772 (2)	0.5884 (4)	0.0920 (13)
F2	0.8728 (3)	−0.2922 (3)	0.5907 (3)	0.0871 (12)
F3	0.7167 (4)	−0.3060 (3)	0.4371 (3)	0.0939 (13)
S1	0.49607 (15)	−0.02018 (11)	0.79536 (15)	0.0645 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0606 (5)	0.0418 (4)	0.0591 (5)	0.0045 (3)	0.0365 (4)	0.0020 (3)
N1	0.047 (3)	0.048 (3)	0.049 (3)	0.001 (2)	0.022 (2)	−0.003 (2)
N2	0.050 (3)	0.048 (3)	0.054 (3)	−0.001 (2)	0.027 (3)	−0.002 (2)
O1	0.066 (3)	0.042 (2)	0.071 (3)	0.0025 (19)	0.044 (2)	−0.0024 (19)
O2	0.079 (3)	0.042 (2)	0.076 (3)	0.001 (2)	0.052 (2)	−0.0025 (19)
Cl1	0.0571 (9)	0.0510 (9)	0.0583 (9)	0.0043 (7)	0.0288 (8)	0.0062 (7)
C1	0.054 (4)	0.050 (4)	0.057 (4)	0.006 (3)	0.025 (3)	−0.006 (3)
C2	0.064 (4)	0.048 (4)	0.062 (4)	0.008 (3)	0.019 (4)	−0.013 (3)
C3	0.059 (4)	0.044 (4)	0.068 (4)	0.005 (3)	0.008 (4)	−0.009 (3)
C4	0.048 (4)	0.043 (3)	0.059 (4)	−0.003 (3)	0.009 (3)	0.000 (3)
C5	0.066 (5)	0.046 (4)	0.076 (5)	−0.005 (3)	0.016 (4)	0.015 (3)
C6	0.072 (5)	0.070 (5)	0.071 (5)	−0.019 (4)	0.028 (4)	0.017 (4)
C7	0.044 (4)	0.067 (4)	0.045 (3)	−0.003 (3)	0.012 (3)	0.008 (3)
C8	0.059 (4)	0.092 (5)	0.043 (4)	−0.015 (4)	0.023 (3)	0.007 (3)
C9	0.048 (4)	0.101 (5)	0.057 (4)	−0.006 (4)	0.030 (3)	−0.007 (4)
C10	0.057 (4)	0.063 (4)	0.060 (4)	0.009 (3)	0.034 (3)	−0.004 (3)
C11	0.039 (3)	0.054 (4)	0.041 (3)	−0.008 (3)	0.012 (3)	−0.002 (3)
C12	0.038 (3)	0.050 (3)	0.039 (3)	−0.004 (3)	0.002 (3)	−0.001 (3)

C13	0.058 (4)	0.049 (4)	0.075 (5)	0.004 (3)	0.036 (4)	−0.009 (3)
C14	0.045 (3)	0.037 (3)	0.048 (3)	0.003 (3)	0.014 (3)	−0.002 (3)
C15	0.049 (4)	0.038 (3)	0.051 (3)	0.003 (3)	0.026 (3)	−0.001 (2)
C16	0.034 (3)	0.049 (3)	0.043 (3)	−0.004 (3)	0.014 (3)	−0.005 (3)
C17	0.047 (3)	0.047 (3)	0.041 (3)	0.001 (3)	0.018 (3)	−0.003 (3)
C18	0.043 (3)	0.046 (3)	0.051 (4)	0.003 (3)	0.021 (3)	−0.004 (3)
C19	0.056 (4)	0.061 (4)	0.061 (4)	−0.007 (3)	0.036 (3)	0.000 (3)
C20	0.058 (4)	0.074 (4)	0.075 (4)	−0.002 (3)	0.042 (4)	−0.011 (3)
F1	0.135 (4)	0.040 (2)	0.151 (4)	0.002 (2)	0.109 (3)	−0.001 (2)
F2	0.066 (3)	0.074 (2)	0.127 (3)	0.013 (2)	0.048 (3)	−0.007 (2)
F3	0.125 (3)	0.089 (3)	0.075 (3)	0.017 (2)	0.051 (3)	−0.024 (2)
S1	0.0722 (11)	0.0507 (9)	0.0895 (12)	−0.0013 (8)	0.0529 (10)	−0.0125 (8)

Geometric parameters (Å, º)

Cu1—O2	1.941 (4)	C7—C11	1.396 (8)
Cu1—O1	1.956 (4)	C8—C9	1.383 (8)
Cu1—N1	2.007 (4)	C8—H8	0.9300
Cu1—N2	2.013 (5)	C9—C10	1.395 (8)
Cu1—Cl1	2.467 (2)	C9—H9	0.9300
N1—C1	1.328 (7)	C10—H10	0.9300
N1—C12	1.364 (7)	C11—C12	1.434 (8)
N2—C10	1.312 (7)	C13—F3	1.312 (7)
N2—C11	1.355 (6)	C13—F1	1.313 (7)
O1—C16	1.263 (6)	C13—F2	1.324 (6)
O2—C14	1.280 (6)	C13—C14	1.533 (7)
C1—C2	1.383 (7)	C14—C15	1.353 (7)
C1—H1	0.9300	C15—C16	1.417 (7)
C2—C3	1.355 (8)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.458 (7)
C3—C4	1.400 (8)	C17—C18	1.363 (7)
C3—H3	0.9300	C17—S1	1.721 (5)
C4—C12	1.399 (7)	C18—C19	1.394 (7)
C4—C5	1.416 (9)	C18—H18	0.9300
C5—C6	1.352 (9)	C19—C20	1.350 (7)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.448 (8)	C20—S1	1.700 (6)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.383 (8)		
O2—Cu1—O1	91.93 (16)	C9—C8—H8	120.0
O2—Cu1—N1	161.00 (17)	C8—C9—C10	117.7 (6)
O1—Cu1—N1	91.92 (18)	C8—C9—H9	121.1
O2—Cu1—N2	89.98 (18)	C10—C9—H9	121.1
O1—Cu1—N2	165.85 (17)	N2—C10—C9	124.0 (6)
N1—Cu1—N2	81.94 (19)	N2—C10—H10	118.0
O2—Cu1—Cl1	99.65 (12)	C9—C10—H10	118.0
O1—Cu1—Cl1	98.15 (14)	N2—C11—C7	123.2 (5)

N1—Cu1—Cl1	98.21 (13)	N2—C11—C12	116.5 (5)
N2—Cu1—Cl1	95.34 (14)	C7—C11—C12	120.2 (5)
C1—N1—C12	117.5 (5)	N1—C12—C4	123.3 (6)
C1—N1—Cu1	129.5 (4)	N1—C12—C11	115.9 (5)
C12—N1—Cu1	112.8 (4)	C4—C12—C11	120.7 (6)
C10—N2—C11	117.5 (5)	F3—C13—F1	107.8 (5)
C10—N2—Cu1	129.6 (4)	F3—C13—F2	105.7 (5)
C11—N2—Cu1	112.6 (4)	F1—C13—F2	106.7 (5)
C16—O1—Cu1	126.1 (3)	F3—C13—C14	111.7 (5)
C14—O2—Cu1	122.0 (4)	F1—C13—C14	114.2 (5)
N1—C1—C2	122.7 (6)	F2—C13—C14	110.2 (5)
N1—C1—H1	118.6	O2—C14—C15	129.9 (5)
C2—C1—H1	118.6	O2—C14—C13	110.8 (5)
C3—C2—C1	119.8 (6)	C15—C14—C13	119.2 (5)
C3—C2—H2	120.1	C14—C15—C16	122.8 (5)
C1—C2—H2	120.1	C14—C15—H15	118.6
C2—C3—C4	120.1 (6)	C16—C15—H15	118.6
C2—C3—H3	119.9	O1—C16—C15	124.0 (5)
C4—C3—H3	119.9	O1—C16—C17	116.3 (5)
C12—C4—C3	116.5 (6)	C15—C16—C17	119.7 (5)
C12—C4—C5	117.8 (6)	C18—C17—C16	129.7 (5)
C3—C4—C5	125.7 (6)	C18—C17—S1	110.6 (4)
C6—C5—C4	122.5 (6)	C16—C17—S1	119.7 (4)
C6—C5—H5	118.7	C17—C18—C19	113.0 (5)
C4—C5—H5	118.7	C17—C18—H18	123.5
C5—C6—C7	120.6 (6)	C19—C18—H18	123.5
C5—C6—H6	119.7	C20—C19—C18	113.0 (5)
C7—C6—H6	119.7	C20—C19—H19	123.5
C8—C7—C11	117.4 (6)	C18—C19—H19	123.5
C8—C7—C6	124.6 (6)	C19—C20—S1	111.8 (5)
C11—C7—C6	118.0 (6)	C19—C20—H20	124.1
C7—C8—C9	120.1 (6)	S1—C20—H20	124.1
C7—C8—H8	120.0	C20—S1—C17	91.6 (3)

O2—Cu1—N1—C1	116.2 (6)	C10—N2—C11—C12	−178.6 (5)
O1—Cu1—N1—C1	14.6 (5)	Cu1—N2—C11—C12	−4.6 (6)
N2—Cu1—N1—C1	−178.1 (5)	C8—C7—C11—N2	−2.3 (8)
Cl1—Cu1—N1—C1	−83.9 (5)	C6—C7—C11—N2	179.4 (5)
O2—Cu1—N1—C12	−69.4 (7)	C8—C7—C11—C12	177.8 (5)
O1—Cu1—N1—C12	−171.0 (3)	C6—C7—C11—C12	−0.5 (8)
N2—Cu1—N1—C12	−3.8 (3)	C1—N1—C12—C4	−0.4 (7)
Cl1—Cu1—N1—C12	90.5 (3)	Cu1—N1—C12—C4	−175.4 (4)
O2—Cu1—N2—C10	−19.5 (5)	C1—N1—C12—C11	177.5 (4)
O1—Cu1—N2—C10	−117.4 (7)	Cu1—N1—C12—C11	2.5 (5)
N1—Cu1—N2—C10	177.7 (5)	C3—C4—C12—N1	1.3 (8)
Cl1—Cu1—N2—C10	80.1 (5)	C5—C4—C12—N1	179.9 (5)
O2—Cu1—N2—C11	167.3 (4)	C3—C4—C12—C11	−176.5 (5)
O1—Cu1—N2—C11	69.5 (8)	C5—C4—C12—C11	2.1 (8)

N1—Cu1—N2—C11	4.6 (3)	N2—C11—C12—N1	1.5 (7)
Cl1—Cu1—N2—C11	−93.0 (3)	C7—C11—C12—N1	−178.7 (4)
O2—Cu1—O1—C16	18.6 (4)	N2—C11—C12—C4	179.4 (5)
N1—Cu1—O1—C16	180.0 (4)	C7—C11—C12—C4	−0.7 (8)
N2—Cu1—O1—C16	116.2 (7)	Cu1—O2—C14—C15	12.5 (8)
Cl1—Cu1—O1—C16	−81.5 (4)	Cu1—O2—C14—C13	−167.2 (3)
O1—Cu1—O2—C14	−17.6 (4)	F3—C13—C14—O2	−52.9 (7)
N1—Cu1—O2—C14	−119.2 (6)	F1—C13—C14—O2	−175.5 (5)
N2—Cu1—O2—C14	176.4 (4)	F2—C13—C14—O2	64.3 (7)
Cl1—Cu1—O2—C14	81.0 (4)	F3—C13—C14—C15	127.4 (6)
C12—N1—C1—C2	−0.7 (8)	F1—C13—C14—C15	4.8 (8)
Cu1—N1—C1—C2	173.4 (4)	F2—C13—C14—C15	−115.3 (6)
N1—C1—C2—C3	0.7 (9)	O2—C14—C15—C16	−0.1 (9)
C1—C2—C3—C4	0.3 (9)	C13—C14—C15—C16	179.6 (5)
C2—C3—C4—C12	−1.3 (8)	Cu1—O1—C16—C15	−12.7 (7)
C2—C3—C4—C5	−179.7 (6)	Cu1—O1—C16—C17	168.8 (3)
C12—C4—C5—C6	−2.4 (9)	C14—C15—C16—O1	−0.1 (8)
C3—C4—C5—C6	176.0 (6)	C14—C15—C16—C17	178.3 (5)
C4—C5—C6—C7	1.3 (10)	O1—C16—C17—C18	177.3 (5)
C5—C6—C7—C8	−178.0 (6)	C15—C16—C17—C18	−1.2 (8)
C5—C6—C7—C11	0.2 (9)	O1—C16—C17—S1	−3.7 (6)
C11—C7—C8—C9	2.0 (8)	C15—C16—C17—S1	177.8 (4)
C6—C7—C8—C9	−179.8 (5)	C16—C17—C18—C19	179.4 (5)
C7—C8—C9—C10	−1.0 (9)	S1—C17—C18—C19	0.3 (6)
C11—N2—C10—C9	−0.3 (8)	C17—C18—C19—C20	−0.3 (7)
Cu1—N2—C10—C9	−173.2 (4)	C18—C19—C20—S1	0.1 (7)
C8—C9—C10—N2	0.1 (9)	C19—C20—S1—C17	0.1 (5)
C10—N2—C11—C7	1.5 (8)	C18—C17—S1—C20	−0.2 (4)
Cu1—N2—C11—C7	175.5 (4)	C16—C17—S1—C20	−179.4 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···Cl1^{i}	0.93	2.68	3.604 (6)	177

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+3/2.