

Tetra- μ -acetato- κ^8 O:O'-bis[(2-amino-1,3-benzothiazole- κ N)copper(II)] butanol disolvate

Yi-Feng Sun,* Jing-Rong Lu and Ze-Bao Zheng

Department of Chemistry, Taishan University, 271021 Taian, Shandong, People's Republic of China

Correspondence e-mail: sunyf50@hotmail.com

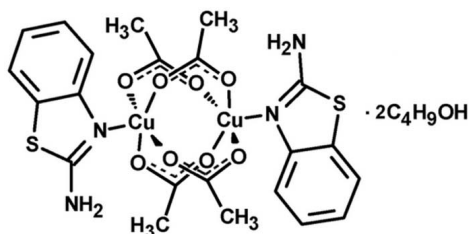
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.020$ Å; R factor = 0.084; wR factor = 0.249; data-to-parameter ratio = 15.5.

The title compound, $[\text{Cu}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_7\text{H}_6\text{N}_2\text{S})_2] \cdot 2\text{C}_4\text{H}_{10}\text{O}$, exhibits distorted square-pyramidal coordination geometry around each Cu^{II} atom, with the basal plane comprising O atoms from four bridging acetate ligands and the apical position occupied by the thiazole N atom of 2-amino-benzothiazole. The dinuclear complex lies on a crystallographic centre of inversion and has a $\text{Cu} \cdots \text{Cu}$ distance of 2.6850 (14) Å. Complexes are linked into one-dimensional chains by a combination of intermolecular $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds involving the butanol solvent molecules.

Related literature

For general literature concerning applications of benzothiazole compounds, see: Rana *et al.* (2007); Kim *et al.* (2005); Costa *et al.* (2006); Wu *et al.* (2003); Marko *et al.* (1996). Similar coordination geometry has been observed for a related dinuclear Cu^{II} complex containing 2-amino-5-chloropyridine (Liu *et al.*, 2003). Other reported 2-aminobenzothiazole complexes with Cu^{II} contain either six-coordinate (Sieroń & Bukowska-Strzyżewska, 1999, 2000; Sieroń, 2007) or four-coordinate Cu^{II} (Usman *et al.*, 2003).



Experimental

Crystal data

$[\text{Cu}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_7\text{H}_6\text{N}_2\text{S})_2] \cdot 2\text{C}_4\text{H}_{10}\text{O}$	$\beta = 91.242$ (7) $^\circ$
$M_r = 811.89$	$V = 1911.8$ (6) Å ³
Monoclinic, $P2_1/c$	$Z = 2$
$a = 10.0998$ (17) Å	Mo $K\alpha$ radiation
$b = 11.465$ (2) Å	$\mu = 1.28$ mm ⁻¹
$c = 16.514$ (3) Å	$T = 273$ (2) K
	$0.32 \times 0.21 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	20441 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3353 independent reflections
$T_{\text{min}} = 0.686$, $T_{\text{max}} = 0.862$	3000 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.084$	5 restraints
$wR(F^2) = 0.249$	H-atom parameters constrained
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.97$ e Å ⁻³
3353 reflections	$\Delta\rho_{\text{min}} = -1.00$ e Å ⁻³
217 parameters	

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1A} \cdots \text{O2}$	0.90	2.23	3.002 (11)	144
$\text{N1}-\text{H1B} \cdots \text{O5}^{\text{i}}$	0.90	1.99	2.850 (12)	159
$\text{O5}-\text{H5} \cdots \text{O1}^{\text{ii}}$	0.85	2.04	2.885 (10)	180

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2187).

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supplementary materials

Acta Cryst. (2007). E63, m1881 [doi:10.1107/S1600536807027948]

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Comment

Interest in the study of compounds containing the benzothiazole group has increased on account of their broad spectrum of biological activities (Rana *et al.*, 2007), and also their potential applications in the areas of sensors (Kim *et al.*, 2005), non-linear optics, laser dyes, electroluminescent devices (Costa *et al.*, 2006) and as chelating agents (Usman *et al.*, 2003). A large number of copper compounds with diverse ligands have been synthesized and studied as potential therapeutic agents (Wu *et al.*, 2003) and catalysts (Marko *et al.*, 1996).

In the title compound (Fig. 1), each Cu^{II} ion is five-coordinated, with a coordination geometry that is best described as distorted square pyramidal. Four O atoms of bridging acetate ligands construct the basal plane of the square pyramid. The 2-aminobenzothiazole molecules are coordinated to Cu^{II} through their thiazole N atom and occupy the axial position. Four acetate ligands act as bridges to connect the two Cu^{II} centers into a dinuclear complex across a crystallographic centre of inversion. All the geometrical parameters lie within expected ranges.

The complexes are linked into one-dimensional chains by a combination of intermolecular O—H \cdots O and N—H \cdots O hydrogen bonds involving the butane solvent molecules (Fig. 2).

Experimental

A solution of 2-aminobenzothiazole (2 mmol) in butanol (10 ml) was added dropwise to Cu(OAc)₂·2H₂O (1 mmol in 10 ml of butanol) with stirring. The resulting solution was left to stand at room temperature and black crystals were obtained after several days.

Refinement

All H atoms were visible in a difference Fourier map. The methyl H atoms were constrained to an ideal geometry with C—H distances of 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. The hydroxyl H atoms were treated as riding atoms with O—H distances normalized to 0.85 Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. All other H atoms were placed geometrically and constrained to ride on their parent atoms with C—H distances of 0.93–0.97 Å and N—H distances of 0.90 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C/N})$. The C—C bonds and 1,3-distances in the butanol molecule were restrained to 1.50 (1) and 2.45 (2) Å, respectively.

Figures

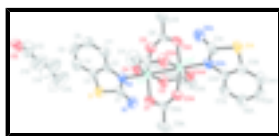


Fig. 1. The molecular structure of the title compound showing displacement ellipsoids at the 50% probability level. H atoms are omitted.

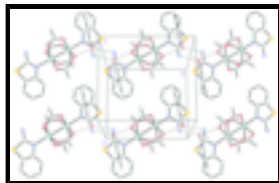


Fig. 2. The chain structure in the title compound formed *via* hydrogen bonds (dashed lines). H atoms are omitted.

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Crystal data

$[\text{Cu}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_7\text{H}_6\text{N}_2\text{S})_2] \cdot 2\text{C}_4\text{H}_{10}\text{O}$

$M_r = 811.89$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.0998$ (17) Å

$b = 11.465$ (2) Å

$c = 16.514$ (3) Å

$\beta = 91.242$ (7)°

$V = 1911.8$ (6) Å³

$Z = 2$

$F_{000} = 844$

$D_x = 1.410$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 8320 reflections

$\theta = 2.2$ – 25.7 °

$\mu = 1.28$ mm⁻¹

$T = 273$ (2) K

Block, black

$0.32 \times 0.21 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.686$, $T_{\max} = 0.862$

20441 measured reflections

3353 independent reflections

3000 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 25.0$ °

$\theta_{\min} = 2.0$ °

$h = -12 \rightarrow 11$

$k = -13 \rightarrow 13$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.084$

$wR(F^2) = 0.249$

$S = 1.15$

3353 reflections

217 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 21.2639P]$

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

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.97$ e Å⁻³

$\Delta\rho_{\min} = -1.00$ e Å⁻³

5 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.93063 (11)	0.90286 (8)	0.98271 (6)	0.0418 (4)
S1	0.7442 (3)	0.5375 (2)	0.9140 (2)	0.0706 (8)
O1	1.0552 (7)	0.8231 (6)	1.0602 (4)	0.0611 (18)
O2	1.0644 (7)	0.8793 (6)	0.8988 (4)	0.0616 (18)
O3	0.8344 (7)	1.0149 (6)	0.9128 (4)	0.0620 (18)
O4	0.8287 (7)	0.9547 (6)	1.0754 (4)	0.0624 (18)
O5	0.0282 (10)	0.3940 (7)	0.8688 (6)	0.088 (3)
H5	0.0037	0.3299	0.8896	0.131*
N1	0.9877 (9)	0.6283 (8)	0.9201 (7)	0.074 (3)
H1A	1.0440	0.6891	0.9240	0.111*
H1B	1.0208	0.5571	0.9100	0.111*
N2	0.8107 (7)	0.7502 (6)	0.9518 (5)	0.0491 (18)
C1	0.8607 (10)	0.6475 (8)	0.9296 (6)	0.050 (2)
C2	0.6731 (9)	0.7435 (8)	0.9545 (6)	0.051 (2)
C3	0.6197 (11)	0.6342 (9)	0.9356 (7)	0.060 (3)
C4	0.4832 (12)	0.6167 (12)	0.9369 (9)	0.085 (4)
H4A	0.4472	0.5442	0.9239	0.102*
C5	0.4020 (12)	0.7085 (12)	0.9576 (10)	0.092 (4)
H5A	0.3108	0.6977	0.9596	0.110*
C6	0.4558 (12)	0.8154 (11)	0.9753 (9)	0.081 (4)
H6A	0.3999	0.8771	0.9875	0.097*
C7	0.5897 (11)	0.8339 (9)	0.9754 (7)	0.063 (3)
H7A	0.6243	0.9065	0.9893	0.076*
C8	0.8556 (10)	1.1205 (8)	0.9024 (6)	0.051 (2)
C9	0.7718 (14)	1.1838 (11)	0.8413 (9)	0.093 (5)
H9A	0.7082	1.1310	0.8176	0.139*
H9B	0.8268	1.2147	0.7998	0.139*
H9C	0.7263	1.2466	0.8673	0.139*
C10	0.8488 (10)	1.0437 (9)	1.1167 (6)	0.054 (2)
C11	0.7607 (14)	1.0663 (13)	1.1869 (8)	0.089 (4)

supplementary materials

H11A	0.6998	1.0027	1.1923	0.134*
H11B	0.7121	1.1373	1.1777	0.134*
H11C	0.8136	1.0736	1.2356	0.134*
C12	0.0949 (18)	0.3587 (19)	0.7984 (11)	0.129 (6)
H12A	0.0785	0.4125	0.7540	0.154*
H12B	0.0684	0.2809	0.7817	0.154*
C13	0.236 (2)	0.361 (3)	0.8257 (12)	0.220 (15)
H13A	0.2570	0.4376	0.8482	0.264*
H13B	0.2509	0.3038	0.8678	0.264*
C14	0.325 (2)	0.337 (3)	0.7572 (13)	0.30 (3)
H14A	0.3449	0.4091	0.7293	0.359*
H14B	0.2805	0.2851	0.7189	0.359*
C15	0.449 (2)	0.282 (3)	0.7884 (18)	0.27 (2)
H15A	0.5061	0.2671	0.7442	0.410*
H15B	0.4279	0.2104	0.8151	0.410*
H15C	0.4918	0.3342	0.8262	0.410*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0566 (7)	0.0260 (5)	0.0427 (6)	-0.0058 (4)	-0.0026 (4)	-0.0019 (4)
S1	0.0751 (18)	0.0379 (13)	0.099 (2)	-0.0159 (12)	0.0041 (15)	-0.0175 (13)
O1	0.079 (5)	0.036 (3)	0.067 (4)	-0.003 (3)	-0.016 (4)	0.011 (3)
O2	0.078 (5)	0.049 (4)	0.059 (4)	-0.011 (3)	0.015 (3)	-0.013 (3)
O3	0.070 (4)	0.046 (4)	0.069 (4)	-0.005 (3)	-0.020 (4)	0.009 (3)
O4	0.068 (4)	0.057 (4)	0.063 (4)	-0.016 (3)	0.011 (3)	-0.006 (4)
O5	0.127 (7)	0.041 (4)	0.095 (6)	0.004 (4)	0.022 (6)	-0.004 (4)
N1	0.065 (6)	0.039 (5)	0.117 (8)	-0.001 (4)	0.014 (5)	-0.014 (5)
N2	0.052 (4)	0.032 (4)	0.063 (5)	-0.004 (3)	-0.002 (4)	-0.001 (3)
C1	0.064 (6)	0.032 (4)	0.054 (5)	-0.004 (4)	0.003 (4)	-0.006 (4)
C2	0.055 (5)	0.038 (5)	0.058 (5)	-0.007 (4)	-0.006 (4)	0.007 (4)
C3	0.068 (6)	0.042 (5)	0.069 (6)	-0.016 (5)	-0.005 (5)	0.006 (5)
C4	0.072 (8)	0.068 (8)	0.112 (11)	-0.027 (7)	-0.015 (7)	0.002 (7)
C5	0.056 (7)	0.080 (9)	0.139 (13)	-0.008 (6)	-0.004 (7)	0.014 (9)
C6	0.067 (7)	0.054 (7)	0.123 (11)	0.000 (6)	0.002 (7)	0.003 (7)
C7	0.072 (7)	0.033 (5)	0.086 (8)	-0.003 (5)	-0.001 (6)	-0.007 (5)
C8	0.062 (6)	0.039 (5)	0.051 (5)	0.001 (4)	-0.006 (4)	0.011 (4)
C9	0.110 (10)	0.059 (7)	0.107 (10)	0.002 (7)	-0.048 (8)	0.026 (7)
C10	0.061 (6)	0.054 (6)	0.048 (5)	-0.003 (5)	0.003 (4)	-0.008 (4)
C11	0.101 (10)	0.103 (10)	0.066 (7)	-0.016 (8)	0.030 (7)	-0.013 (7)
C12	0.145 (16)	0.131 (16)	0.111 (13)	-0.019 (13)	0.019 (12)	-0.008 (12)
C13	0.20 (3)	0.31 (4)	0.15 (2)	0.05 (3)	0.02 (2)	0.09 (3)
C14	0.38 (5)	0.37 (6)	0.14 (2)	0.19 (5)	-0.06 (3)	-0.06 (3)
C15	0.14 (2)	0.44 (6)	0.24 (4)	0.03 (3)	0.00 (2)	0.12 (4)

Geometric parameters (\AA , $^\circ$)

Cu1—O4	1.956 (7)	C6—C7	1.369 (15)
Cu1—O3	1.970 (7)	C6—H6A	0.930

Cu1—O2	1.975 (7)	C7—H7A	0.930
Cu1—O1	1.996 (7)	C8—O1 ⁱ	1.260 (11)
Cu1—N2	2.183 (7)	C8—C9	1.491 (13)
Cu1—Cu1 ⁱ	2.6862 (19)	C9—H9A	0.960
S1—C3	1.720 (12)	C9—H9B	0.960
S1—C1	1.740 (9)	C9—H9C	0.960
O1—C8 ⁱ	1.260 (11)	C10—O2 ⁱ	1.274 (12)
O2—C10 ⁱ	1.274 (12)	C10—C11	1.499 (15)
O3—C8	1.242 (11)	C11—H11A	0.960
O4—C10	1.241 (12)	C11—H11B	0.960
O5—C12	1.415 (18)	C11—H11C	0.960
O5—H5	0.850	C12—C13	1.487 (10)
N1—C1	1.314 (12)	C12—H12A	0.970
N1—H1A	0.900	C12—H12B	0.970
N1—H1B	0.900	C13—C14	1.482 (10)
N2—C1	1.336 (11)	C13—H13A	0.970
N2—C2	1.394 (12)	C13—H13B	0.970
C2—C7	1.383 (14)	C14—C15	1.483 (10)
C2—C3	1.397 (13)	C14—H14A	0.970
C3—C4	1.394 (15)	C14—H14B	0.970
C4—C5	1.383 (19)	C15—H15A	0.960
C4—H4A	0.930	C15—H15B	0.960
C5—C6	1.370 (18)	C15—H15C	0.960
C5—H5A	0.930		
O4—Cu1—O3	90.0 (3)	C6—C7—C2	119.4 (10)
O4—Cu1—O2	166.1 (3)	C6—C7—H7A	120.3
O3—Cu1—O2	90.8 (3)	C2—C7—H7A	120.3
O4—Cu1—O1	88.4 (3)	O3—C8—O1 ⁱ	123.8 (8)
O3—Cu1—O1	166.1 (3)	O3—C8—C9	118.1 (9)
O2—Cu1—O1	87.4 (3)	O1 ⁱ —C8—C9	118.1 (9)
O4—Cu1—N2	97.4 (3)	C8—C9—H9A	109.5
O3—Cu1—N2	97.0 (3)	C8—C9—H9B	109.5
O2—Cu1—N2	96.4 (3)	H9A—C9—H9B	109.5
O1—Cu1—N2	97.0 (3)	C8—C9—H9C	109.5
O4—Cu1—Cu1 ⁱ	82.1 (2)	H9A—C9—H9C	109.5
O3—Cu1—Cu1 ⁱ	80.4 (2)	H9B—C9—H9C	109.5
O2—Cu1—Cu1 ⁱ	84.3 (2)	O4—C10—O2 ⁱ	124.3 (9)
O1—Cu1—Cu1 ⁱ	85.7 (2)	O4—C10—C11	118.3 (10)
N2—Cu1—Cu1 ⁱ	177.3 (2)	O2 ⁱ —C10—C11	117.3 (9)
C3—S1—C1	89.8 (5)	C10—C11—H11A	109.5
C8 ⁱ —O1—Cu1	120.9 (6)	C10—C11—H11B	109.5
C10 ⁱ —O2—Cu1	122.0 (6)	H11A—C11—H11B	109.5
C8—O3—Cu1	129.2 (6)	C10—C11—H11C	109.5
C10—O4—Cu1	126.7 (7)	H11A—C11—H11C	109.5
C12—O5—H5	103.5	H11B—C11—H11C	109.5
C1—N1—H1A	118.6	O5—C12—C13	102.5 (14)

supplementary materials

C1—N1—H1B	122.8	O5—C12—H12A	111.3
H1A—N1—H1B	118.6	C13—C12—H12A	111.3
C1—N2—C2	110.1 (8)	O5—C12—H12B	111.3
C1—N2—Cu1	124.0 (6)	C13—C12—H12B	111.3
C2—N2—Cu1	125.8 (6)	H12A—C12—H12B	109.2
N1—C1—N2	123.8 (8)	C14—C13—C12	110.8 (14)
N1—C1—S1	121.3 (7)	C14—C13—H13A	109.5
N2—C1—S1	114.9 (7)	C12—C13—H13A	109.5
C7—C2—N2	125.4 (8)	C14—C13—H13B	109.5
C7—C2—C3	119.6 (9)	C12—C13—H13B	109.5
N2—C2—C3	115.0 (9)	H13A—C13—H13B	108.1
C4—C3—C2	120.2 (11)	C13—C14—C15	109.4 (14)
C4—C3—S1	129.6 (9)	C13—C14—H14A	109.8
C2—C3—S1	110.1 (8)	C15—C14—H14A	109.8
C5—C4—C3	119.1 (11)	C13—C14—H14B	109.8
C5—C4—H4A	120.5	C15—C14—H14B	109.8
C3—C4—H4A	120.5	H14A—C14—H14B	108.2
C6—C5—C4	120.0 (11)	C14—C15—H15A	109.5
C6—C5—H5A	120.0	C14—C15—H15B	109.5
C4—C5—H5A	120.0	H15A—C15—H15B	109.5
C7—C6—C5	121.7 (12)	C14—C15—H15C	109.5
C7—C6—H6A	119.1	H15A—C15—H15C	109.5
C5—C6—H6A	119.1	H15B—C15—H15C	109.5
O4—Cu1—O1—C8 ⁱ	-80.3 (8)	C2—N2—C1—N1	178.5 (10)
O3—Cu1—O1—C8 ⁱ	3.3 (18)	Cu1—N2—C1—N1	-3.5 (14)
O2—Cu1—O1—C8 ⁱ	86.3 (8)	C2—N2—C1—S1	-1.7 (10)
N2—Cu1—O1—C8 ⁱ	-177.6 (8)	Cu1—N2—C1—S1	176.4 (4)
Cu1 ⁱ —Cu1—O1—C8 ⁱ	1.9 (8)	C3—S1—C1—N1	-178.7 (10)
O4—Cu1—O2—C10 ⁱ	-20.0 (18)	C3—S1—C1—N2	1.5 (8)
O3—Cu1—O2—C10 ⁱ	73.2 (8)	C1—N2—C2—C7	179.9 (10)
O1—Cu1—O2—C10 ⁱ	-92.9 (8)	Cu1—N2—C2—C7	1.9 (14)
N2—Cu1—O2—C10 ⁱ	170.3 (8)	C1—N2—C2—C3	1.0 (12)
Cu1 ⁱ —Cu1—O2—C10 ⁱ	-7.0 (8)	Cu1—N2—C2—C3	-177.0 (7)
O4—Cu1—O3—C8	83.1 (9)	C7—C2—C3—C4	0.7 (16)
O2—Cu1—O3—C8	-82.9 (9)	N2—C2—C3—C4	179.6 (10)
O1—Cu1—O3—C8	0(2)	C7—C2—C3—S1	-178.8 (8)
N2—Cu1—O3—C8	-179.4 (9)	N2—C2—C3—S1	0.1 (11)
Cu1 ⁱ —Cu1—O3—C8	1.2 (9)	C1—S1—C3—C4	179.7 (12)
O3—Cu1—O4—C10	-79.9 (9)	C1—S1—C3—C2	-0.8 (8)
O2—Cu1—O4—C10	13.4 (19)	C2—C3—C4—C5	-0.5 (19)
O1—Cu1—O4—C10	86.3 (9)	S1—C3—C4—C5	179.0 (11)
N2—Cu1—O4—C10	-176.9 (9)	C3—C4—C5—C6	1(2)
Cu1 ⁱ —Cu1—O4—C10	0.4 (8)	C4—C5—C6—C7	-2(2)
O4—Cu1—N2—C1	-138.9 (8)	C5—C6—C7—C2	2(2)
O3—Cu1—N2—C1	130.2 (8)	N2—C2—C7—C6	179.7 (11)
O2—Cu1—N2—C1	38.6 (8)	C3—C2—C7—C6	-1.5 (17)

O1—Cu1—N2—C1	-49.6 (8)	Cu1—O3—C8—O1 ⁱ	-3.1 (16)
Cu1 ⁱ —Cu1—N2—C1	143 (4)	Cu1—O3—C8—C9	176.2 (9)
O4—Cu1—N2—C2	38.9 (8)	Cu1—O4—C10—O2 ⁱ	5.0 (16)
O3—Cu1—N2—C2	-52.0 (8)	Cu1—O4—C10—C11	-178.6 (8)
O2—Cu1—N2—C2	-143.6 (7)	O5—C12—C13—C14	-175 (2)
O1—Cu1—N2—C2	128.2 (7)	C12—C13—C14—C15	-152 (3)
Cu1 ⁱ —Cu1—N2—C2	-40 (5)		

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

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>
N1—H1A \cdots O2	0.90	2.23	3.002 (11)	144
N1—H1B \cdots O5 ⁱⁱ	0.90	1.99	2.850 (12)	159
O5—H5 \cdots O1 ⁱⁱⁱ	0.85	2.04	2.885 (10)	180

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

Fig. 1

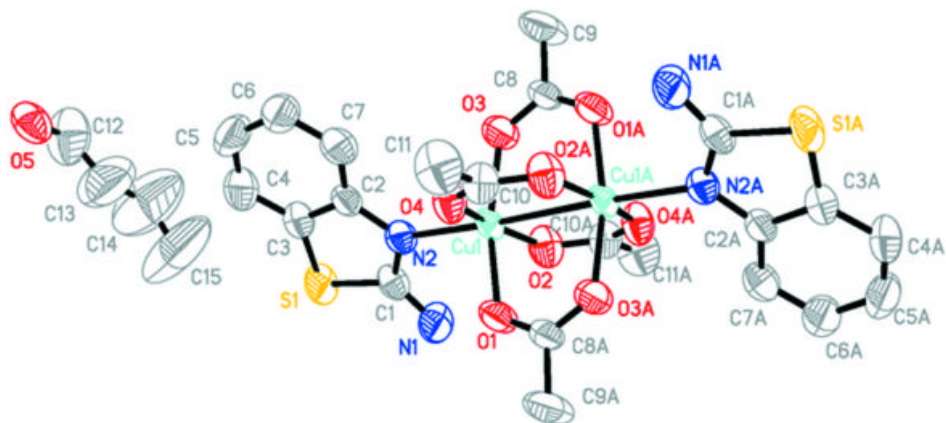


Fig. 2

