

Bis[μ -4-chloro- N' -[(E)-1-(5-chloro-2-oxidophenyl)ethylidene]benzohydrazidato]bis[pyridinecopper(II)]

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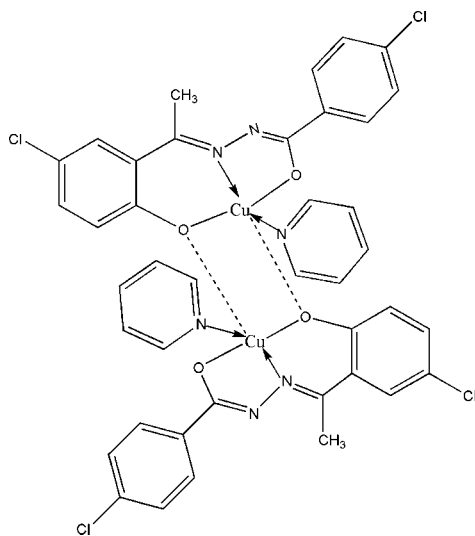
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.026; wR factor = 0.064; data-to-parameter ratio = 13.4.

The crystal structure of the title complex, $[\text{Cu}_2(\text{C}_{15}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}_2)_2(\text{C}_5\text{H}_5\text{N})_2]$, features centrosymmetric dimers. The Cu^{II} ion is pentacoordinated in a quadratic pyramidal mode. The quadratic plane is formed by the O, O', N -tridentate ligand and a pyridine molecule. The fifth coordination site is occupied by the O atom of another ligand showing a significantly longer Cu—O bond.

Related literature

For further details of the chemistry of the title compound, see: Salem (1998). For a related structure, see: Chang (2008).



Experimental

Crystal data

 $[\text{Cu}_2(\text{C}_{15}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}_2)_2(\text{C}_5\text{H}_5\text{N})_2]$
 $M_r = 927.58$

 Monoclinic, $P2_1/c$
 $a = 11.913$ (2) Å

 $b = 8.0783$ (16) Å

 $c = 19.997$ (4) Å

 $\beta = 95.66$ (3)°

 $V = 1915.1$ (7) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 1.44$ mm⁻¹
 $T = 298$ K

 $0.28 \times 0.25 \times 0.18$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

 $T_{\text{min}} = 0.688$, $T_{\text{max}} = 0.782$

9685 measured reflections

3411 independent reflections

 2976 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.064$
 $S = 1.02$

3411 reflections

255 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³
Table 1

Selected bond lengths (Å).

Cu1—O2	1.8824 (14)	Cu1—N3	2.0275 (17)
Cu1—O1	1.9209 (15)	Cu1—O2 ¹	2.6055 (16)
Cu1—N2	1.9475 (17)		

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

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: SHELXTL (Sheldrick, 2008); 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: BT5720).

References

- Bruker (2005). APEX2 and SAINT Bruker AXS Inc., Madison, Wisconsin, USA.
 Chang, J.-G. (2008). *Acta Cryst.* **E64**, o198.
 Salem, A. A. (1998). *Microchem. J.* **60**, 51–66.
 Sheldrick, G. M. (2003). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2011). E67, m1886 [doi:10.1107/S1600536811050720]

Bis{ μ -4-chloro-*N'*-[(*E*)-1-(5-chloro-2-oxidophenyl)ethylidene]benzohydrazidato}bis[pyridinecopper(II)]

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Comment

The chemistry of aroylhydrazones has gained a special attraction due to their coordination abilities to metal ions (Salem, 1998). As an extension of work on the structural characterization of aroylhydrazone derivatives (Chang, 2008), the title compound, (I), was synthesized and its crystal structure is reported here.

The new complex, (I), the Cu II ion exhibits a distorted *trans*-Cu₂O₂ square-planar geometry arising from the O, O, N-tridentate ligand and a pyridine molecule. (see Fig. 1). Two molecules form a weak-bridged dimer with weak Cu—O interactions. (see Fig. 2).

Experimental

The ligand 4-chloro-*N'*-[(1*E*)-1-(5-chloro-2-hydroxyphenyl)ethylidene]benzohydrazide was prepared by the reaction of 1-(5-chloro-2-hydroxyphenyl)ethanone and 4-chlorobenzohydrazide in a molar ratio of 1:1 under reflux in ethanol for 4 h. The white precipitate was collected, washed several times with ethanol and dried *in vacuo* (yield 83%). A DMF solution (5 ml) of the ligand (0.25 mmol, 0.081 g) was mixed with a methanol solution (5 ml) of Cu(OAc)₂ (0.25 mmol, 0.05 g). The mixture was stirred at 298 K for 4 h and then filtered. A blue precipitate was produced after about 10 d. A pyridine mixture (5 ml) was used to dissolve the precipitate at 330 K. Blue block-shaped crystals were obtained after one month (yield 25%).

Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms, with *C*—*H*(methyl) = 0.96 Å, *C*—*H*(aromatic) = 0.93 Å and with *U*_{iso}(H) = 1.5*U*_{eq}(*C*_{methyl}) and 1.2*U*_{eq}(*C*_{aromatic}).

Figures

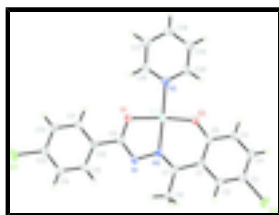


Fig. 1. The molecular structure of compound (I). Displacement ellipsoids are drawn at the 30% probability level.

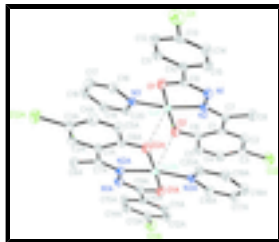


Fig. 2. The dimeric structure of the title compound. H atoms have been omitted for clarity. [Dashed lines show Cu—O weak interactions].

Bis{ μ -4-chloro-*N'*-[(*E*)-1-(5-chloro-2-oxidophenyl)ethylidene]benzohydrazidato}bis[pyridinecopper(II)]

Crystal data

[Cu₂(C₁₅H₁₀Cl₂N₂O₂)₂(C₅H₅N)₂]

$M_r = 927.58$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.913$ (2) Å

$b = 8.0783$ (16) Å

$c = 19.997$ (4) Å

$\beta = 95.66$ (3)°

$V = 1915.1$ (7) Å³

$Z = 2$

$F(000) = 940$

$D_x = 1.609$ Mg m⁻³

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

Cell parameters from 4831 reflections

$\theta = 2.5$ – 27.9 °

$\mu = 1.44$ mm⁻¹

$T = 298$ K

Block, blue

$0.28 \times 0.25 \times 0.18$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)

$T_{\min} = 0.688$, $T_{\max} = 0.782$

9685 measured reflections

3411 independent reflections

2976 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 25.1$ °, $\theta_{\min} = 2.1$ °

$h = -13 \rightarrow 14$

$k = -9 \rightarrow 9$

$l = -22 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.064$

$S = 1.02$

3411 reflections

255 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 1.1862P]$

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

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

$\Delta\rho_{\max} = 0.22$ e Å⁻³

$\Delta\rho_{\min} = -0.23$ e Å⁻³

0 restraints

Extinction correction: *SHELXL97* (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0011 (3)

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_{iso}^*/U_{eq}
Cu1	0.09353 (2)	0.14880 (3)	0.017875 (12)	0.03476 (10)
Cl1	0.49728 (6)	0.08946 (11)	0.39268 (3)	0.0677 (2)
Cl2	0.23787 (6)	-0.18478 (10)	-0.29800 (3)	0.0638 (2)
C1	0.19626 (16)	-0.0360 (3)	-0.10969 (10)	0.0334 (4)
C2	0.24154 (18)	-0.0995 (3)	-0.16734 (10)	0.0389 (5)
H2	0.3158	-0.1368	-0.1638	0.047*
C13	0.43005 (18)	0.0975 (3)	0.31108 (10)	0.0425 (5)
C6	0.08344 (17)	0.0220 (3)	-0.11671 (10)	0.0349 (5)
C9	0.26194 (17)	0.1119 (3)	0.11379 (10)	0.0355 (5)
C10	0.32367 (17)	0.1101 (3)	0.18203 (10)	0.0350 (5)
C7	0.26861 (16)	-0.0379 (3)	-0.04553 (10)	0.0340 (4)
C3	0.17827 (19)	-0.1071 (3)	-0.22803 (10)	0.0425 (5)
C14	0.47580 (18)	0.0123 (3)	0.26053 (11)	0.0496 (6)
H14	0.5416	-0.0489	0.2696	0.060*
C12	0.33351 (19)	0.1898 (3)	0.29860 (11)	0.0439 (5)
H12	0.3045	0.2480	0.3331	0.053*
C16	-0.04746 (19)	0.3803 (3)	0.08770 (11)	0.0442 (5)
H16	0.0054	0.3580	0.1239	0.053*
C11	0.27997 (18)	0.1952 (3)	0.23412 (11)	0.0410 (5)
H11	0.2140	0.2564	0.2254	0.049*
C15	0.42230 (18)	0.0195 (3)	0.19631 (11)	0.0457 (6)
H15	0.4527	-0.0373	0.1619	0.055*
C5	0.02189 (19)	0.0115 (3)	-0.18052 (11)	0.0447 (5)
H5	-0.0523	0.0491	-0.1857	0.054*
C17	-0.1338 (2)	0.4880 (3)	0.09677 (13)	0.0531 (6)
H17	-0.1394	0.5365	0.1385	0.064*
C4	0.0679 (2)	-0.0524 (3)	-0.23534 (11)	0.0472 (6)
H4	0.0254	-0.0587	-0.2768	0.057*
C8	0.38055 (18)	-0.1255 (3)	-0.04096 (11)	0.0470 (6)

supplementary materials

H8A	0.4069	-0.1434	0.0054	0.071*
H8B	0.4341	-0.0589	-0.0617	0.071*
H8C	0.3720	-0.2301	-0.0637	0.071*
C19	-0.20175 (18)	0.4478 (3)	-0.01709 (12)	0.0477 (6)
H19	-0.2536	0.4692	-0.0540	0.057*
C18	-0.21219 (19)	0.5235 (3)	0.04330 (13)	0.0515 (6)
H18	-0.2709	0.5971	0.0481	0.062*
C20	-0.11366 (17)	0.3397 (3)	-0.02264 (11)	0.0401 (5)
H20	-0.1077	0.2882	-0.0637	0.048*
O2	0.02859 (12)	0.07997 (19)	-0.06722 (7)	0.0410 (4)
O1	0.16834 (12)	0.19404 (19)	0.10550 (7)	0.0408 (4)
N2	0.23464 (13)	0.0347 (2)	0.00719 (8)	0.0347 (4)
N1	0.30604 (14)	0.0264 (2)	0.06694 (8)	0.0389 (4)
N3	-0.03615 (14)	0.3059 (2)	0.02877 (8)	0.0346 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03293 (15)	0.03761 (16)	0.03257 (15)	0.00326 (11)	-0.00261 (10)	-0.00316 (11)
Cl1	0.0542 (4)	0.1114 (6)	0.0349 (3)	-0.0007 (4)	-0.0088 (3)	-0.0007 (3)
Cl2	0.0581 (4)	0.0963 (5)	0.0374 (3)	-0.0031 (4)	0.0078 (3)	-0.0195 (3)
C1	0.0347 (11)	0.0345 (11)	0.0307 (10)	-0.0046 (9)	0.0023 (8)	0.0004 (9)
C2	0.0362 (11)	0.0438 (13)	0.0367 (11)	-0.0040 (9)	0.0041 (9)	-0.0007 (10)
C13	0.0376 (12)	0.0582 (14)	0.0304 (11)	-0.0076 (10)	-0.0039 (9)	0.0000 (10)
C6	0.0381 (11)	0.0345 (11)	0.0316 (11)	-0.0027 (9)	0.0009 (9)	0.0012 (9)
C9	0.0335 (11)	0.0367 (12)	0.0353 (11)	-0.0029 (9)	-0.0015 (9)	-0.0004 (9)
C10	0.0330 (10)	0.0374 (12)	0.0341 (11)	-0.0039 (9)	0.0007 (9)	-0.0034 (9)
C7	0.0329 (10)	0.0356 (11)	0.0336 (11)	-0.0051 (9)	0.0030 (8)	0.0001 (9)
C3	0.0475 (13)	0.0507 (14)	0.0298 (11)	-0.0068 (10)	0.0068 (9)	-0.0030 (10)
C14	0.0348 (12)	0.0676 (17)	0.0445 (13)	0.0090 (11)	-0.0053 (10)	-0.0052 (12)
C12	0.0475 (13)	0.0497 (14)	0.0349 (12)	0.0007 (11)	0.0062 (10)	-0.0066 (10)
C16	0.0432 (12)	0.0481 (14)	0.0404 (13)	0.0050 (10)	-0.0004 (10)	-0.0030 (10)
C11	0.0378 (12)	0.0446 (13)	0.0400 (12)	0.0041 (10)	0.0008 (9)	-0.0037 (10)
C15	0.0376 (12)	0.0615 (15)	0.0372 (12)	0.0080 (11)	-0.0004 (9)	-0.0107 (11)
C5	0.0394 (12)	0.0570 (15)	0.0360 (12)	0.0051 (11)	-0.0046 (9)	0.0027 (11)
C17	0.0502 (14)	0.0567 (16)	0.0528 (14)	0.0076 (12)	0.0071 (11)	-0.0121 (12)
C4	0.0502 (14)	0.0619 (16)	0.0281 (11)	-0.0018 (11)	-0.0039 (10)	0.0026 (11)
C8	0.0367 (12)	0.0669 (16)	0.0366 (12)	0.0067 (11)	-0.0011 (9)	-0.0077 (11)
C19	0.0350 (12)	0.0509 (14)	0.0557 (15)	0.0033 (10)	-0.0034 (10)	0.0052 (12)
C18	0.0365 (12)	0.0491 (14)	0.0697 (17)	0.0082 (11)	0.0092 (11)	-0.0007 (13)
C20	0.0369 (11)	0.0402 (12)	0.0424 (12)	-0.0003 (9)	0.0003 (9)	0.0013 (10)
O2	0.0348 (8)	0.0523 (9)	0.0348 (8)	0.0070 (7)	-0.0024 (6)	-0.0080 (7)
O1	0.0370 (8)	0.0468 (9)	0.0370 (8)	0.0084 (7)	-0.0043 (6)	-0.0071 (7)
N2	0.0331 (9)	0.0400 (10)	0.0298 (9)	-0.0012 (7)	-0.0028 (7)	-0.0018 (8)
N1	0.0337 (9)	0.0506 (11)	0.0309 (9)	0.0029 (8)	-0.0041 (7)	-0.0044 (8)
N3	0.0324 (9)	0.0340 (9)	0.0370 (10)	-0.0005 (7)	0.0005 (7)	0.0014 (8)

Geometric parameters (Å, °)

Cu1—O2	1.8824 (14)	C14—C15	1.377 (3)
Cu1—O1	1.9209 (15)	C14—H14	0.9300
Cu1—N2	1.9475 (17)	C12—C11	1.382 (3)
Cu1—N3	2.0275 (17)	C12—H12	0.9300
Cu1—O2 ⁱ	2.6055 (16)	C16—N3	1.342 (3)
C11—C13	1.747 (2)	C16—C17	1.373 (3)
C12—C3	1.747 (2)	C16—H16	0.9300
C1—C2	1.417 (3)	C11—H11	0.9300
C1—C6	1.417 (3)	C15—H15	0.9300
C1—C7	1.473 (3)	C5—C4	1.374 (3)
C2—C3	1.365 (3)	C5—H5	0.9300
C2—H2	0.9300	C17—C18	1.379 (3)
C13—C12	1.373 (3)	C17—H17	0.9300
C13—C14	1.379 (3)	C4—H4	0.9300
C6—O2	1.324 (2)	C8—H8A	0.9600
C6—C5	1.410 (3)	C8—H8B	0.9600
C9—O1	1.294 (2)	C8—H8C	0.9600
C9—N1	1.315 (3)	C19—C18	1.370 (3)
C9—C10	1.485 (3)	C19—C20	1.378 (3)
C10—C15	1.390 (3)	C19—H19	0.9300
C10—C11	1.391 (3)	C18—H18	0.9300
C7—N2	1.305 (3)	C20—N3	1.341 (3)
C7—C8	1.504 (3)	C20—H20	0.9300
C3—C4	1.381 (3)	N2—N1	1.398 (2)
O2—Cu1—O1	173.26 (6)	C12—C11—C10	120.7 (2)
O2—Cu1—N2	92.48 (7)	C12—C11—H11	119.7
O1—Cu1—N2	82.09 (7)	C10—C11—H11	119.7
O2—Cu1—N3	91.86 (7)	C14—C15—C10	121.2 (2)
O1—Cu1—N3	94.17 (7)	C14—C15—H15	119.4
N2—Cu1—N3	169.49 (7)	C10—C15—H15	119.4
C2—C1—C6	118.22 (18)	C4—C5—C6	122.1 (2)
C2—C1—C7	117.89 (18)	C4—C5—H5	118.9
C6—C1—C7	123.88 (18)	C6—C5—H5	118.9
C3—C2—C1	121.2 (2)	C16—C17—C18	119.2 (2)
C3—C2—H2	119.4	C16—C17—H17	120.4
C1—C2—H2	119.4	C18—C17—H17	120.4
C12—C13—C14	121.5 (2)	C5—C4—C3	119.1 (2)
C12—C13—C11	119.26 (17)	C5—C4—H4	120.4
C14—C13—C11	119.23 (18)	C3—C4—H4	120.4
O2—C6—C5	116.53 (18)	C7—C8—H8A	109.5
O2—C6—C1	125.16 (18)	C7—C8—H8B	109.5
C5—C6—C1	118.24 (19)	H8A—C8—H8B	109.5
O1—C9—N1	125.31 (18)	C7—C8—H8C	109.5
O1—C9—C10	117.72 (18)	H8A—C8—H8C	109.5
N1—C9—C10	116.95 (18)	H8B—C8—H8C	109.5
C15—C10—C11	118.53 (19)	C18—C19—C20	119.3 (2)

supplementary materials

C15—C10—C9	121.73 (19)	C18—C19—H19	120.3
C11—C10—C9	119.68 (19)	C20—C19—H19	120.3
N2—C7—C1	119.81 (18)	C19—C18—C17	118.5 (2)
N2—C7—C8	120.39 (18)	C19—C18—H18	120.7
C1—C7—C8	119.80 (18)	C17—C18—H18	120.7
C2—C3—C4	121.1 (2)	N3—C20—C19	122.7 (2)
C2—C3—C12	119.72 (18)	N3—C20—H20	118.7
C4—C3—C12	119.21 (17)	C19—C20—H20	118.7
C15—C14—C13	118.8 (2)	C6—O2—Cu1	126.23 (13)
C15—C14—H14	120.6	C9—O1—Cu1	109.62 (13)
C13—C14—H14	120.6	C7—N2—N1	117.24 (16)
C13—C12—C11	119.2 (2)	C7—N2—Cu1	129.88 (14)
C13—C12—H12	120.4	N1—N2—Cu1	112.82 (12)
C11—C12—H12	120.4	C9—N1—N2	109.36 (16)
N3—C16—C17	122.8 (2)	C20—N3—C16	117.44 (18)
N3—C16—H16	118.6	C20—N3—Cu1	121.31 (14)
C17—C16—H16	118.6	C16—N3—Cu1	121.24 (14)
C6—C1—C2—C3	-0.8 (3)	C18—C19—C20—N3	-0.6 (3)
C7—C1—C2—C3	177.68 (19)	C5—C6—O2—Cu1	-166.71 (15)
C2—C1—C6—O2	177.84 (19)	C1—C6—O2—Cu1	16.1 (3)
C7—C1—C6—O2	-0.6 (3)	N2—Cu1—O2—C6	-17.20 (17)
C2—C1—C6—C5	0.7 (3)	N3—Cu1—O2—C6	153.23 (17)
C7—C1—C6—C5	-177.69 (19)	N1—C9—O1—Cu1	7.5 (3)
O1—C9—C10—C15	177.2 (2)	C10—C9—O1—Cu1	-170.89 (14)
N1—C9—C10—C15	-1.3 (3)	N2—Cu1—O1—C9	-7.65 (14)
O1—C9—C10—C11	0.0 (3)	N3—Cu1—O1—C9	-177.77 (14)
N1—C9—C10—C11	-178.6 (2)	C1—C7—N2—N1	178.98 (17)
C2—C1—C7—N2	172.96 (19)	C8—C7—N2—N1	-0.2 (3)
C6—C1—C7—N2	-8.6 (3)	C1—C7—N2—Cu1	1.9 (3)
C2—C1—C7—C8	-7.8 (3)	C8—C7—N2—Cu1	-177.31 (16)
C6—C1—C7—C8	170.6 (2)	O2—Cu1—N2—C7	8.57 (19)
C1—C2—C3—C4	0.3 (3)	O1—Cu1—N2—C7	-175.44 (19)
C1—C2—C3—C12	179.44 (17)	N3—Cu1—N2—C7	-105.7 (4)
C12—C13—C14—C15	-0.6 (4)	O2—Cu1—N2—N1	-168.59 (13)
C11—C13—C14—C15	-179.93 (19)	O1—Cu1—N2—N1	7.40 (13)
C14—C13—C12—C11	1.1 (4)	N3—Cu1—N2—N1	77.1 (4)
C11—C13—C12—C11	-179.58 (18)	O1—C9—N1—N2	-1.4 (3)
C13—C12—C11—C10	-0.8 (3)	C10—C9—N1—N2	176.98 (16)
C15—C10—C11—C12	0.0 (3)	C7—N2—N1—C9	176.99 (18)
C9—C10—C11—C12	177.4 (2)	Cu1—N2—N1—C9	-5.5 (2)
C13—C14—C15—C10	-0.2 (4)	C19—C20—N3—C16	0.8 (3)
C11—C10—C15—C14	0.5 (3)	C19—C20—N3—Cu1	-178.99 (17)
C9—C10—C15—C14	-176.8 (2)	C17—C16—N3—C20	-0.2 (3)
O2—C6—C5—C4	-177.5 (2)	C17—C16—N3—Cu1	179.63 (18)
C1—C6—C5—C4	-0.1 (3)	O2—Cu1—N3—C20	-10.18 (16)
N3—C16—C17—C18	-0.6 (4)	O1—Cu1—N3—C20	172.84 (16)
C6—C5—C4—C3	-0.5 (4)	N2—Cu1—N3—C20	104.2 (4)
C2—C3—C4—C5	0.4 (4)	O2—Cu1—N3—C16	170.03 (17)
C12—C3—C4—C5	-178.78 (19)	O1—Cu1—N3—C16	-6.95 (17)

C20—C19—C18—C17 -0.2 (4)

C16—C17—C18—C19 0.8 (4)

N2—Cu1—N3—C16

-75.6 (4)

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

Fig. 1

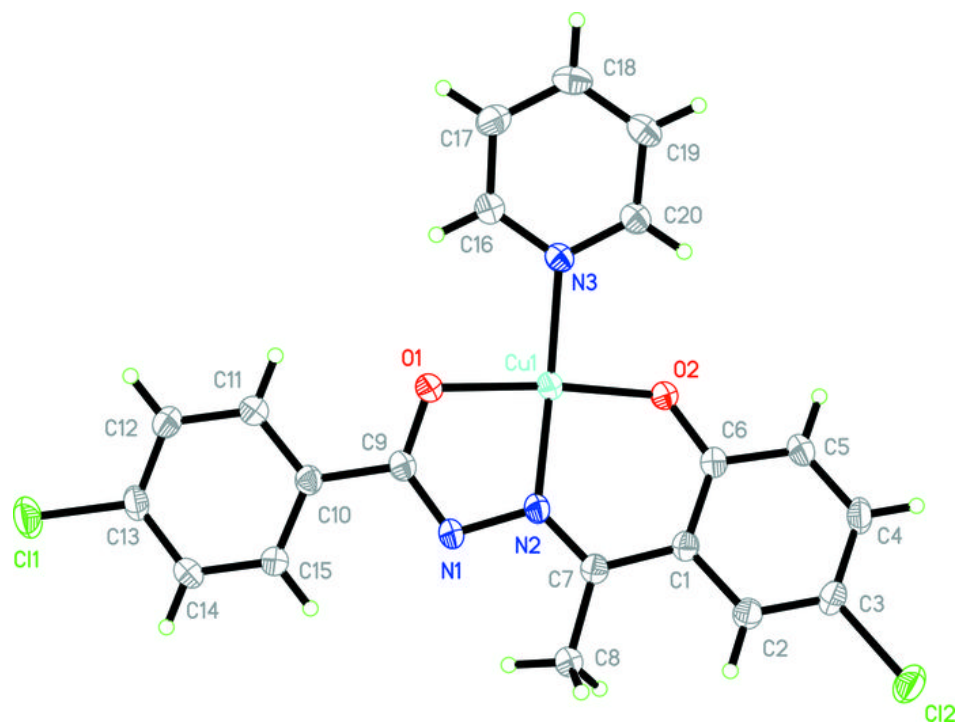


Fig. 2

