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Bis[2-(5-methylsulfanyl-1,3,4-oxadiazol-2-yl-κN^3)phenolato-κO^1]copper(II)

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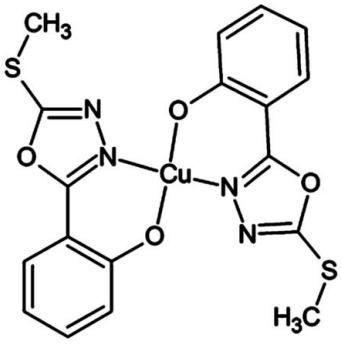
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.066; data-to-parameter ratio = 14.3.

In the title complex, $[Cu(C_9H_7N_2O_2S)_2]$, the Cu^{II} ion, located on an inversion center, adopts an N_2O_2 square-planar coordination. The 2-(5-methylsulfanyl-1,3,4-oxadiazol-2-yl)phenolate ligand is chelated to the central Cu^{II} ion in an *N*,*O*-bidentate manner.

Related literature

For general background to derivatives of dithiocarbazate ligands and their metal complexes, see: Beghidja *et al.* (2005; 2006); Bouchameni *et al.* (2011); Beghidja, Bouslimani & Welter (2007); Beghidja, Rogez & Welter (2007). For similar structures, see: Kala *et al.* (2007); Liu *et al.* (2008); Zhang *et al.* (2001). For the preparation of the ligand, see: Dolman *et al.* (2006); Young & Wood (1955).



Experimental

Crystal data

$[Cu(C_9H_7N_2O_2S)_2]$
M_r = 478.02
Monoclinic, $P2_1/n$
a = 12.5695 (7) Å
b = 4.4216 (3) Å
c = 17.3861 (9) Å
β = 106.005 (6)°
V = 928.81 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 170 K
0.18 × 0.12 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.926, T_{max} = 1.000
6693 measured reflections
1906 independent reflections
1250 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.066
S = 0.99
1906 reflections
133 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O2	1.896 (2)	Cu1—N1	1.9746 (19)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 1995); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HP2039).

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supplementary materials

Acta Cryst. (2012). E**68**, m943 [doi:10.1107/S1600536812026815]

Bis[2-(5-methylsulfanyl-1,3,4-oxadiazol-2-yl-κN^3)phenolato-κO^1]copper(II)

Souheila Ouilia, Chahrazed Beghidja, Adel Beghidja and François Michaud

Comment

The molecular structure of the complex (1) shows that the Cu^{II} ion is located on an inversion center and chelated by two bidentate anions HL^- (Fig. 1). This ligand has been obtained from the *in situ* cyclization of 2-hydroxy [bis(methyl-sulfanyl)methylene]hydrazide $HL^{(1)}$ described previously by (Young *et al.*,1955; Dolman *et al.*, 2006). The title mononuclear complex, [Cu $(C_9H_7O_2N_2S)_2$] (1) has a square-plane geometry formed by the N_2O_2 donor atoms (N1, O2). Several mononuclear compounds with similar structures have been reported previously (Kala *et al.*, 2007; Liu *et al.*, 2008). The whole molecule is planar with a small deviation at C8 from the mean plane. The distances in the coordination planes around the Cu^{II} ion [Cu_1—N_1= 1.975 (19) Å and Cu_1—O_2= 1.896 (2) Å] are in agreement with other square-planar complexes, such as [Cu($C_{15}H_{22}O$)2] [Cu—O = 1.88 (3) Å and Cu—N = 2.00 (3) Å; (Zhang *et al.*, 2001)]. From a supramolecular point of view, this structure can be described as a zigzag chain within which the molecular complexes are connected to each other *via* the weak hydrogen bonding C—H···O. In the crystal the layers are held together by normal van der Waals interactions (Fig. 2).

Experimental

The ligand $HL^{(1)}$ (0.128 g, 0.05 mmol) was dissolved in minimum of DMF. The solution of $CuCl_2.2H_2O$ (0.0085 g, 0.05 mmol) in DMF was added to the first when the ligand was dissolved completely. Green crystals of the complex 1 were isolated from the solution after two weeks.

Refinement

All H atoms were placed at calculated positions and treated as riding on their parent atoms with C—H = 0.93–0.96 Å, and U_{iso} (H) = 1.5Ueq(C) for methyl H atoms and 1.2Ueq(C) for the others.

Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 1995); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

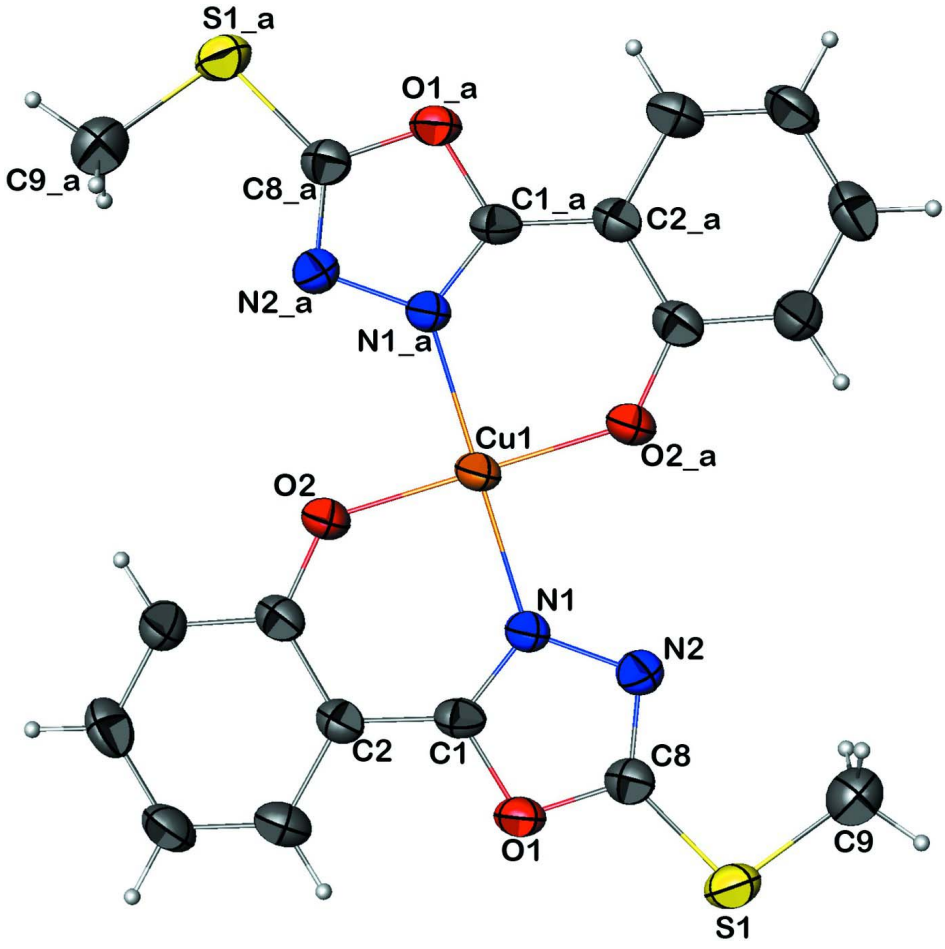

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

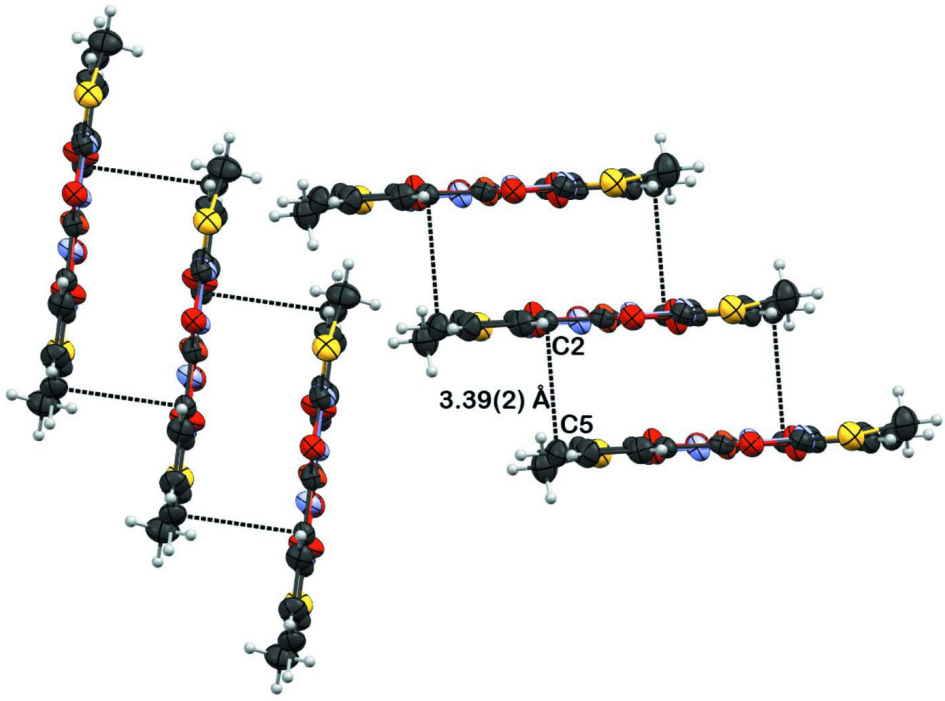

Figure 2

Linking of the layers in the structure *via* van der Waals interactions.

Bis[2-(5-methylsulfanyl-1,3,4-oxadiazol-2-yl-κN^3)phenolato- κO^1]copper(II)

Crystal data

$[Cu(C_9H_7N_2O_2S)_2]$
$M_r = 478.02$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.5695$ (7) Å
$b = 4.4216$ (3) Å
$c = 17.3861$ (9) Å
$\beta = 106.005$ (6)°
$V = 928.81$ (9) Å^3
$Z = 2$
$F(000) = 486$

Least Squares Treatment of 25 SET4 setting angles.
$D_x = 1.709$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2354 reflections
$\theta = 3.3$–$31.6°$
$\mu = 1.44$ mm^{-1}
$T = 170$ K
Plates, green
0.18 × 0.12 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.926$, $T_{max} = 1.000$

6693 measured reflections
1906 independent reflections
1250 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.4°$, $\theta_{min} = 3.4°$
$h = -15 \rightarrow 15$
$k = -5 \rightarrow 5$
$l = -21 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.066$
$S = 0.99$
1906 reflections
133 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
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.50000	0.00000	1.00000	0.0381 (1)
S1	0.45296 (6)	0.47186 (17)	0.68566 (4)	0.0455 (3)
O1	0.58495 (13)	0.1114 (4)	0.79047 (9)	0.0362 (6)
O2	0.62190 (14)	−0.2686 (5)	1.01766 (9)	0.0506 (7)
N1	0.51554 (16)	0.0936 (5)	0.89257 (11)	0.0347 (7)
N2	0.44837 (16)	0.2890 (5)	0.83525 (11)	0.0387 (8)
C1	0.59434 (18)	−0.0065 (6)	0.86434 (13)	0.0315 (7)
C2	0.68113 (19)	−0.2153 (6)	0.89831 (14)	0.0326 (8)
C3	0.68883 (19)	−0.3359 (6)	0.97479 (15)	0.0356 (8)
C4	0.7755 (2)	−0.5413 (6)	1.00571 (15)	0.0424 (9)
C5	0.8503 (2)	−0.6167 (6)	0.96422 (17)	0.0474 (10)
C6	0.8424 (2)	−0.4940 (7)	0.88955 (16)	0.0455 (9)
C7	0.7584 (2)	−0.2969 (6)	0.85724 (16)	0.0429 (10)
C8	0.4933 (2)	0.2903 (6)	0.77720 (14)	0.0346 (8)
C9	0.3251 (2)	0.6276 (7)	0.69352 (17)	0.0602 (11)
H4	0.78230	−0.62840	1.05550	0.0510*
H5	0.90710	−0.75200	0.98660	0.0570*
H6	0.89350	−0.54500	0.86190	0.0550*
H7	0.75220	−0.21510	0.80690	0.0510*
H9A	0.29080	0.74020	0.64590	0.0900*
H9B	0.33910	0.75940	0.73910	0.0900*
H9C	0.27680	0.46690	0.69980	0.0900*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0309 (2)	0.0596 (3)	0.0265 (2)	0.0096 (2)	0.0123 (2)	0.0020 (3)
S1	0.0469 (4)	0.0576 (5)	0.0340 (4)	−0.0015 (4)	0.0146 (3)	0.0092 (4)
O1	0.0361 (10)	0.0457 (11)	0.0307 (9)	−0.0003 (8)	0.0158 (8)	0.0006 (8)
O2	0.0442 (11)	0.0785 (14)	0.0346 (10)	0.0221 (10)	0.0200 (9)	0.0092 (11)
N1	0.0300 (11)	0.0482 (14)	0.0274 (11)	0.0054 (10)	0.0104 (9)	0.0020 (10)
N2	0.0340 (12)	0.0521 (15)	0.0303 (12)	0.0051 (11)	0.0093 (10)	0.0039 (11)
C1	0.0301 (12)	0.0398 (14)	0.0261 (12)	−0.0068 (14)	0.0102 (10)	−0.0058 (14)
C2	0.0285 (13)	0.0385 (15)	0.0316 (13)	−0.0021 (11)	0.0098 (11)	−0.0059 (12)
C3	0.0289 (13)	0.0443 (16)	0.0341 (14)	−0.0017 (12)	0.0095 (11)	−0.0084 (13)
C4	0.0397 (15)	0.0520 (19)	0.0342 (13)	0.0079 (13)	0.0078 (12)	0.0011 (14)
C5	0.0398 (16)	0.0462 (17)	0.0562 (19)	0.0112 (13)	0.0135 (14)	−0.0070 (15)
C6	0.0398 (14)	0.0508 (17)	0.0535 (16)	0.0065 (15)	0.0256 (13)	−0.0016 (17)
C7	0.0426 (16)	0.0489 (18)	0.0438 (16)	0.0004 (14)	0.0230 (13)	−0.0031 (14)
C8	0.0320 (14)	0.0401 (16)	0.0315 (14)	−0.0036 (12)	0.0086 (12)	−0.0033 (12)
C9	0.060 (2)	0.069 (2)	0.0527 (19)	0.0110 (16)	0.0175 (16)	0.0157 (16)

Geometric parameters (Å, º)

Cu1—O2	1.896 (2)	C2—C3	1.411 (3)
Cu1—N1	1.9746 (19)	C2—C7	1.402 (4)
Cu1—O2^{i}	1.896 (2)	C3—C4	1.406 (4)
Cu1—N1^{i}	1.9746 (19)	C4—C5	1.375 (4)
S1—C8	1.729 (3)	C5—C6	1.385 (4)
S1—C9	1.788 (3)	C6—C7	1.365 (4)
O1—C1	1.361 (3)	C4—H4	0.9300
O1—C8	1.364 (3)	C5—H5	0.9300
O2—C3	1.303 (3)	C6—H6	0.9300
N1—N2	1.410 (3)	C7—H7	0.9300
N1—C1	1.298 (3)	C9—H9A	0.9600
N2—C8	1.285 (3)	C9—H9B	0.9600
C1—C2	1.427 (4)	C9—H9C	0.9600
Cu1···O2^{ii}	3.555 (2)	C3···Cu1^{vi}	3.876 (3)
Cu1···C3^{ii}	3.876 (3)	C3···N1^{vi}	3.381 (3)
Cu1···C4^{ii}	3.991 (3)	C3···C1^{vi}	3.554 (4)
Cu1···O2^{iii}	3.555 (2)	C3···Cu1^{iii}	3.876 (3)
Cu1···C3^{iii}	3.876 (3)	C4···C2^{vi}	3.543 (4)
Cu1···C4^{iii}	3.991 (3)	C4···Cu1^{vi}	3.991 (3)
S1···H6^{iv}	3.1400	C4···C1^{vi}	3.517 (4)
S1···H4^{v}	3.0600	C4···Cu1^{iii}	3.991 (3)
O1···N2	2.215 (3)	C5···C7^{vi}	3.557 (4)
O1···C7^{ii}	3.399 (3)	C5···C2^{vi}	3.391 (4)
O2···N2^{i}	2.928 (3)	C7···O1^{vi}	3.399 (3)
O2···C1	2.839 (3)	C7···C5^{ii}	3.557 (4)
O2···Cu1^{vi}	3.555 (2)	C8···C1^{ii}	3.538 (4)
O2···N1	2.735 (3)	C8···C2^{ii}	3.471 (4)
O2···Cu1^{iii}	3.555 (2)	C9···N2^{x}	3.410 (3)

O2···N1^{i}	2.740 (3)	C3···H9A^{viii}	2.9300
O1···H6^{vii}	2.8200	C4···H9A^{viii}	2.7400
O1···H7	2.5000	C8···H9B^{vi}	3.0000
O2···H9A^{viii}	2.6200	C9···H9C^{x}	2.9400
N1···O1	2.185 (3)	H4···S1^{xi}	3.0600
N1···O2	2.735 (3)	H4···H9A^{viii}	2.3100
N1···C3	2.946 (3)	H6···S1^{xii}	3.1400
N1···C3^{ii}	3.381 (3)	H6···O1^{xiii}	2.8200
N1···O2^{i}	2.740 (3)	H7···O1	2.5000
N2···O1	2.215 (3)	H9A···O2^{xiv}	2.6200
N2···O2^{i}	2.928 (3)	H9A···C3^{xiv}	2.9300
N2···C9^{ix}	3.410 (3)	H9A···C4^{xiv}	2.7400
N2···H9C	2.8300	H9A···H4^{xiv}	2.3100
N2···H9B	2.7800	H9B···N2	2.7800
C1···C3^{ii}	3.554 (4)	H9B···C8^{ii}	3.0000
C1···C4^{ii}	3.517 (4)	H9B···H9C^{x}	2.2200
C1···C8^{vi}	3.538 (4)	H9C···N2	2.8300
C2···C4^{ii}	3.543 (4)	H9C···C9^{ix}	2.9400
C2···C5^{ii}	3.391 (4)	H9C···H9B^{ix}	2.2200
C2···C8^{vi}	3.471 (4)		

O2—Cu1—N1	89.90 (8)	C3—C4—C5	121.7 (2)
O2—Cu1—O2^{i}	180.00	C4—C5—C6	121.0 (2)
O2—Cu1—N1^{i}	90.11 (8)	C5—C6—C7	118.9 (2)
O2^{i}—Cu1—N1	90.11 (8)	C2—C7—C6	121.4 (2)
N1—Cu1—N1^{i}	180.00	S1—C8—O1	116.41 (17)
O2^{i}—Cu1—N1^{i}	89.90 (8)	S1—C8—N2	130.1 (2)
C8—S1—C9	98.63 (13)	O1—C8—N2	113.5 (2)
C1—O1—C8	103.37 (18)	C3—C4—H4	119.00
Cu1—O2—C3	132.15 (16)	C5—C4—H4	119.00
Cu1—N1—N2	126.93 (15)	C4—C5—H5	120.00
Cu1—N1—C1	124.81 (17)	C6—C5—H5	119.00
N2—N1—C1	108.19 (19)	C5—C6—H6	121.00
N1—N2—C8	104.5 (2)	C7—C6—H6	121.00
O1—C1—N1	110.5 (2)	C2—C7—H7	119.00
O1—C1—C2	119.7 (2)	C6—C7—H7	119.00
N1—C1—C2	129.8 (2)	S1—C9—H9A	109.00
C1—C2—C3	118.7 (2)	S1—C9—H9B	109.00
C1—C2—C7	120.9 (2)	S1—C9—H9C	109.00
C3—C2—C7	120.4 (2)	H9A—C9—H9B	109.00
O2—C3—C2	124.4 (2)	H9A—C9—H9C	110.00
O2—C3—C4	118.9 (2)	H9B—C9—H9C	109.00
C2—C3—C4	116.7 (2)		

N1—Cu1—O2—C3	3.7 (2)	Cu1—N1—C1—O1	−176.81 (15)
N1^{i}—Cu1—O2—C3	−176.3 (2)	N1—N2—C8—O1	0.2 (3)
O2—Cu1—N1—N2	178.6 (2)	N1—N2—C8—S1	177.9 (2)
O2^{i}—Cu1—N1—N2	−1.4 (2)	O1—C1—C2—C7	1.2 (4)
O2—Cu1—N1—C1	−4.9 (2)	N1—C1—C2—C7	179.4 (3)

O2^{i}—Cu1—N1—C1	175.1 (2)	O1—C1—C2—C3	−179.6 (2)
C9—S1—C8—O1	173.0 (2)	N1—C1—C2—C3	−1.4 (4)
C9—S1—C8—N2	−4.7 (3)	C3—C2—C7—C6	0.2 (4)
C8—O1—C1—N1	−0.1 (3)	C1—C2—C3—C4	179.8 (2)
C1—O1—C8—N2	−0.1 (3)	C1—C2—C7—C6	179.3 (3)
C8—O1—C1—C2	178.4 (2)	C1—C2—C3—O2	−0.4 (4)
C1—O1—C8—S1	−178.12 (18)	C7—C2—C3—O2	178.8 (2)
Cu1—O2—C3—C2	−1.8 (4)	C7—C2—C3—C4	−1.0 (4)
Cu1—O2—C3—C4	177.95 (18)	O2—C3—C4—C5	−178.6 (2)
C1—N1—N2—C8	−0.3 (3)	C2—C3—C4—C5	1.2 (4)
Cu1—N1—N2—C8	176.71 (18)	C3—C4—C5—C6	−0.5 (4)
N2—N1—C1—C2	−178.1 (3)	C4—C5—C6—C7	−0.3 (4)
N2—N1—C1—O1	0.2 (3)	C5—C6—C7—C2	0.5 (4)
Cu1—N1—C1—C2	4.9 (4)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+2; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, −*y*−1, −*z*+2; (iv) −*x*+3/2, *y*+3/2, −*z*+3/2; (v) *x*−1/2, −*y*−1/2, *z*−1/2; (vi) *x*, *y*−1, *z*; (vii) −*x*+3/2, *y*+1/2, −*z*+3/2; (viii) *x*+1/2, −*y*+1/2, *z*+1/2; (ix) −*x*+1/2, *y*−1/2, −*z*+3/2; (x) −*x*+1/2, *y*+1/2, −*z*+3/2; (xi) *x*+1/2, −*y*−1/2, *z*+1/2; (xii) −*x*+3/2, *y*−3/2, −*z*+3/2; (xiii) −*x*+3/2, *y*−1/2, −*z*+3/2; (xiv) *x*−1/2, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1	0.93	2.50	2.822 (3)	100