Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{μ-*N*′-[1-(5-bromo-2-oxidophenyl)ethylidene]benzenesulfonohydrazidato}-$\kappa^3O^2,N':N;\kappa^3N:O^2,N'$-bis[(dimethyl sulfoxide-κO)copper(II)]

Hapipah M. Ali, Musalem Laila, Razali M. Rizal and Seik Weng Ng*

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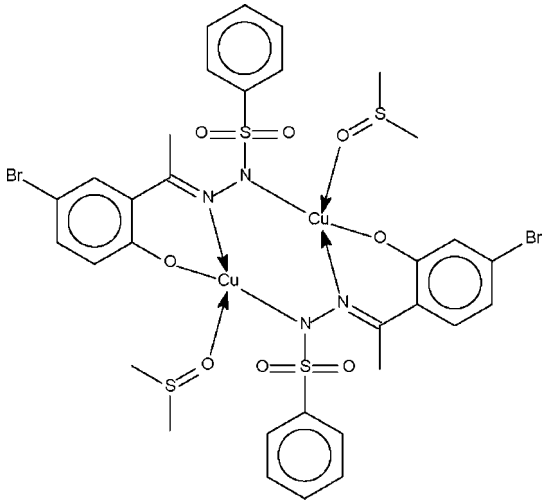
Received 7 January 2008; accepted 21 January 2008

Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.006 Å; R factor = 0.039; wR factor = 0.151; data-to-parameter ratio = 18.1.

In the title centrosymmetric dinuclear complex, $[Cu_2(C_{15}H_{11}BrN_2O_3S)_2(C_2H_6OS)_2]$, the Cu^{II} ion is *N*,*O*-chelated by a dianionic ligand, monocoordinated by the sulfonamide N atom of a symmetry-related ligand and coordinated by an O atom from a dimethyl sulfoxide ligand, forming a distorted square-planar coordination geometry.

Related literature

For the structure of 2′-[1-(2-hydroxyphenyl)ethylidene]-benzenesulfonohydrazide, see: Ali *et al.* (2007).



Experimental

Crystal data

$[Cu_2(C_{15}H_{11}BrN_2O_3S)_2(C_2H_6OS)_2]$
M_r = 1017.77
Triclinic, $P\overline{1}$
a = 8.0831 (1) Å
b = 10.4972 (2) Å
c = 12.9481 (2) Å
α = 68.157 (1)°
β = 74.928 (1)°
γ = 70.691 (1)°
V = 950.56 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 3.49 mm^{-1}
T = 123 (2) K
0.40 × 0.31 × 0.20 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.335, T_{max} = 0.542
(expected range = 0.308–0.497)
12330 measured reflections
4318 independent reflections
3788 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.151
S = 1.21
4318 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.894 (3)	Cu1—N1	1.967 (3)
Cu1—O4	1.986 (3)	Cu1—N2^{i}	2.026 (3)

Symmetry code: (i) $-x+2, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

The authors thank the University of Canterbury, New Zealand, for the diffraction measurements, and the Science Fund (12–02-03–2031) and the Fundamental Research Grant Scheme (FP064/2006 A) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2588).

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supporting information

Acta Cryst. (2008). E**64**, m414 [doi:10.1107/S1600536808002201]

Bis{μ-*N*′-[1-(5-bromo-2-oxidophenyl)ethylidene]benzenesulfonohydrazidato}-$\kappa^3O^2,N'{:}N;\kappa^3N{:}O^2,N'$-bis[(dimethyl sulfoxide-κO)copper(II)]

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S1. Experimental

The Schiff base ligand was synthesized by refluxing 5-bromo-2-hydroxyacetophenone (0.6 g, 2.8 mmol) with benzene sulfonohydrazide (0.48 g,2.8 mmol)in ethanol for 2 h. The ligand then was refluxed with Copper (II) acetate for 5 h. The brown crystal were obtained by recrystalization the product from DMSO.

S2. Refinement

All H atoms were placed in calculated positions (C–H = 0.95–0.98 Å) and were included in the refinement in the riding-model approximation with U_{iso}(H) set to 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.

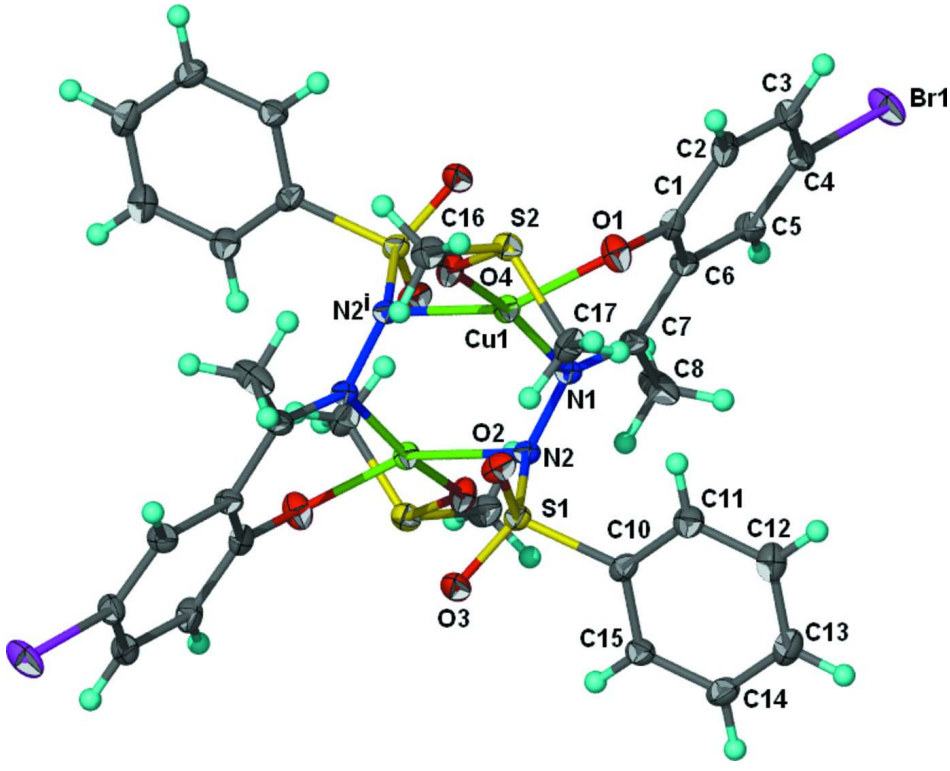

Figure 1

The molecular structure with displacement ellipsoids drawn at the 50% probability level, and H atoms shown as spheres of arbitrary radii [symmetry code: (i) -*x* + 2, -*y* + 1, -*z*].

Bis{μ-*N*′-[1-(5-bromo-2- oxidophenyl)ethylidene]benzenesulfonohydrazidato}- $\kappa^3O^2,N′:N;\kappa^3N:N′,O^2$-bis[(dimethyl sulfoxide-κO)copper(II)]

Crystal data

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M_r = 1017.77
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.0831 (1) Å
b = 10.4972 (2) Å
c = 12.9481 (2) Å
α = 68.157 (1)°
β = 74.928 (1)°
γ = 70.691 (1)°
V = 950.56 (3) Å^3
Z = 1
F(000) = 510
D_x = 1.778 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7546 reflections
θ = 2.7–31.0°
μ = 3.49 mm^{-1}
T = 123 K
Block, green
0.40 × 0.31 × 0.20 mm

Data collection

Bruker APEXII diffractometer
Radiation source: medium-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.335, T_{max} = 0.542
12330 measured reflections
4318 independent reflections
3788 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 1.7°
h = −10→10
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.151
S = 1.21
4318 reflections
238 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
$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 1.8365P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.33316 (6)	0.23924 (5)	0.54963 (4)	0.03789 (17)
Cu1	1.09563 (6)	0.32031 (5)	0.10740 (4)	0.02020 (15)
S1	1.13219 (13)	0.63204 (10)	0.05283 (8)	0.0213 (2)
S2	1.41379 (13)	0.06832 (10)	0.18255 (8)	0.0230 (2)
O1	1.0528 (4)	0.2167 (3)	0.2622 (3)	0.0285 (6)
O2	1.2628 (4)	0.4956 (3)	0.0677 (3)	0.0278 (6)
O3	1.1615 (4)	0.7489 (3)	−0.0472 (3)	0.0292 (7)
O4	1.3150 (4)	0.1704 (3)	0.0840 (2)	0.0253 (6)
N1	0.9142 (4)	0.4879 (3)	0.1354 (3)	0.0195 (6)
N2	0.9352 (4)	0.6205 (3)	0.0558 (3)	0.0198 (6)
C1	0.8917 (5)	0.2298 (4)	0.3191 (3)	0.0219 (8)

C2	0.8558 (6)	0.1098 (5)	0.4082 (3)	0.0269 (9)
H2	0.9472	0.0236	0.4212	0.032*
C3	0.6946 (6)	0.1120 (5)	0.4770 (3)	0.0274 (9)
H3	0.6759	0.0294	0.5370	0.033*
C4	0.5591 (6)	0.2368 (5)	0.4575 (3)	0.0249 (8)
C5	0.5843 (5)	0.3557 (4)	0.3695 (4)	0.0243 (8)
H5	0.4889	0.4393	0.3569	0.029*
C6	0.7481 (5)	0.3565 (4)	0.2975 (3)	0.0208 (7)
C7	0.7691 (5)	0.4889 (4)	0.2075 (3)	0.0217 (8)
C8	0.6221 (7)	0.6230 (5)	0.1999 (5)	0.0392 (12)
H8A	0.6631	0.7033	0.1428	0.059*
H8B	0.5875	0.6396	0.2731	0.059*
H8C	0.5198	0.6135	0.1788	0.059*
C10	1.1190 (5)	0.6831 (4)	0.1713 (3)	0.0220 (8)
C11	1.1381 (6)	0.5793 (5)	0.2752 (4)	0.0269 (8)
H11	1.1558	0.4822	0.2833	0.032*
C12	1.1307 (6)	0.6200 (5)	0.3673 (4)	0.0318 (9)
H12	1.1418	0.5505	0.4393	0.038*
C13	1.1072 (6)	0.7618 (5)	0.3547 (4)	0.0327 (10)
H13	1.1064	0.7884	0.4174	0.039*
C14	1.0849 (6)	0.8649 (5)	0.2507 (4)	0.0304 (9)
H14	1.0656	0.9622	0.2429	0.036*
C15	1.0910 (6)	0.8258 (4)	0.1583 (4)	0.0249 (8)
H15	1.0761	0.8957	0.0869	0.030*
C16	1.6285 (6)	0.0005 (5)	0.1132 (4)	0.0294 (9)
H16A	1.6190	−0.0542	0.0690	0.044*
H16B	1.7060	−0.0613	0.1694	0.044*
H16C	1.6786	0.0797	0.0631	0.044*
C17	1.4719 (6)	0.1775 (5)	0.2371 (4)	0.0310 (9)
H17A	1.3669	0.2215	0.2823	0.046*
H17B	1.5168	0.2519	0.1746	0.046*
H17C	1.5640	0.1193	0.2844	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0284 (3)	0.0359 (3)	0.0357 (3)	−0.01063 (19)	0.00829 (19)	−0.0030 (2)
Cu1	0.0171 (3)	0.0210 (3)	0.0222 (3)	−0.00342 (18)	−0.00075 (18)	−0.00929 (19)
S1	0.0190 (5)	0.0249 (5)	0.0240 (5)	−0.0098 (4)	0.0014 (3)	−0.0118 (4)
S2	0.0192 (5)	0.0238 (5)	0.0253 (5)	−0.0066 (4)	−0.0020 (4)	−0.0070 (4)
O1	0.0205 (14)	0.0309 (15)	0.0248 (14)	0.0000 (12)	−0.0005 (11)	−0.0063 (12)
O2	0.0179 (14)	0.0312 (16)	0.0391 (17)	−0.0064 (12)	0.0007 (12)	−0.0200 (13)
O3	0.0320 (17)	0.0352 (16)	0.0255 (15)	−0.0200 (14)	0.0015 (13)	−0.0095 (13)
O4	0.0220 (14)	0.0278 (14)	0.0245 (14)	0.0011 (11)	−0.0040 (11)	−0.0130 (12)
N1	0.0206 (16)	0.0187 (15)	0.0205 (15)	−0.0074 (12)	−0.0020 (12)	−0.0063 (12)
N2	0.0201 (16)	0.0205 (15)	0.0214 (15)	−0.0094 (12)	−0.0014 (12)	−0.0074 (12)
C1	0.0202 (18)	0.0271 (19)	0.0204 (18)	−0.0047 (15)	−0.0025 (14)	−0.0113 (15)
C2	0.030 (2)	0.0246 (19)	0.0213 (19)	0.0012 (16)	−0.0058 (16)	−0.0085 (15)

C3	0.036 (2)	0.0252 (19)	0.0199 (18)	−0.0089 (17)	−0.0040 (17)	−0.0047 (15)
C4	0.024 (2)	0.029 (2)	0.0213 (18)	−0.0088 (16)	0.0002 (15)	−0.0081 (16)
C5	0.0196 (18)	0.0247 (19)	0.028 (2)	−0.0055 (15)	−0.0014 (15)	−0.0090 (16)
C6	0.0190 (18)	0.0193 (17)	0.0245 (18)	−0.0061 (14)	−0.0008 (15)	−0.0081 (14)
C7	0.0190 (18)	0.0202 (18)	0.0255 (19)	−0.0070 (14)	0.0012 (15)	−0.0084 (15)
C8	0.030 (2)	0.021 (2)	0.046 (3)	−0.0012 (18)	0.011 (2)	−0.0033 (19)
C10	0.0177 (18)	0.0252 (19)	0.0275 (19)	−0.0056 (15)	−0.0009 (15)	−0.0149 (16)
C11	0.025 (2)	0.026 (2)	0.029 (2)	−0.0045 (16)	−0.0016 (16)	−0.0115 (16)
C12	0.029 (2)	0.038 (2)	0.027 (2)	−0.0038 (19)	−0.0042 (17)	−0.0122 (18)
C13	0.030 (2)	0.044 (3)	0.032 (2)	−0.0112 (19)	−0.0001 (18)	−0.023 (2)
C14	0.030 (2)	0.030 (2)	0.037 (2)	−0.0118 (18)	0.0038 (18)	−0.0194 (19)
C15	0.024 (2)	0.0241 (19)	0.027 (2)	−0.0099 (16)	0.0023 (16)	−0.0099 (16)
C16	0.023 (2)	0.027 (2)	0.038 (2)	−0.0021 (16)	−0.0020 (17)	−0.0153 (18)
C17	0.031 (2)	0.038 (2)	0.031 (2)	−0.0086 (19)	−0.0062 (18)	−0.0181 (19)

Geometric parameters (Å, º)

Br1—C4	1.902 (4)	C5—H5	0.9500
Cu1—O1	1.894 (3)	C6—C7	1.472 (5)
Cu1—O4	1.986 (3)	C7—C8	1.501 (6)
Cu1—N1	1.967 (3)	C8—H8A	0.9800
Cu1—N2^{i}	2.026 (3)	C8—H8B	0.9800
S1—O3	1.445 (3)	C8—H8C	0.9800
S1—O2	1.450 (3)	C10—C11	1.388 (6)
S1—N2	1.626 (3)	C10—C15	1.390 (6)
S1—C10	1.772 (4)	C11—C12	1.391 (6)
S2—O4	1.537 (3)	C11—H11	0.9500
S2—C17	1.779 (4)	C12—C13	1.387 (7)
S2—C16	1.781 (4)	C12—H12	0.9500
O1—C1	1.310 (5)	C13—C14	1.389 (7)
N1—C7	1.295 (5)	C13—H13	0.9500
N1—N2	1.423 (4)	C14—C15	1.388 (6)
N2—Cu1^{i}	2.026 (3)	C14—H14	0.9500
C1—C2	1.410 (6)	C15—H15	0.9500
C1—C6	1.438 (5)	C16—H16A	0.9800
C2—C3	1.372 (6)	C16—H16B	0.9800
C2—H2	0.9500	C16—H16C	0.9800
C3—C4	1.388 (6)	C17—H17A	0.9800
C3—H3	0.9500	C17—H17B	0.9800
C4—C5	1.374 (6)	C17—H17C	0.9800
C5—C6	1.407 (6)		
O1—Cu1—N1	89.77 (13)	C1—C6—C7	122.5 (4)
O1—Cu1—O4	91.02 (13)	N1—C7—C6	119.4 (3)
N1—Cu1—O4	167.44 (13)	N1—C7—C8	120.8 (4)
O1—Cu1—N2^{i}	153.28 (14)	C6—C7—C8	119.7 (4)
N1—Cu1—N2^{i}	93.89 (13)	C7—C8—H8A	109.5
O4—Cu1—N2^{i}	91.03 (13)	C7—C8—H8B	109.5

O3—S1—O2	118.67 (19)	H8A—C8—H8B	109.5
O3—S1—N2	105.18 (18)	C7—C8—H8C	109.5
O2—S1—N2	112.07 (17)	H8A—C8—H8C	109.5
O3—S1—C10	107.86 (19)	H8B—C8—H8C	109.5
O2—S1—C10	106.05 (19)	C11—C10—C15	121.3 (4)
N2—S1—C10	106.37 (18)	C11—C10—S1	119.2 (3)
O4—S2—C17	105.9 (2)	C15—C10—S1	119.5 (3)
O4—S2—C16	102.9 (2)	C10—C11—C12	118.8 (4)
C17—S2—C16	98.1 (2)	C10—C11—H11	120.6
C1—O1—Cu1	121.3 (3)	C12—C11—H11	120.6
S2—O4—Cu1	120.97 (17)	C13—C12—C11	120.3 (4)
C7—N1—N2	117.5 (3)	C13—C12—H12	119.8
C7—N1—Cu1	127.0 (3)	C11—C12—H12	119.8
N2—N1—Cu1	114.7 (2)	C12—C13—C14	120.3 (4)
N1—N2—S1	108.2 (2)	C12—C13—H13	119.9
N1—N2—Cu1^{i}	122.8 (2)	C14—C13—H13	119.9
S1—N2—Cu1^{i}	105.85 (17)	C15—C14—C13	119.9 (4)
O1—C1—C2	117.5 (4)	C15—C14—H14	120.0
O1—C1—C6	125.2 (4)	C13—C14—H14	120.0
C2—C1—C6	117.3 (4)	C14—C15—C10	119.3 (4)
C3—C2—C1	122.9 (4)	C14—C15—H15	120.4
C3—C2—H2	118.5	C10—C15—H15	120.4
C1—C2—H2	118.5	S2—C16—H16A	109.5
C2—C3—C4	119.0 (4)	S2—C16—H16B	109.5
C2—C3—H3	120.5	H16A—C16—H16B	109.5
C4—C3—H3	120.5	S2—C16—H16C	109.5
C5—C4—C3	120.7 (4)	H16A—C16—H16C	109.5
C5—C4—Br1	119.9 (3)	H16B—C16—H16C	109.5
C3—C4—Br1	119.3 (3)	S2—C17—H17A	109.5
C4—C5—C6	121.5 (4)	S2—C17—H17B	109.5
C4—C5—H5	119.2	H17A—C17—H17B	109.5
C6—C5—H5	119.2	S2—C17—H17C	109.5
C5—C6—C1	118.4 (4)	H17A—C17—H17C	109.5
C5—C6—C7	119.0 (4)	H17B—C17—H17C	109.5

N1—Cu1—O1—C1	40.0 (3)	C3—C4—C5—C6	−1.3 (7)
O4—Cu1—O1—C1	−152.5 (3)	Br1—C4—C5—C6	−178.1 (3)
N2^{i}—Cu1—O1—C1	−58.2 (5)	C4—C5—C6—C1	−1.1 (6)
C17—S2—O4—Cu1	−58.7 (3)	C4—C5—C6—C7	−177.5 (4)
C16—S2—O4—Cu1	−161.2 (2)	O1—C1—C6—C5	−177.2 (4)
O1—Cu1—O4—S2	−23.1 (2)	C2—C1—C6—C5	3.2 (6)
N1—Cu1—O4—S2	70.5 (7)	O1—C1—C6—C7	−0.9 (6)
N2^{i}—Cu1—O4—S2	−176.4 (2)	C2—C1—C6—C7	179.6 (4)
O1—Cu1—N1—C7	−34.4 (4)	N2—N1—C7—C6	−174.7 (3)
O4—Cu1—N1—C7	−128.1 (6)	Cu1—N1—C7—C6	15.4 (5)
N2^{i}—Cu1—N1—C7	119.1 (3)	N2—N1—C7—C8	5.6 (6)
O1—Cu1—N1—N2	155.5 (3)	Cu1—N1—C7—C8	−164.3 (4)
O4—Cu1—N1—N2	61.8 (7)	C5—C6—C7—N1	−174.6 (4)

N2^{i}—Cu1—N1—N2	−51.0 (3)	C1—C6—C7—N1	9.1 (6)
C7—N1—N2—S1	132.6 (3)	C5—C6—C7—C8	5.1 (6)
Cu1—N1—N2—S1	−56.4 (3)	C1—C6—C7—C8	−171.2 (4)
C7—N1—N2—Cu1^{i}	−103.8 (4)	O3—S1—C10—C11	−163.2 (3)
Cu1—N1—N2—Cu1^{i}	67.3 (3)	O2—S1—C10—C11	−35.1 (4)
O3—S1—N2—N1	166.0 (2)	N2—S1—C10—C11	84.4 (4)
O2—S1—N2—N1	35.8 (3)	O3—S1—C10—C15	16.4 (4)
C10—S1—N2—N1	−79.7 (3)	O2—S1—C10—C15	144.5 (3)
O3—S1—N2—Cu1^{i}	32.7 (2)	N2—S1—C10—C15	−96.0 (3)
O2—S1—N2—Cu1^{i}	−97.6 (2)	C15—C10—C11—C12	−0.7 (6)
C10—S1—N2—Cu1^{i}	146.95 (18)	S1—C10—C11—C12	178.8 (3)
Cu1—O1—C1—C2	148.7 (3)	C10—C11—C12—C13	−0.9 (7)
Cu1—O1—C1—C6	−30.8 (5)	C11—C12—C13—C14	2.1 (7)
O1—C1—C2—C3	177.1 (4)	C12—C13—C14—C15	−1.7 (7)
C6—C1—C2—C3	−3.3 (6)	C13—C14—C15—C10	0.1 (7)
C1—C2—C3—C4	1.1 (7)	C11—C10—C15—C14	1.1 (6)
C2—C3—C4—C5	1.3 (7)	S1—C10—C15—C14	−178.5 (3)
C2—C3—C4—Br1	178.2 (3)		

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