

Crystal structure of a copper complex containing the 4-bromo-2-[[[(2-hydroxyethyl)imino]methyl]phenol base Schiff ligand

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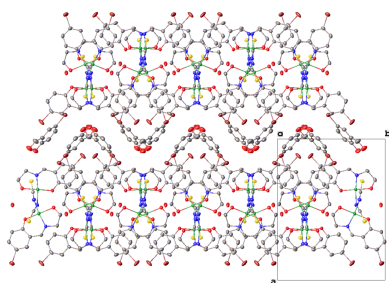
The coordination co-crystal (4-bromo-2-[[[(2-hydroxyethyl)imino]methyl]phenololato- $\kappa^3 O, N, O'$)(thiocyanato- κN)copper(II)–5-bromo-2-hydroxybenzaldehyde–water (2/1/1), $[\text{Cu}(\text{C}_9\text{H}_9\text{BrNO}_2)(\text{NCS})] \cdot 0.5\text{C}_7\text{H}_5\text{BrO}_2 \cdot 0.5\text{H}_2\text{O}$ or $[\text{Cu}(\text{HL})(\text{SCN})]_2 \cdot \text{C}_7\text{H}_5\text{BrO}_2 \cdot \text{H}_2\text{O}$, crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains two mononuclear units of the complex, each consisting of one deprotonated ligand, one thiocyanate anion (SCN^-) coordinated through its nitrogen atom, one free water molecule, and one free 5-bromosalicylaldehyde molecule, forming a co-crystal. The copper atom is four-coordinate, adopting a slightly distorted square-planar geometry defined by the tridentate ligand and the nitrogen atom of the thiocyanate anion. Bond length values show that the thiocyanate ion has a linear $\text{S}-\text{C}\equiv\text{N}$ arrangement, typical of a terminal, N-bound isothiocyanate group. The water molecule plays a key role in linking the two complex units through $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. In the crystal, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ hydrogen bonds allow the free 5-bromosalicylaldehyde molecule to form a bridge between two adjacent layers. Additional $\text{O}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{S}$, $\text{O}-\text{H}\cdots\text{S}$, and $\text{C}-\text{H}\cdots\text{N}$ interactions further consolidate the overall structure.

1. Chemical context

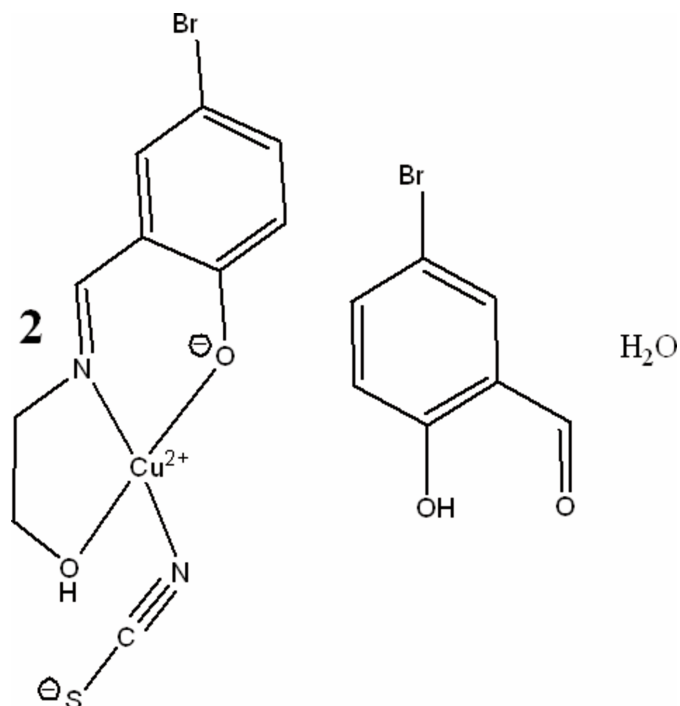
The use of salicylaldehyde-derived ligands in the synthesis of coordination complexes has become increasingly important and represents a frequent research topic, particularly in copper-catalysed reactions (Juyal *et al.*, 2023). Indeed, these ligands contain donor sites such as the phenolic oxygen atom and the imine nitrogen atom, enabling the formation of stable complexes with various geometries, notably polynuclear copper(II) complexes.

Numerous applications have been reported, including in catalysis (Shelar *et al.*, 2021), materials science (Abu-Dief & Mohamed, 2015), and medicine (More *et al.*, 2019). The formation of a co-crystal associated with a polynuclear copper complex represents an important aspect of supramolecular chemistry, as such systems are stabilized by networks of non-covalent interactions, including hydrogen bonds (Benito *et al.*, 2025).

In the field of crystal engineering, co-crystals defined as single-phase crystalline materials comprising two or more neutral molecular species have long been exploited to tune physicochemical attributes while preserving the molecular identity of active components (Taylor & Day, 2018). We have synthesized a tridentate Schiff base ligand, (*E*)-4-bromo-2-[[[(2-hydroxyethyl)imino]methyl]phenol, derived from salicyl-



aldehyde, which forms a polynuclear complex with copper(II) chloride and potassium thiocyanate.



2. Structural commentary

The title compound (Fig. 1) crystallizes in the monoclinic system, space group $P2_1/c$. The asymmetric unit, $[\text{Cu}(\text{HL})(\text{SCN})]_2(\text{C}_7\text{H}_5\text{BrO}_2) \cdot \text{H}_2\text{O}$, contains two monodeprotonated ligand molecules, two independent copper(II) ions, two monodentate thiocyanate anions, one co-crystallized bromo-hydroxybenzaldehyde molecule and one free water molecule.

The Schiff base ligand acts in a tridentate fashion through the phenolate oxygen atom, the azomethine nitrogen atom, and the alcoholic oxygen atom, resulting in one five-membered (CuOCCN) and one six-membered (CuOCCCN) chelate ring around each Cu^{II} ion.

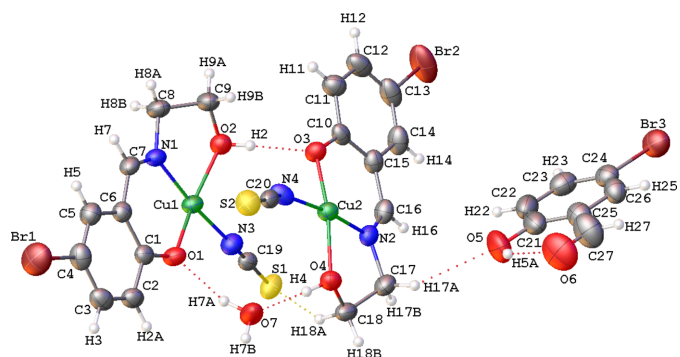


Figure 1

The molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 1

Selected geometric parameters ($\text{\AA}$, $^\circ$).

Cu1—O1	1.911 (2)	Cu2—O3	1.923 (2)
Cu1—O2	2.038 (2)	Cu2—O4	2.005 (2)
Cu1—N1	1.928 (3)	Cu2—N4	1.995 (3)
Cu1—N3	1.952 (3)	Cu2—N2	1.927 (3)
O1—Cu1—O2	166.82 (10)	O3—Cu2—O4	166.23 (10)
N3—Cu1—O2	89.45 (11)	O3—Cu2—N4	91.49 (10)
O1—Cu1—N1	93.58 (10)	O3—Cu2—N2	93.35 (11)
O1—Cu1—N3	94.69 (11)	N4—Cu2—O4	92.01 (10)
N1—Cu1—O2	82.51 (10)	N2—Cu2—O4	82.24 (11)
N1—Cu1—N3	171.73 (12)	N2—Cu2—N4	173.38 (11)

Each copper atom is four-coordinate, bound by an N_2O_2 donor set comprising one azomethine (imine) nitrogen and two oxygen atoms (one phenolate, one alcoholic) from the Schiff base ligand, together with one nitrogen atom from its own thiocyanate group, forming an essentially square-planar, moderately distorted coordination plane. The bond lengths within this square plane are $\text{Cu1—O1} = 1.911 (2) \text{ \AA}$, $\text{Cu1—N1} = 1.928 (3) \text{ \AA}$, $\text{Cu1—N3} = 1.952 (3) \text{ \AA}$, and $\text{Cu1—O2} = 2.038 (2) \text{ \AA}$. For the corresponding values for Cu2, see Table 1).

A single, additional axial contact to the nitrogen atom of the thiocyanate group of the neighbouring mononuclear unit is present at each copper centre, but this contact is long and markedly asymmetric between the two independent centres [$2.961 (3) \text{ \AA}$ for Cu1 *versus* $3.100 (3) \text{ \AA}$ for Cu2]. The latter value exceeds the sum of the van der Waals radii for $\text{Cu} \cdots \text{N}$ and cannot reasonably be described as a coordination bond. The geometry is therefore described as distorted square-planar (four-coordinate, N_2O_2), with a weak, asymmetric secondary axial contact of semi-coordinate character, rather than as distorted square-planar.

It is this weak, asymmetric $\text{N} \cdots \text{Cu}$ axial contact, not a Cu—S bond, that links each mononuclear $[\text{Cu}(\text{HL})(\text{SCN})]$ unit to its neighbour and propagates the one-dimensional polymeric chain.

The deviations of the angles from the ideal value of 90° [$\text{O1—Cu1—N1} = 93.58 (10)^\circ$, $\text{O2—Cu1—N3} = 89.45 (11)^\circ$, $\text{N1—Cu1—O2} = 82.51 (10)^\circ$, and $\text{O1—Cu1—N3} = 94.69 (11)^\circ$] confirm the distortion of the coordination geometry.

The Cu1 ion is displaced from the least-squares plane defined by O1, N1, O2 and N3 (r.m.s. deviation $0.117 \text{ \AA}$) by $0.006 (12) \text{ \AA}$, indicating that the metal centre lies essentially within the equatorial plane. The dihedral angle of $175.63 (17)^\circ$ between the phenolate ring plane (O1/C1—C6) and the plane of the open-chain fragment (C7/N1/C8/C9/O2) reveals a slight but measurable deviation from planarity, indicative of a twist in the ligand backbone.

The $\text{Cu1} \cdots \text{Cu2}$ separation between two adjacent units is $3.7765 (5) \text{ \AA}$, a distance too long to invoke any meaningful metal–metal interaction. The *cis* angles span the range $82.51 (10)–94.69 (11)^\circ$, in good agreement with values reported for related complexes. The *trans* angles $\text{O1—Cu1—O2} = 166.82 (10)^\circ$ and $\text{N3—Cu1—N1} = 171.73 (12)^\circ$ deviate significantly from the ideal value of 180° , further confirming that Cu1 resides in a severely distorted

square-planar coordination environment. The environment about Cu2 is similar, see Table 1).

The bond lengths within the two thiocyanate groups are S1—C19 = 1.629 (3) Å, C19—N3 = 1.153 (4) Å, and S2—C20 = 1.643 (4) Å, C20—N4 = 1.106 (4) Å. These values are consistent with the linear S—C≡N arrangement typical of a terminal, N-bound isothiocyanate group.

The sulfur atoms S1 and S2 are not bonded to any copper atom. The bridging mode is therefore not the classical μ -1,3 (S,N) mode frequently found in Cu—SCN polymers, but an asymmetric end-on μ -1,1 (N,N') bridge, in which each thiocyanate nitrogen atom is strongly bonded to its own copper center and forms a second, much weaker, semi-coordinate contact with the neighbouring copper center, as summarized below.

3. Supramolecular features

We note four strong interactions of the O—H—O type (Table 2). The water molecule connects unit Cu2 *via* O4—H4 $\cdots$ O7 to unit Cu1 *via* O7—H7A $\cdots$ O1. The O2—H2 $\cdots$ O3 hydrogen bond similarly connects the two units. The O5—H5A $\cdots$ O6 interaction corresponds to the classical intramolecular hydrogen bond within the co-crystallized aldehyde fragment, confirming its nature as an isolated unit maintained in the network mainly by the weak C—H $\cdots$ Br, C—H $\cdots$ S, C—H $\cdots$ N and C—H $\cdots$ O contacts and extending the three-dimensional network and further enhances the cohesion of the structure. The packing is shown in Fig. 2.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.46, updates of November 2024 and February 2025; Groom *et al.*, 2016) yielded 25 hits containing crystal structures of coordination complexes bearing the 4-bromo-2-[(2-hydroxyethyl)imino]methyl]phenol ligand. The first result corresponds to the structure of the free ligand reported by Thakur *et al.*

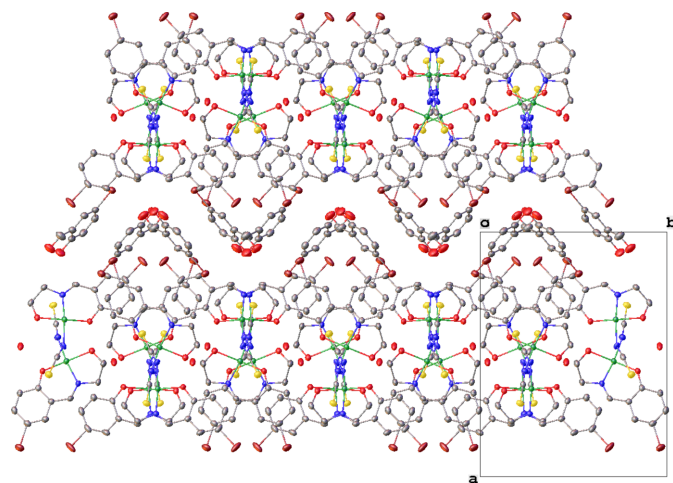


Figure 2
Partial packing diagram for the title compound along [001].

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O4—H4 $\cdots$ O7	0.82	1.75	2.562 (4)	174
O2—H2 $\cdots$ O3	0.82	1.84	2.647 (3)	169
O7—H7A $\cdots$ O1	0.85	1.88	2.709 (4)	163
O7—H7B $\cdots$ S2 ⁱ	0.85	2.64	3.290 (3)	135
O5—H5A $\cdots$ O6	0.82	1.94	2.655 (6)	146
C18—H18A $\cdots$ Br3 ⁱⁱ	0.97	3.32	3.856 (4)	117
C18—H18A $\cdots$ S1	0.97	2.98	3.801 (4)	143
C18—H18A $\cdots$ N3	0.97	3.22	3.785 (5)	119
C17—H17A $\cdots$ O5	0.97	2.73	3.368 (5)	124
C16—H16 $\cdots$ O6 ⁱⁱⁱ	0.93	2.52	3.376 (5)	153
C2—H2A $\cdots$ O2 ^{iv}	0.93	2.92	3.726 (4)	146
C2—H2A $\cdots$ O7	0.93	3.08	3.548 (5)	113
C9—H9A $\cdots$ N4 ^v	0.97	3.20	3.851 (4)	126
C9—H9B $\cdots$ O3 ^v	0.97	3.03	3.613 (5)	120
C9—H9B $\cdots$ N4	0.97	3.20	3.700 (5)	114
C11—H11 $\cdots$ S2 ^v	0.93	3.11	3.709 (4)	124
C8—H8A $\cdots$ S1 ^{vi}	0.97	3.29	3.881 (3)	121
C8—H8A $\cdots$ O3 ^v	0.97	3.07	3.773 (5)	130
C8—H8B $\cdots$ S2 ⁱⁱⁱ	0.97	3.30	3.784 (4)	113
C8—H8B $\cdots$ O7 ^{vi}	0.97	2.96	3.739 (6)	138
C14—H14 $\cdots$ O6 ⁱⁱⁱ	0.93	3.12	3.827 (6)	134
C12—H12 $\cdots$ S2 ^v	0.93	2.93	3.616 (5)	131
C22—H22 $\cdots$ O6 ⁱⁱⁱ	0.93	2.97	3.847 (6)	158
C27—H27 $\cdots$ Br2 ^{vii}	0.93	3.04	3.949 (6)	166

Symmetry codes: (i) $-x + 1, -y + 2, -z + 1$; (ii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iv) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (v) $-x + 1, -y + 1, -z + 1$; (vi) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (vii) $-x, -y + 1, -z + 1$.

2024 (refcode YAWNOB01). 23 of the remaining hits correspond to coordination complexes of first-row transition metals. Only one second-row transition metal complex is noted, namely a cadmium complex (AWOHIE; Yu *et al.*, 2011). Half of the hits correspond to mononuclear complexes in which two molecules of the tridentate ligand chelate the metal ion including refcodes BAVGUD, BAVROI (Abbasi *et al.*, 2017); HEDKUX (Liang *et al.*, 2006); HEDKUX01 (Chumakov *et al.*, 2007); HEDKUX02 (Zabierowski *et al.*, 2013); MIWSEQ (De *et al.*, 2001), among others. Polynuclear complexes are also reported, including a dinuclear copper complex (FOQKAY; Thakurta *et al.*, 2009a,b), a tetranuclear copper complex (LICWAW; Yoshida *et al.*), and a tetranuclear iron complex (EBUWII; Oshio *et al.*, 2004).

5. Synthesis and crystallization

The Schiff base ligand HL was prepared by adding 2.5 g (13.5 mmol) of 5-bromosalicylaldehyde and 0.8 g (13.5 mmol) of 2-aminoethanol, along with a few drops of glacial acetic acid, to 20 mL of ethanol in a flask. The mixture was refluxed, then evaporated to dryness using a rotary evaporator, giving a light-brown oil in 80% yield. This oil was dissolved in ethanol (100 mL) to give a 0.108 mol l⁻¹ ligand solution.

For the complex synthesis, 0.17 g (1 mmol) of copper(II) chloride dihydrate and 0.19 g (2 mmol) of potassium thiocyanate were dissolved in 10 mL of methanol and stirred under reflux for 30 minutes, giving a brown solution. Then, 9.2 mL of the ligand solution was added dropwise to the metal solution. After refluxing for 1 h, a green precipitate formed, which was filtered, washed with methanol, and dried, giving

0.14 g of product. Green single crystals suitable for X-ray diffraction were obtained after two weeks.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

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Table 3

Experimental details.

Crystal data	
Chemical formula	[Cu(C ₉ H ₉ BrNO ₂)(NCS)]·0.5C ₇ H ₅ BrO ₂ ·0.5H ₂ O
M_r	948.44
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	18.4400 (5), 13.7346 (3), 13.6402 (3)
β (°)	103.136 (1)
V (Å ³)	3364.20 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	5.00
Crystal size (mm)	0.2 × 0.2 × 0.2
Data collection	
Diffractometer	Bruker D8 Venture Equipped with PhotonII Detector
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	60122, 6909, 5316
R_{int}	0.070
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.034, 0.081, 1.01
No. of reflections	6909
No. of parameters	412
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.62, -0.61

Computer programs: *APEX* and *SAINT* (Bruker, 2014), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2018/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

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Crystal structure of a copper complex containing the 4-bromo-2-[(2-hydroxyethyl)imino]methyl}phenol base Schiff ligand

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Computing details

(4-Bromo-2-[(2-hydroxyethyl)imino]methyl}phenololato- $\kappa^3 O, N, O'$)(thiocyanato- κN)copper(II)–5-bromo-2-hydroxybenzaldehyde–water (2/1/1)

Crystal data

[Cu(C₉H₉BrNO₂)(NCS)]·0.5C₇H₅BrO₂·0.5H₂O
 M_r = 948.44
 Monoclinic, $P2_1/c$
 a = 18.4400 (5) Å
 b = 13.7346 (3) Å
 c = 13.6402 (3) Å
 β = 103.136 (1)°
 V = 3364.20 (14) Å³
 Z = 4

$F(000)$ = 1864
 D_x = 1.873 Mg m⁻³
 Mo $K\alpha$ radiation, λ = 0.71073 Å
 Cell parameters from 60122 reflections
 θ = 1.9–26.4°
 μ = 5.00 mm⁻¹
 T = 296 K
 Prism, green
 0.2 × 0.2 × 0.2 mm

Data collection

Bruker D8 Venture Equipped with PhotonII
 Detector
 diffractometer
 profile data from ω -scans
 Absorption correction: multi-scan
 (SADABS; Krause *et al.*, 2015)

6909 independent reflections
 5316 reflections with $I > 2\sigma(I)$
 R_{int} = 0.070
 θ_{max} = 26.4°, θ_{min} = 1.9°
 h = -23→23
 k = -17→17
 l = -17→15

60122 measured reflections

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)]$ = 0.034
 $wR(F^2)$ = 0.081
 S = 1.01
 6909 reflections
 412 parameters
 0 restraints

Hydrogen site location: mixed
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 4.7568P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}}$ = 0.001
 $\Delta\rho_{\text{max}}$ = 0.62 e Å⁻³
 $\Delta\rho_{\text{min}}$ = -0.61 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu2	0.35837 (2)	0.72579 (3)	0.41858 (3)	0.03257 (10)
Cu1	0.52874 (2)	0.71541 (3)	0.30893 (3)	0.03342 (10)
Br3	−0.17062 (2)	0.47243 (3)	0.42161 (4)	0.06458 (14)
Br1	0.88193 (3)	0.96575 (4)	0.53387 (5)	0.07697 (16)
Br2	0.11977 (3)	0.30742 (4)	0.22273 (4)	0.08438 (19)
S1	0.29927 (5)	0.78586 (7)	0.09224 (7)	0.0424 (2)
S2	0.58322 (6)	0.80940 (7)	0.62694 (8)	0.0485 (2)
O3	0.36588 (12)	0.59043 (15)	0.38633 (18)	0.0365 (5)
O4	0.35052 (13)	0.87140 (16)	0.41724 (18)	0.0386 (5)
H4	0.388208	0.901725	0.414008	0.058*
O1	0.56911 (13)	0.84305 (15)	0.33838 (18)	0.0376 (5)
O2	0.48631 (13)	0.57876 (16)	0.31199 (19)	0.0399 (6)
H2	0.446357	0.578002	0.328833	0.060*
N4	0.46559 (16)	0.73030 (19)	0.4895 (2)	0.0353 (6)
N1	0.61991 (15)	0.65156 (18)	0.3749 (2)	0.0340 (6)
N2	0.25666 (15)	0.7357 (2)	0.3433 (2)	0.0338 (6)
N3	0.43073 (16)	0.7612 (2)	0.2376 (2)	0.0397 (7)
O7	0.46760 (17)	0.96055 (19)	0.3943 (3)	0.0702 (10)
H7A	0.502551	0.934333	0.372361	0.105*
H7B	0.481742	1.019032	0.407084	0.105*
O5	0.0839 (2)	0.7473 (3)	0.4295 (3)	0.0837 (11)
H5A	0.093367	0.779032	0.481825	0.126*
C19	0.37653 (18)	0.7704 (2)	0.1765 (2)	0.0305 (7)
C1	0.63814 (19)	0.8652 (2)	0.3819 (2)	0.0336 (7)
C6	0.69389 (18)	0.7959 (2)	0.4217 (2)	0.0339 (7)
C7	0.68112 (18)	0.6930 (2)	0.4166 (3)	0.0354 (7)
H7	0.720737	0.653006	0.446251	0.042*
C10	0.30904 (19)	0.5317 (2)	0.3505 (2)	0.0345 (7)
C18	0.2894 (2)	0.9050 (2)	0.3404 (3)	0.0412 (8)
H18A	0.302755	0.905842	0.275613	0.049*
H18B	0.275062	0.970303	0.355478	0.049*
C17	0.2264 (2)	0.8346 (2)	0.3389 (3)	0.0424 (8)
H17A	0.204564	0.846199	0.396192	0.051*
H17B	0.188028	0.843103	0.277853	0.051*
O6	0.0669 (2)	0.8034 (3)	0.6092 (3)	0.0965 (12)
C15	0.23619 (19)	0.5640 (3)	0.3092 (3)	0.0376 (8)
C16	0.21500 (19)	0.6653 (3)	0.3038 (3)	0.0385 (8)
H16	0.166982	0.680496	0.268639	0.046*
C2	0.6592 (2)	0.9643 (2)	0.3897 (3)	0.0399 (8)

H2A	0.623644	1.011294	0.363949	0.048*
C20	0.5114 (2)	0.7642 (2)	0.5457 (3)	0.0385 (8)
C5	0.7662 (2)	0.8277 (3)	0.4681 (3)	0.0426 (8)
H5	0.802604	0.782312	0.495451	0.051*
C9	0.5384 (2)	0.5164 (3)	0.3777 (3)	0.0470 (9)
H9A	0.528637	0.448840	0.358511	0.056*
H9B	0.533871	0.524355	0.446689	0.056*
C11	0.3229 (2)	0.4310 (3)	0.3530 (3)	0.0450 (9)
H11	0.370795	0.408127	0.379841	0.054*
C8	0.6145 (2)	0.5446 (2)	0.3682 (3)	0.0452 (9)
H8A	0.651666	0.515002	0.421687	0.054*
H8B	0.622919	0.522553	0.304106	0.054*
C3	0.7297 (2)	0.9935 (3)	0.4337 (3)	0.0446 (9)
H3	0.741978	1.059317	0.437188	0.054*
C4	0.7831 (2)	0.9240 (3)	0.4734 (3)	0.0461 (9)
C14	0.1799 (2)	0.4965 (3)	0.2705 (3)	0.0495 (10)
H14	0.131914	0.517809	0.241540	0.059*
C24	−0.0898 (2)	0.5597 (3)	0.4264 (3)	0.0462 (9)
C13	0.1959 (2)	0.3992 (3)	0.2754 (3)	0.0521 (10)
C12	0.2665 (2)	0.3655 (3)	0.3162 (3)	0.0518 (10)
H12	0.276256	0.299005	0.319076	0.062*
C25	−0.0669 (2)	0.6183 (3)	0.5070 (3)	0.0488 (9)
H25	−0.090676	0.615755	0.560213	0.059*
C26	−0.0078 (2)	0.6828 (3)	0.5107 (3)	0.0511 (10)
C21	0.0275 (2)	0.6859 (3)	0.4308 (4)	0.0555 (11)
C23	−0.0552 (2)	0.5622 (3)	0.3469 (3)	0.0559 (11)
H23	−0.071640	0.521800	0.291633	0.067*
C22	0.0035 (2)	0.6245 (3)	0.3492 (4)	0.0611 (12)
H22	0.027240	0.625415	0.295851	0.073*
C27	0.0160 (3)	0.7449 (4)	0.5975 (4)	0.0801 (15)
H27	−0.009566	0.739894	0.648683	0.096*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu2	0.0329 (2)	0.0294 (2)	0.0334 (2)	−0.00098 (16)	0.00347 (17)	−0.00299 (17)
Cu1	0.0343 (2)	0.0288 (2)	0.0348 (2)	0.00313 (16)	0.00299 (17)	0.00019 (17)
Br3	0.0459 (2)	0.0590 (3)	0.0845 (3)	−0.0085 (2)	0.0057 (2)	−0.0066 (2)
Br1	0.0490 (3)	0.0770 (3)	0.0974 (4)	−0.0180 (2)	0.0010 (2)	−0.0192 (3)
Br2	0.0856 (4)	0.0834 (3)	0.0933 (4)	−0.0563 (3)	0.0395 (3)	−0.0404 (3)
S1	0.0369 (5)	0.0564 (6)	0.0320 (5)	0.0095 (4)	0.0035 (4)	−0.0040 (4)
S2	0.0446 (5)	0.0535 (6)	0.0441 (5)	−0.0064 (4)	0.0029 (4)	−0.0037 (4)
O3	0.0330 (12)	0.0300 (11)	0.0454 (14)	−0.0018 (9)	0.0066 (10)	−0.0056 (10)
O4	0.0419 (14)	0.0305 (12)	0.0446 (14)	−0.0008 (10)	0.0124 (11)	−0.0016 (11)
O1	0.0366 (13)	0.0297 (11)	0.0434 (14)	0.0029 (10)	0.0026 (11)	−0.0007 (10)
O2	0.0391 (14)	0.0338 (12)	0.0475 (15)	−0.0012 (11)	0.0111 (11)	−0.0019 (11)
N4	0.0459 (17)	0.0333 (15)	0.0233 (14)	−0.0138 (13)	0.0007 (13)	−0.0050 (12)
N1	0.0369 (16)	0.0277 (13)	0.0372 (16)	0.0042 (11)	0.0075 (12)	0.0027 (12)

N2	0.0313 (15)	0.0385 (15)	0.0319 (15)	0.0023 (12)	0.0078 (12)	−0.0005 (12)
N3	0.0369 (16)	0.0424 (16)	0.0379 (17)	0.0038 (13)	0.0044 (14)	0.0008 (13)
O7	0.0595 (19)	0.0332 (14)	0.131 (3)	0.0022 (13)	0.048 (2)	0.0022 (17)
O5	0.063 (2)	0.084 (3)	0.112 (3)	−0.0221 (18)	0.038 (2)	0.012 (2)
C19	0.0388 (19)	0.0279 (15)	0.0267 (16)	0.0020 (13)	0.0114 (15)	−0.0019 (13)
C1	0.0390 (19)	0.0350 (17)	0.0289 (17)	0.0013 (14)	0.0123 (15)	0.0002 (14)
C6	0.0345 (18)	0.0370 (17)	0.0307 (17)	0.0011 (14)	0.0086 (14)	−0.0002 (14)
C7	0.0327 (18)	0.0366 (17)	0.0365 (19)	0.0083 (14)	0.0069 (15)	0.0067 (15)
C10	0.0414 (19)	0.0331 (17)	0.0327 (18)	−0.0085 (14)	0.0161 (15)	−0.0065 (14)
C18	0.051 (2)	0.0343 (18)	0.041 (2)	0.0109 (16)	0.0169 (17)	0.0069 (16)
C17	0.037 (2)	0.0419 (19)	0.048 (2)	0.0089 (15)	0.0089 (16)	0.0030 (17)
O6	0.078 (3)	0.102 (3)	0.099 (3)	−0.041 (2)	−0.001 (2)	−0.012 (2)
C15	0.0362 (19)	0.0426 (19)	0.0358 (19)	−0.0062 (15)	0.0117 (15)	−0.0088 (15)
C16	0.0281 (17)	0.050 (2)	0.0364 (19)	−0.0015 (15)	0.0051 (14)	−0.0060 (16)
C2	0.049 (2)	0.0314 (17)	0.041 (2)	0.0011 (15)	0.0136 (17)	−0.0020 (15)
C20	0.044 (2)	0.0340 (17)	0.043 (2)	0.0084 (16)	0.0222 (18)	0.0087 (16)
C5	0.0369 (19)	0.047 (2)	0.044 (2)	0.0020 (16)	0.0080 (16)	−0.0002 (17)
C9	0.048 (2)	0.0324 (18)	0.063 (3)	0.0054 (16)	0.0182 (19)	0.0097 (18)
C11	0.052 (2)	0.0371 (19)	0.046 (2)	−0.0023 (16)	0.0118 (18)	−0.0015 (16)
C8	0.046 (2)	0.0290 (17)	0.061 (3)	0.0065 (15)	0.0132 (18)	0.0037 (17)
C3	0.057 (2)	0.0362 (19)	0.042 (2)	−0.0074 (17)	0.0153 (18)	−0.0066 (16)
C4	0.040 (2)	0.053 (2)	0.044 (2)	−0.0118 (17)	0.0093 (17)	−0.0111 (18)
C14	0.037 (2)	0.060 (2)	0.053 (2)	−0.0152 (18)	0.0127 (18)	−0.018 (2)
C24	0.037 (2)	0.046 (2)	0.053 (2)	0.0041 (16)	0.0040 (18)	0.0042 (18)
C13	0.060 (3)	0.052 (2)	0.051 (2)	−0.027 (2)	0.025 (2)	−0.0200 (19)
C12	0.073 (3)	0.0360 (19)	0.052 (2)	−0.0137 (19)	0.024 (2)	−0.0082 (18)
C25	0.040 (2)	0.058 (2)	0.047 (2)	−0.0010 (18)	0.0089 (17)	0.0069 (19)
C26	0.041 (2)	0.057 (2)	0.053 (2)	−0.0026 (18)	0.0039 (18)	0.005 (2)
C21	0.041 (2)	0.056 (2)	0.070 (3)	0.0054 (19)	0.013 (2)	0.017 (2)
C23	0.060 (3)	0.052 (2)	0.054 (3)	0.012 (2)	0.009 (2)	0.001 (2)
C22	0.060 (3)	0.065 (3)	0.066 (3)	0.019 (2)	0.031 (2)	0.019 (2)
C27	0.069 (3)	0.093 (4)	0.074 (4)	−0.030 (3)	0.008 (3)	−0.006 (3)

Geometric parameters (Å, °)

Cu1—O1	1.911 (2)	C18—H18B	0.9700
Cu1—O2	2.038 (2)	C18—C17	1.508 (5)
Cu1—N1	1.928 (3)	C17—H17A	0.9700
Cu1—N3	1.952 (3)	C17—H17B	0.9700
Cu2—O3	1.923 (2)	O6—C27	1.217 (5)
Cu2—O4	2.005 (2)	C15—C16	1.442 (5)
Cu2—N4	1.995 (3)	C15—C14	1.403 (5)
Cu2—N2	1.927 (3)	C16—H16	0.9300
Br3—C24	1.903 (4)	C2—H2A	0.9300
Br1—C4	1.910 (4)	C2—C3	1.363 (5)
Br2—C13	1.902 (4)	C5—H5	0.9300
S1—C19	1.629 (3)	C5—C4	1.358 (5)
S2—C20	1.643 (4)	C9—H9A	0.9700

O3—C10	1.325 (4)	C9—H9B	0.9700
O4—H4	0.8200	C9—C8	1.490 (5)
O4—C18	1.430 (4)	C11—H11	0.9300
O1—C1	1.312 (4)	C11—C12	1.380 (5)
O2—H2	0.8200	C8—H8A	0.9700
O2—C9	1.437 (4)	C8—H8B	0.9700
N4—C20	1.106 (4)	C3—H3	0.9300
N1—C7	1.277 (4)	C3—C4	1.390 (5)
N1—C8	1.474 (4)	C14—H14	0.9300
N2—C17	1.464 (4)	C14—C13	1.367 (6)
N2—C16	1.276 (4)	C24—C25	1.350 (5)
N3—C19	1.153 (4)	C24—C23	1.378 (6)
O7—H7A	0.8502	C13—C12	1.375 (6)
O7—H7B	0.8501	C12—H12	0.9300
O5—H5A	0.8200	C25—H25	0.9300
O5—C21	1.343 (5)	C25—C26	1.396 (5)
C1—C6	1.416 (5)	C26—C21	1.391 (6)
C1—C2	1.412 (5)	C26—C27	1.445 (7)
C6—C7	1.431 (5)	C21—C22	1.387 (6)
C6—C5	1.409 (5)	C23—H23	0.9300
C7—H7	0.9300	C23—C22	1.375 (6)
C10—C15	1.405 (5)	C22—H22	0.9300
C10—C11	1.406 (5)	C27—H27	0.9300
C18—H18A	0.9700		
O1—Cu1—O2	166.82 (10)	C15—C16—H16	117.3
N3—Cu1—O2	89.45 (11)	C1—C2—H2A	118.8
O1—Cu1—N1	93.58 (10)	C3—C2—C1	122.4 (3)
O1—Cu1—N3	94.69 (11)	C3—C2—H2A	118.8
N1—Cu1—O2	82.51 (10)	N4—C20—S2	176.2 (3)
N1—Cu1—N3	171.73 (12)	C6—C5—H5	119.7
O3—Cu2—O4	166.23 (10)	C4—C5—C6	120.6 (3)
O3—Cu2—N4	91.49 (10)	C4—C5—H5	119.7
O3—Cu2—N2	93.35 (11)	O2—C9—H9A	110.2
N4—Cu2—O4	92.01 (10)	O2—C9—H9B	110.2
N2—Cu2—O4	82.24 (11)	O2—C9—C8	107.5 (3)
N2—Cu2—N4	173.38 (11)	H9A—C9—H9B	108.5
C10—O3—Cu2	125.5 (2)	C8—C9—H9A	110.2
Cu2—O4—H4	116.5	C8—C9—H9B	110.2
C18—O4—Cu2	111.8 (2)	C10—C11—H11	119.5
C18—O4—H4	109.5	C12—C11—C10	121.0 (4)
C1—O1—Cu1	126.8 (2)	C12—C11—H11	119.5
Cu1—O2—H2	113.0	N1—C8—C9	107.8 (3)
C9—O2—Cu1	110.9 (2)	N1—C8—H8A	110.1
C9—O2—H2	109.5	N1—C8—H8B	110.1
C20—N4—Cu2	150.0 (3)	C9—C8—H8A	110.1
C7—N1—Cu1	126.4 (2)	C9—C8—H8B	110.1
C7—N1—C8	120.9 (3)	H8A—C8—H8B	108.5

C8—N1—Cu1	112.6 (2)	C2—C3—H3	120.3
C17—N2—Cu2	113.8 (2)	C2—C3—C4	119.3 (3)
C16—N2—Cu2	126.2 (2)	C4—C3—H3	120.3
C16—N2—C17	119.9 (3)	C5—C4—Br1	120.0 (3)
C19—N3—Cu1	161.4 (3)	C5—C4—C3	121.0 (3)
H7A—O7—H7B	104.5	C3—C4—Br1	119.0 (3)
C21—O5—H5A	109.5	C15—C14—H14	120.2
N3—C19—S1	178.3 (3)	C13—C14—C15	119.6 (4)
O1—C1—C6	124.2 (3)	C13—C14—H14	120.2
O1—C1—C2	118.7 (3)	C25—C24—Br3	120.1 (3)
C2—C1—C6	117.1 (3)	C25—C24—C23	120.7 (4)
C1—C6—C7	123.2 (3)	C23—C24—Br3	119.2 (3)
C5—C6—C1	119.6 (3)	C14—C13—Br2	119.8 (3)
C5—C6—C7	117.2 (3)	C14—C13—C12	121.5 (3)
N1—C7—C6	125.5 (3)	C12—C13—Br2	118.7 (3)
N1—C7—H7	117.2	C11—C12—H12	120.2
C6—C7—H7	117.2	C13—C12—C11	119.6 (4)
O3—C10—C15	124.0 (3)	C13—C12—H12	120.2
O3—C10—C11	117.7 (3)	C24—C25—H25	119.9
C15—C10—C11	118.2 (3)	C24—C25—C26	120.3 (4)
O4—C18—H18A	110.5	C26—C25—H25	119.9
O4—C18—H18B	110.5	C25—C26—C27	119.6 (4)
O4—C18—C17	106.2 (3)	C21—C26—C25	119.4 (4)
H18A—C18—H18B	108.7	C21—C26—C27	120.9 (4)
C17—C18—H18A	110.5	O5—C21—C26	122.1 (4)
C17—C18—H18B	110.5	O5—C21—C22	118.5 (4)
N2—C17—C18	108.0 (3)	C22—C21—C26	119.3 (4)
N2—C17—H17A	110.1	C24—C23—H23	120.0
N2—C17—H17B	110.1	C22—C23—C24	120.1 (4)
C18—C17—H17A	110.1	C22—C23—H23	120.0
C18—C17—H17B	110.1	C21—C22—H22	119.9
H17A—C17—H17B	108.4	C23—C22—C21	120.1 (4)
C10—C15—C16	123.3 (3)	C23—C22—H22	119.9
C14—C15—C10	120.0 (3)	O6—C27—C26	125.4 (5)
C14—C15—C16	116.7 (3)	O6—C27—H27	117.3
N2—C16—C15	125.4 (3)	C26—C27—H27	117.3
N2—C16—H16	117.3		
Cu2—O3—C10—C15	15.2 (4)	C10—C15—C14—C13	1.7 (6)
Cu2—O3—C10—C11	−165.6 (2)	C10—C11—C12—C13	0.8 (6)
Cu2—O4—C18—C17	39.3 (3)	C17—N2—C16—C15	−175.2 (3)
Cu2—N2—C17—C18	31.8 (3)	C15—C10—C11—C12	−0.2 (5)
Cu2—N2—C16—C15	0.8 (5)	C15—C14—C13—Br2	−179.9 (3)
Cu1—O1—C1—C6	−5.0 (5)	C15—C14—C13—C12	−1.0 (6)
Cu1—O1—C1—C2	174.7 (2)	C16—N2—C17—C18	−151.7 (3)
Cu1—O2—C9—C8	−35.9 (3)	C16—C15—C14—C13	−178.5 (3)
Cu1—N1—C7—C6	−0.5 (5)	C2—C1—C6—C7	−178.3 (3)
Cu1—N1—C8—C9	−37.5 (4)	C2—C1—C6—C5	1.1 (5)

Br3—C24—C25—C26	−179.8 (3)	C2—C3—C4—Br1	179.5 (3)
Br3—C24—C23—C22	−179.7 (3)	C2—C3—C4—C5	0.5 (6)
Br2—C13—C12—C11	178.7 (3)	C5—C6—C7—N1	−177.9 (3)
O3—C10—C15—C16	−1.6 (5)	C11—C10—C15—C16	179.1 (3)
O3—C10—C15—C14	178.2 (3)	C11—C10—C15—C14	−1.1 (5)
O3—C10—C11—C12	−179.5 (3)	C8—N1—C7—C6	175.9 (3)
O4—C18—C17—N2	−45.1 (4)	C14—C15—C16—N2	173.2 (3)
O1—C1—C6—C7	1.5 (5)	C14—C13—C12—C11	−0.2 (6)
O1—C1—C6—C5	−179.2 (3)	C24—C25—C26—C21	−0.1 (6)
O1—C1—C2—C3	−180.0 (3)	C24—C25—C26—C27	−179.9 (4)
O2—C9—C8—N1	46.9 (4)	C24—C23—C22—C21	−0.9 (6)
O5—C21—C22—C23	−178.5 (4)	C25—C24—C23—C22	0.4 (6)
C1—C6—C7—N1	1.5 (5)	C25—C26—C21—O5	179.1 (4)
C1—C6—C5—C4	−1.2 (5)	C25—C26—C21—C22	−0.4 (6)
C1—C2—C3—C4	−0.6 (5)	C25—C26—C27—O6	179.7 (5)
C6—C1—C2—C3	−0.2 (5)	C26—C21—C22—C23	0.9 (6)
C6—C5—C4—Br1	−178.6 (3)	C21—C26—C27—O6	−0.1 (8)
C6—C5—C4—C3	0.4 (6)	C23—C24—C25—C26	0.2 (6)
C7—N1—C8—C9	145.7 (3)	C27—C26—C21—O5	−1.1 (7)
C7—C6—C5—C4	178.2 (3)	C27—C26—C21—C22	179.4 (4)
C10—C15—C16—N2	−7.0 (6)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O4—H4 $\cdots$ O7	0.82	1.75	2.562 (4)	174
O2—H2 $\cdots$ O3	0.82	1.84	2.647 (3)	169
O7—H7A $\cdots$ O1	0.85	1.88	2.709 (4)	163
O7—H7B $\cdots$ S2 ⁱ	0.85	2.64	3.290 (3)	135
O5—H5A $\cdots$ O6	0.82	1.94	2.655 (6)	146
C18—H18A $\cdots$ Br3 ⁱⁱ	0.97	3.32	3.856 (4)	117
C18—H18A $\cdots$ S1	0.97	2.98	3.801 (4)	143
C18—H18A $\cdots$ N3	0.97	3.22	3.785 (5)	119
C17—H17A $\cdots$ O5	0.97	2.73	3.368 (5)	124
C16—H16 $\cdots$ O6 ⁱⁱⁱ	0.93	2.52	3.376 (5)	153
C2—H2A $\cdots$ O2 ^{iv}	0.93	2.92	3.726 (4)	146
C2—H2A $\cdots$ O7	0.93	3.08	3.548 (5)	113
C9—H9A $\cdots$ N4 ^v	0.97	3.20	3.851 (4)	126
C9—H9B $\cdots$ O3 ^v	0.97	3.03	3.613 (5)	120
C9—H9B $\cdots$ N4	0.97	3.20	3.700 (5)	114
C11—H11 $\cdots$ S2 ^v	0.93	3.11	3.709 (4)	124
C8—H8A $\cdots$ S1 ^{vi}	0.97	3.29	3.881 (3)	121
C8—H8A $\cdots$ O3 ^v	0.97	3.07	3.773 (5)	130
C8—H8B $\cdots$ S2 ⁱⁱⁱ	0.97	3.30	3.784 (4)	113
C8—H8B $\cdots$ O7 ^{vi}	0.97	2.96	3.739 (6)	138
C14—H14 $\cdots$ O6 ⁱⁱⁱ	0.93	3.12	3.827 (6)	134
C12—H12 $\cdots$ S2 ^v	0.93	2.93	3.616 (5)	131

C22—H22 $\cdots$ O6 ⁱⁱⁱ	0.93	2.97	3.847 (6)	158
C27—H27 $\cdots$ Br2 ^{vii}	0.93	3.04	3.949 (6)	166

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x, y+1/2, -z+1/2$; (iii) $x, -y+3/2, z-1/2$; (iv) $-x+1, y+1/2, -z+1/2$; (v) $-x+1, -y+1, -z+1$; (vi) $-x+1, y-1/2, -z+1/2$; (vii) $-x, -y+1, -z+1$.