



Bis{ μ -2,2'-[(3,4-dithiahexane-1,6-diyl)bis(nitrilomethanylylidene)]bis(4-bromophenolato)- κ^4 O,N,N',O'}dicopper(II)

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Keywords: crystal structure; dinuclear copper(II) complex; Schiff base; 5-bromosalicylaldehyde; cysteamine (2-aminoethanethiol).

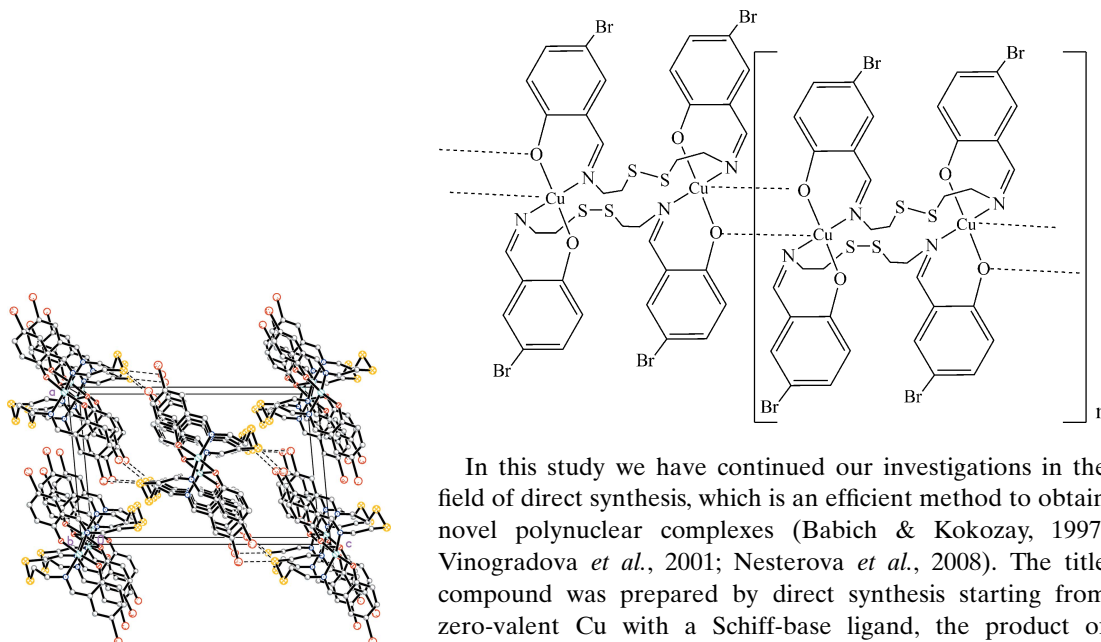
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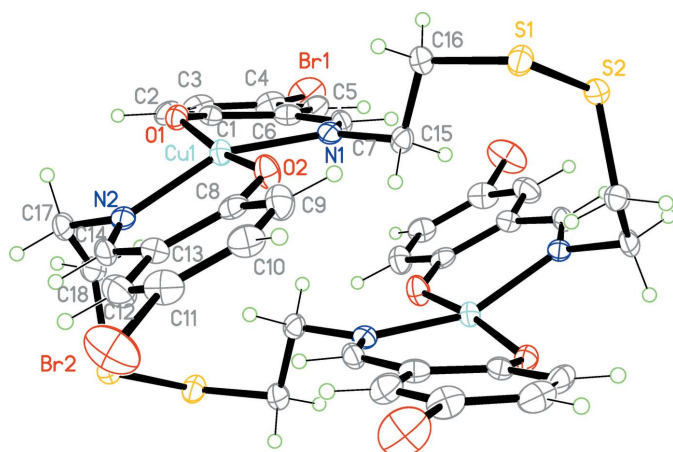
The crystal structure of the title compound, $[\text{Cu}_2(\text{C}_{18}\text{H}_{12}\text{Br}_2\text{N}_4\text{O}_2\text{S}_2)_2]$, consists of binuclear complex units which lie across inversion centres and are connected by weak Cu—O coordination bonds forming chains along the *b* axis. The Cu^{II} ion is five-coordinated by two N atoms and two O atoms of the chelating ligand and one symmetry-related O atom forming a square-pyramidal coordination geometry. In the crystal, short S...Br contacts connect neighbouring chains into a two-dimensional network parallel to (101).

1. Chemical context

Schiff bases and their metal complexes represent one of the most widely used classes of compound because of their synthetic flexibility and wide range of applications (Mitra *et al.*, 1997; Bera *et al.*, 1998; Prabhakaran *et al.*, 2004). Such complexes having sulfur-containing ligands are of considerable interest because of their diverse coordination modes and bridging ability. The formation and cleavage of disulfide bonds are known to be important for the biological activity of several sulfur-containing peptides and proteins (Gilbert *et al.*, 1999; Jacob *et al.*, 2003).



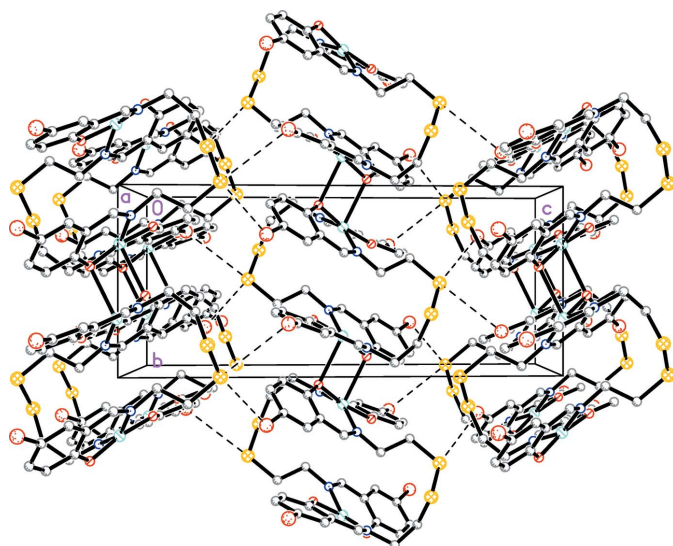
In this study we have continued our investigations in the field of direct synthesis, which is an efficient method to obtain novel polynuclear complexes (Babich & Kokozya, 1997; Vinogradova *et al.*, 2001; Nesterova *et al.*, 2008). The title compound was prepared by direct synthesis starting from zero-valent Cu with a Schiff-base ligand, the product of condensation between 5-bromosalicylaldehyde and cysteamine, formed *in situ* in a methanol/dimethylformamide (DMF) mixture.


Figure 1

The molecular structure of the binuclear complex unit of the title compound, showing 50% probability displacement ellipsoids. Unlabelled atoms are related to labelled ones by the symmetry operation $(2 - x, -y, 2 - z)$.

2. Structural commentary

In the title compound, binuclear complex units lie across an inversion centre (Fig. 1). The coordination geometry around the Cu^{II} ion is comparable to that found in copper complexes reported earlier (CSD refcode FEDCIB; Dhar *et al.*, 2005; Rusanova & Bederak, 2017). Despite the close structural similarity, neighboring centrosymmetric binuclear fragments are connected by additional weak $\text{Cu} \cdots \text{O}$ $(2 - x, 1 - y, 2 - z)$ coordination bonds with the oxygen atoms of the ligand [2.520 (3) Å] and organized in chains along the b -axis direction (Fig. 2). Thus, each Cu^{II} ion is five-coordinated by two nitrogen atoms (N1, N2), two oxygen atoms (O1, O2) and one symmetry-related O atom [O1 $(2 - x, 1 - y, 2 - z)$], forming a distorted square-pyramidal geometry.


Figure 2

The crystal packing of the title compound viewed along the a axis. Short $\text{S} \cdots \text{Br}$ contacts are shown as dashed lines. H atoms are not shown.

The chelating fragments coordinated to the Cu^{II} ions are twisted relative to each other, as defined by the dihedral angle of $28.9 (2)^\circ$ formed between the mean planes of atoms O1/N1/C1/C6/C7 and O2/N2/C8/C13/C14. The thiosulfonate moiety is not involved in any metal–ligand interactions.

The separation between the two symmetry-related Cu^{II} ions within the binuclear fragment is 5.2161 (11) Å and between neighboring fragments is 3.4458 (11) Å. In general, all bonding parameters and the dimensions of the angles in the title complex are in good agreement with those encountered in related complexes (Dhar *et al.*, 2005; Zhang *et al.*, 2010).

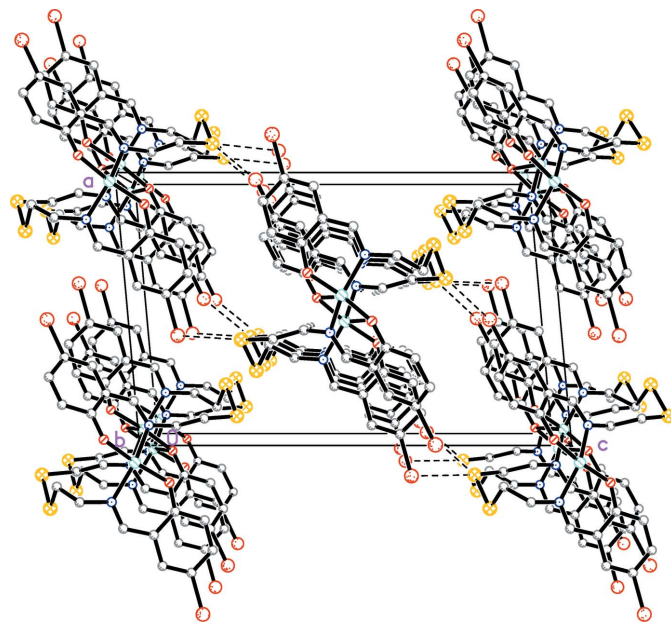
3. Supramolecular features

In the crystal, short $\text{S} \cdots \text{Br}$ $(-\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z)$ contacts with a distance of 3.5108 (13) Å connect neighboring chains, forming a two-dimensional network parallel to (101) (Fig. 3).

In contrast to the previously reported complex (Rusanova & Bederak, 2017), there are no hydrogen-bond or π - π stacking interactions in the title complex. In terms of $\text{C}-\text{H} \cdots \text{Br}$ interactions, the intermolecular $\text{C16}-\text{H16B} \cdots \text{Br2}(x + 1, y, z)$ distance of 3.03 Å and $\text{C17}-\text{H17B} \cdots \text{S1}(-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z)$ distance of 2.95 Å are almost equal to the sum of the van der Waals radii for the atoms involved and may be worthy of note.

4. Database survey

A search of the Cambridge Structural Database (Version 5.38; last update November 2016; Groom *et al.*, 2016) for related complexes with an aminoethanethiol group gave 165 hits, including two closely related structures with a disulfide moiety, *viz.* bis[(μ^2 -sulfato)(6-salicylideneamino-3,4-dithiahexylammonium)copper(II)] and bis(μ^2 - N,N' -(3,4-dithiahexane-1,6-


Figure 3

The crystal packing of the title compound viewed along the b axis. Short $\text{S} \cdots \text{Br}$ contacts are shown as dashed lines. H atoms are not shown.

Table 1
Experimental details.

Crystal data	
Chemical formula	[Cu ₂ (C ₁₈ H ₁₆ Br ₂ N ₂ O ₂ S ₂) ₂]
<i>M</i> _r	1159.61
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.3596 (5), 8.3442 (3), 19.5002 (7)
β (°)	95.156 (2)
<i>V</i> (Å ³)	2002.94 (13)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	5.31
Crystal size (mm)	0.45 × 0.10 × 0.06
Data collection	
Diffractometer	Bruker SMART APEXII
Absorption correction	Multi-scan <i>SADABS</i>
<i>T</i> _{min} , <i>T</i> _{max}	0.36, 0.74
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	18553, 3939, 2644
<i>R</i> _{int}	0.075
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.617
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.046, 0.098, 1.05
No. of reflections	3939
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.82, -0.66

Computer programs: *SMART* and *SAINT* (Bruker, 2008), *SHELXT* (Sheldrick, 2015a), *SHELXL2016* (Sheldrick, 2015b), *SHELXTL* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

diyl)bis(salicylideneiminato)-*N,N',O,O'*dicopper(II) (Dhar *et al.*, 2004, 2005). The length of the S...Br contact in the title compound is in good agreement with those in related complexes (CSD refcodes WEMCAT and QELVIN; Salivon *et al.*, 2006, 2007; CSD refcode PODDAO; Xia *et al.*, 2008)

5. Synthesis and crystallization

A solution of KOH (0.12 g, 2 mmol) in a minimum amount of methanol was added to a solution of aminoethanethiol hydrochloride (0.23g, 2 mmol) in methanol (5 ml) and stirred on an ice bath for 10 min. The white precipitate of solid KCl was removed by filtration and 5-bromosalicylaldehyde (0.402 g, 2 mmol) in dimethylformamide (10 ml) were added to the filtrate and stirred magnetically for 50 min. Copper powder (0.064 g, 1 mmol) were added to the yellow solution of the Schiff base formed *in situ*, and the resulting deep green-brown solution was stirred magnetically and heated in air at 323–333 K for 2 h, resulting in a dark-green precipitate. Crystals suitable for crystallographic study were grown from a saturated solution in DMF after successive addition of CH₂Cl₂. The crystals were filtered off, washed with dry *i*-PrOH and finally dried at room temperature (yield: 20%).

The IR spectrum of the title compound (as KBr pellets) is consistent with the above structural data. In the range 4000–400 cm⁻¹ it shows all characteristic functional groups peaks: ν (CH) due to aromatic =C–H stretching at 3000–3100cm⁻¹, the aromatic ring vibrations in the 1600–1400 cm⁻¹ region, weak S–S absorptions at 500–540 cm⁻¹ as well absorbance at 1630 cm⁻¹ assigned to the azomethine ν (C=N) group. Analysis calculated for C₃₆H₃₂Br₄Cu₂N₄O₄S₄: C 37.28, H 2.78, N 4.83, S 11.06%; found: C 37.32, H 3.01, N 4.70, S 11.10%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All hydrogen atoms were placed at calculated positions (C–H = 0.93–0.97 Å) and refined as riding with *U*_{iso}(H) = 1.2*U*_{eq}(C).

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Bis{ μ -2,2'-[(3,4-dithiahexane-1,6-diyl)bis(nitrilomethanylylidene)]bis(4-bromophenolato)- $\kappa^4 O,N,N',O'$ }dicopper(II)

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Computing details

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Bis{ μ -2,2'-[(3,4-dithiahexane-1,6-diyl)bis(nitrilomethanylylidene)]bis(4-bromophenolato)- $\kappa^4 O,N,N',O'$ }dicopper(II)

Crystal data

[Cu₂(C₁₈H₁₆Br₂N₂O₂S₂)₂]

$M_r = 1159.61$

Monoclinic, $P2_1/n$

$a = 12.3596$ (5) Å

$b = 8.3442$ (3) Å

$c = 19.5002$ (7) Å

$\beta = 95.156$ (2)°

$V = 2002.94$ (13) Å³

$Z = 2$

$F(000) = 1140$

$D_x = 1.923$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2534 reflections

$\theta = 2.7$ – 23.6 °

$\mu = 5.31$ mm⁻¹

$T = 296$ K

Needle, green

$0.45 \times 0.10 \times 0.06$ mm

Data collection

Bruker SMART APEXII
diffractometer

Radiation source: sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan
sadabs

$T_{\min} = 0.36$, $T_{\max} = 0.74$

18553 measured reflections

3939 independent reflections

2644 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.075$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 1.9$ °

$h = -15 \rightarrow 8$

$k = -10 \rightarrow 10$

$l = -23 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.098$

$S = 1.05$

3939 reflections

244 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.004$

$\Delta\rho_{\max} = 0.82$ e Å⁻³

$\Delta\rho_{\min} = -0.66$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
BR1	1.46222 (5)	0.24549 (7)	0.82836 (3)	0.04443 (19)
BR2	0.40450 (5)	0.21977 (8)	1.11957 (3)	0.0456 (2)
CU1	0.95419 (5)	0.30506 (7)	1.00084 (3)	0.01799 (16)
N1	1.0809 (3)	0.1638 (4)	1.03365 (18)	0.0184 (9)
N2	0.8169 (3)	0.3643 (4)	0.94366 (18)	0.0174 (9)
O1	1.0408 (2)	0.4239 (3)	0.94197 (15)	0.0184 (7)
O2	0.8768 (3)	0.2123 (4)	1.07014 (16)	0.0239 (8)
S1	1.10722 (11)	−0.01078 (14)	1.23102 (6)	0.0231 (3)
S2	1.21861 (10)	−0.17845 (15)	1.20755 (6)	0.0229 (3)
C1	1.1308 (4)	0.3764 (5)	0.9170 (2)	0.0187 (11)
C2	1.1648 (4)	0.4542 (5)	0.8585 (2)	0.0241 (12)
H2	1.120805	0.533137	0.836940	0.029*
C3	1.2610 (4)	0.4166 (6)	0.8324 (2)	0.0279 (13)
H3	1.282029	0.470919	0.794135	0.033*
C4	1.3278 (4)	0.2961 (6)	0.8634 (3)	0.0265 (12)
C5	1.2960 (4)	0.2146 (6)	0.9191 (3)	0.0261 (12)
H5	1.340017	0.133916	0.939219	0.031*
C6	1.1973 (4)	0.2517 (5)	0.9464 (2)	0.0205 (11)
C7	1.1680 (4)	0.1571 (5)	1.0031 (2)	0.0184 (11)
H7	1.218760	0.081147	1.019849	0.022*
C8	0.7732 (4)	0.2183 (5)	1.0778 (2)	0.0193 (11)
C9	0.7380 (4)	0.1630 (6)	1.1407 (2)	0.0260 (12)
H9	0.788849	0.123649	1.174609	0.031*
C10	0.6303 (4)	0.1663 (6)	1.1528 (3)	0.0247 (12)
H10	0.608900	0.131899	1.194901	0.030*
C11	0.5537 (4)	0.2208 (6)	1.1021 (3)	0.0282 (12)
C12	0.5833 (4)	0.2746 (6)	1.0406 (3)	0.0287 (13)
H12	0.530635	0.311494	1.007245	0.034*
C13	0.6938 (4)	0.2746 (5)	1.0273 (2)	0.0214 (11)
C14	0.7216 (4)	0.3439 (5)	0.9635 (2)	0.0206 (11)
H14	0.663784	0.377719	0.933102	0.025*
C15	1.0733 (4)	0.0487 (5)	1.0908 (2)	0.0191 (11)
H15A	1.121681	−0.040961	1.085098	0.023*
H15B	0.999770	0.007538	1.089495	0.023*
C16	1.1034 (4)	0.1278 (6)	1.1595 (2)	0.0222 (12)
H16A	1.051164	0.211612	1.166482	0.027*
H16B	1.174199	0.177672	1.158804	0.027*
C17	0.8220 (4)	0.4465 (5)	0.8773 (2)	0.0219 (11)
H17A	0.865362	0.542817	0.884674	0.026*

H17B	0.749153	0.478879	0.860140	0.026*
C18	0.8697 (4)	0.3449 (5)	0.8229 (2)	0.0212 (11)
H18A	0.939036	0.302111	0.841906	0.025*
H18B	0.883066	0.412405	0.784101	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
BR1	0.0376 (4)	0.0474 (4)	0.0522 (4)	-0.0041 (3)	0.0256 (3)	-0.0010 (3)
BR2	0.0234 (3)	0.0744 (5)	0.0400 (4)	-0.0008 (3)	0.0092 (3)	-0.0080 (3)
CU1	0.0192 (3)	0.0175 (3)	0.0170 (3)	0.0009 (3)	0.0002 (2)	0.0026 (3)
N1	0.028 (2)	0.017 (2)	0.010 (2)	-0.0013 (18)	-0.0003 (18)	-0.0023 (16)
N2	0.024 (2)	0.015 (2)	0.013 (2)	0.0012 (17)	-0.0001 (18)	-0.0034 (16)
O1	0.0209 (19)	0.0170 (18)	0.0174 (17)	0.0007 (14)	0.0019 (15)	0.0013 (14)
O2	0.0197 (19)	0.029 (2)	0.0229 (18)	0.0018 (15)	0.0025 (15)	0.0086 (15)
S1	0.0316 (7)	0.0187 (7)	0.0190 (7)	0.0033 (6)	0.0029 (6)	0.0010 (5)
S2	0.0253 (7)	0.0192 (7)	0.0229 (7)	0.0026 (6)	-0.0044 (6)	-0.0016 (6)
C1	0.022 (3)	0.018 (3)	0.015 (3)	-0.001 (2)	-0.002 (2)	-0.004 (2)
C2	0.037 (3)	0.018 (3)	0.018 (3)	-0.007 (2)	0.004 (2)	0.002 (2)
C3	0.040 (3)	0.026 (3)	0.020 (3)	-0.009 (3)	0.010 (3)	-0.003 (2)
C4	0.029 (3)	0.027 (3)	0.025 (3)	-0.003 (2)	0.010 (2)	-0.006 (2)
C5	0.027 (3)	0.020 (3)	0.031 (3)	-0.001 (2)	0.005 (2)	-0.003 (2)
C6	0.020 (3)	0.022 (3)	0.020 (3)	-0.004 (2)	0.003 (2)	-0.007 (2)
C7	0.017 (3)	0.019 (3)	0.018 (3)	0.004 (2)	-0.002 (2)	0.000 (2)
C8	0.021 (3)	0.014 (3)	0.024 (3)	0.000 (2)	0.004 (2)	-0.006 (2)
C9	0.029 (3)	0.027 (3)	0.022 (3)	0.003 (2)	0.001 (2)	0.004 (2)
C10	0.023 (3)	0.026 (3)	0.026 (3)	-0.006 (2)	0.008 (2)	-0.001 (2)
C11	0.024 (3)	0.033 (3)	0.029 (3)	-0.002 (2)	0.009 (2)	-0.006 (2)
C12	0.021 (3)	0.033 (3)	0.030 (3)	0.001 (2)	-0.003 (2)	-0.003 (2)
C13	0.021 (3)	0.021 (3)	0.022 (3)	-0.002 (2)	-0.002 (2)	-0.002 (2)
C14	0.018 (3)	0.019 (3)	0.023 (3)	0.006 (2)	-0.005 (2)	-0.002 (2)
C15	0.014 (3)	0.017 (3)	0.026 (3)	0.002 (2)	0.002 (2)	0.002 (2)
C16	0.026 (3)	0.021 (3)	0.019 (3)	0.002 (2)	-0.002 (2)	0.003 (2)
C17	0.029 (3)	0.021 (3)	0.015 (3)	0.004 (2)	-0.004 (2)	0.003 (2)
C18	0.024 (3)	0.022 (3)	0.018 (3)	-0.004 (2)	0.001 (2)	0.004 (2)

Geometric parameters (Å, °)

BR1—C4	1.900 (5)	C6—C7	1.433 (6)
BR2—C11	1.905 (5)	C7—H7	0.9300
CU1—O2	1.890 (3)	C8—C13	1.408 (6)
CU1—O1	1.915 (3)	C8—C9	1.415 (6)
CU1—N2	2.006 (4)	C9—C10	1.372 (6)
CU1—N1	2.018 (4)	C9—H9	0.9300
CU1—O1 ⁱ	2.520 (3)	C10—C11	1.382 (7)
N1—C7	1.277 (5)	C10—H10	0.9300
N1—C15	1.480 (5)	C11—C12	1.362 (7)
N2—C14	1.284 (5)	C12—C13	1.413 (6)

N2—C17	1.471 (5)	C12—H12	0.9300
O1—C1	1.315 (5)	C13—C14	1.441 (6)
O2—C8	1.304 (5)	C14—H14	0.9300
S1—C16	1.808 (5)	C15—C16	1.511 (6)
S1—S2	2.0435 (17)	C15—H15A	0.9700
S2—C18 ⁱⁱ	1.832 (5)	C15—H15B	0.9700
C1—C2	1.410 (6)	C16—H16A	0.9700
C1—C6	1.415 (6)	C16—H16B	0.9700
C2—C3	1.371 (6)	C17—C18	1.517 (6)
C2—H2	0.9300	C17—H17A	0.9700
C3—C4	1.403 (7)	C17—H17B	0.9700
C3—H3	0.9300	C18—S2 ⁱⁱ	1.832 (5)
C4—C5	1.369 (7)	C18—H18A	0.9700
C5—C6	1.407 (6)	C18—H18B	0.9700
C5—H5	0.9300		
O2—CU1—O1	170.63 (14)	C13—C8—C9	117.8 (4)
O2—CU1—N2	92.36 (15)	C10—C9—C8	121.4 (5)
O1—CU1—N2	91.68 (14)	C10—C9—H9	119.3
O2—CU1—N1	87.85 (14)	C8—C9—H9	119.3
O1—CU1—N1	91.88 (14)	C9—C10—C11	119.7 (5)
N2—CU1—N1	156.01 (14)	C9—C10—H10	120.1
O2—CU1—O1 ⁱ	92.59 (12)	C11—C10—H10	120.1
O1—CU1—O1 ⁱ	78.91 (12)	C12—C11—C10	121.2 (5)
N2—CU1—O1 ⁱ	90.61 (12)	C12—C11—BR2	120.0 (4)
N1—CU1—O1 ⁱ	113.35 (13)	C10—C11—BR2	118.8 (4)
C7—N1—C15	115.8 (4)	C11—C12—C13	120.2 (5)
C7—N1—CU1	122.7 (3)	C11—C12—H12	119.9
C15—N1—CU1	121.2 (3)	C13—C12—H12	119.9
C14—N2—C17	116.0 (4)	C8—C13—C12	119.7 (4)
C14—N2—CU1	123.6 (3)	C8—C13—C14	122.2 (4)
C17—N2—CU1	120.2 (3)	C12—C13—C14	117.9 (4)
C1—O1—CU1	127.1 (3)	N2—C14—C13	127.6 (4)
C8—O2—CU1	129.2 (3)	N2—C14—H14	116.2
C16—S1—S2	103.67 (16)	C13—C14—H14	116.2
C18 ⁱⁱ —S2—S1	101.41 (16)	N1—C15—C16	110.9 (4)
O1—C1—C2	119.0 (4)	N1—C15—H15A	109.5
O1—C1—C6	123.5 (4)	C16—C15—H15A	109.5
C2—C1—C6	117.5 (4)	N1—C15—H15B	109.5
C3—C2—C1	121.8 (5)	C16—C15—H15B	109.5
C3—C2—H2	119.1	H15A—C15—H15B	108.0
C1—C2—H2	119.1	C15—C16—S1	113.1 (3)
C2—C3—C4	120.0 (4)	C15—C16—H16A	109.0
C2—C3—H3	120.0	S1—C16—H16A	109.0
C4—C3—H3	120.0	C15—C16—H16B	109.0
C5—C4—C3	119.9 (5)	S1—C16—H16B	109.0
C5—C4—BR1	119.9 (4)	H16A—C16—H16B	107.8
C3—C4—BR1	120.2 (4)	N2—C17—C18	113.8 (4)

C4—C5—C6	120.7 (5)	N2—C17—H17A	108.8
C4—C5—H5	119.7	C18—C17—H17A	108.8
C6—C5—H5	119.7	N2—C17—H17B	108.8
C5—C6—C1	120.1 (4)	C18—C17—H17B	108.8
C5—C6—C7	117.3 (4)	H17A—C17—H17B	107.7
C1—C6—C7	122.7 (4)	C17—C18—S2 ⁱⁱ	113.1 (3)
N1—C7—C6	128.2 (4)	C17—C18—H18A	109.0
N1—C7—H7	115.9	S2 ⁱⁱ —C18—H18A	109.0
C6—C7—H7	115.9	C17—C18—H18B	109.0
O2—C8—C13	124.2 (4)	S2 ⁱⁱ —C18—H18B	109.0
O2—C8—C9	118.0 (4)	H18A—C18—H18B	107.8

Symmetry codes: (i) $-x+2, -y+1, -z+2$; (ii) $-x+2, -y, -z+2$.