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Dibromido[2-hydroxy-*N'*-[phenyl(2-pyridyl)methylene]benzohydrazide]-copper(II)

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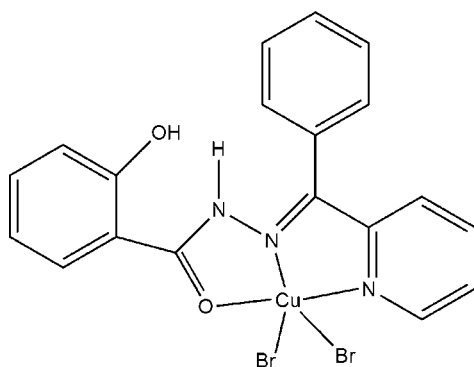
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.034; wR factor = 0.082; data-to-parameter ratio = 14.1.

In the title complex, $[\text{CuBr}_2(\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2)]$, the metal ion is coordinated by the *N,N',O*-tridentate 2-hydroxy-*N'*-[phenyl(2-pyridyl)methylene]benzohydrazide ligand and two bromide ions, resulting in a distorted CuN_2OBr_2 square-based pyramidal coordination geometry with one bromide ion in the apical site. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond occurs in the ligand. In the crystal, molecules are connected by intermolecular $\text{C}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{Br}$ and $\text{O}-\text{H}\cdots\text{Br}$ interactions.

Related literature

For the crystal structures of metal complexes with 2-benzoylpyridine salicyloylhydrazone, see: Sur *et al.* (1993); Seth & Chakraborty (1984); Dan *et al.* (1989).



Experimental

Crystal data

 $[\text{CuBr}_2(\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2)]$
 $M_r = 540.70$

Monoclinic, $P2_1/n$
 $a = 8.0779$ (11) Å
 $b = 16.302$ (2) Å
 $c = 15.0376$ (18) Å
 $\beta = 97.624$ (2)°
 $V = 1962.8$ (4) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.20$ mm⁻¹
 $T = 298$ K
 $0.23 \times 0.19 \times 0.15$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2003)
 $T_{\min} = 0.381$, $T_{\max} = 0.509$

8676 measured reflections
 3446 independent reflections
 2426 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.082$
 $S = 1.01$
 3446 reflections

244 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.94$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.58$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cu1—N2	1.966 (3)	Cu1—Br1	2.3469 (6)
Cu1—N3	2.018 (3)	Cu1—Br2	2.5931 (8)
Cu1—O1	2.083 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O2}$	0.86	1.92	2.574 (4)	131
$\text{O2}-\text{H2}\cdots\text{Br2}^{\text{i}}$	0.82	2.35	3.153 (3)	166
$\text{C11}-\text{H11}\cdots\text{O1}^{\text{ii}}$	0.93	2.58	3.503 (5)	170
$\text{C10}-\text{H10}\cdots\text{Br1}^{\text{ii}}$	0.93	2.81	3.575 (4)	141
$\text{C15}-\text{H15}\cdots\text{Br2}^{\text{iii}}$	0.93	2.82	3.742 (4)	171

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

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); 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: HB5107).

References

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supplementary materials

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Dibromido{2-hydroxy-*N'*-[phenyl(2-pyridyl)methylene]benzohydrazide}copper(II)

L.-Q. Kong, X.-P. Ju and D.-C. Li

Comment

A large number of salicyloylhydrazone complexes have been reported and studied. However, the metal complexes of 2-benzoylpyridine salicyloylhydrazone reported are limited to Zn (Sur *et al.*, 1993), Ni (Seth *et al.*, 1984) and (Dan *et al.*, 1989). Here, we have synthesized and will report a new 2-benzoylpyridine salicyloylhydrazone complex $\text{Cu}(\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2)\text{Br}_2$, which was characterized by X-ray diffraction and elemental analysis. The crystals suitable for X-ray diffraction studies were obtained by slow evaporation of the mother liquid. In this paper, we will display the crystal structure of the title complex.

The title complex (Fig.1), $\text{Cu}(\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2)\text{Br}_2$ is composed of a Cu atom, a 2-benzoylpyridine salicyloylhydrazone ligand molecule and two bromines. The ligand is bound to Cu atom by a carbonyl O, a pyridine N and a hydrazone N to form two juxtaposed five-membered chelate rings. Cu lies in a five-coordinated and square-pyramid coordination geometry with the $\text{O}_2\text{N}_2\text{Br}_2$ set of donor atoms. The equatorial coordination sites are occupied by O1, N2, N3, Br1 and the axial coordination atom is Br2 with the distance of $\text{Cu1}-\text{Br2}$ 2.5931 (8) Å. In the structure, there are intramolecular $\text{N}-\text{H}\cdots\text{O}$ interactions. Except that, the complex is linked into one-dimensional chain by intermolecular $\text{C}-\text{H}\cdots\text{Br}$ interactions, and the neighboring chains form a two-dimensional network structure *via* $\text{C}-\text{H}\cdots\text{Br}$ and $\text{O}-\text{H}\cdots\text{Br}$ interactions. A three-dimensional network structure is connected *via* $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ interactions between adjacent two-dimensional networks. So the complex is linked into a three-dimensional network structure *via* intermolecular $\text{C}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{Br}$ and $\text{O}-\text{H}\cdots\text{Br}$ interactions.

Experimental

$\text{CuBr}_2\cdot\text{H}_2\text{O}$ (0.25 mmol 0.065 g) was dissolved in 10 ml MeOH and a 10 ml 1,1-dichloroethane solution of 2-benzoylpyridine salicyloylhydrazone (0.25 mmol 0.080 g) was added dropwise to the former. The mixture was stirred for six hours until the solution color became dark green. The dark green solution was stirred for five hours and filtered. The filtrate layered with Et_2O to result in dark green blocks of (I) at room temperature. m.p. > 573 K. Elemental analysis for $\text{C}_{19}\text{H}_{15}\text{CuN}_3\text{O}_2\text{Br}_2$ calculated: C 42.21, H 2.80, N 7.77%; found: C 42.32, H 2.54, N 7.68%.

Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms with $\text{C}-\text{H} = 0.93$ Å, $\text{O}-\text{H} = 0.82$ Å and $\text{N}-\text{H} = 0.86$ Å [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$].

Figures

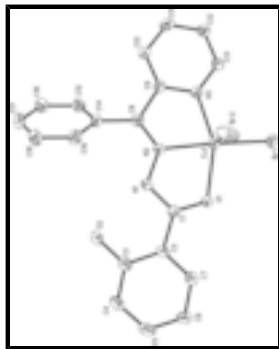


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids. C-bound H atoms have been omitted for clarity.

Dibromido{2-hydroxy-*N*'-[phenyl(2-pyridyl)methylene]benzohydrazide}copper(II)

Crystal data

[CuBr₂(C₁₉H₁₅N₃O₂)]

M_r = 540.70

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2yn

a = 8.0779 (11) Å

b = 16.302 (2) Å

c = 15.0376 (18) Å

β = 97.624 (2)°

V = 1962.8 (4) Å³

Z = 4

*F*₀₀₀ = 1060

D_x = 1.830 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 2246 reflections

θ = 2.5–25.1°

μ = 5.20 mm⁻¹

T = 298 K

Block, dark green

0.23 × 0.19 × 0.15 mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 298 K

ω scans

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

*T*_{min} = 0.381, *T*_{max} = 0.509

8676 measured reflections

3446 independent reflections

2426 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.034

θ_{max} = 25.0°

θ_{min} = 1.9°

h = -9→9

k = -17→19

l = -17→11

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.034

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.082$	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3446 reflections	$(\Delta/\sigma)_{\max} = 0.001$
244 parameters	$\Delta\rho_{\max} = 0.94 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.58 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.63317 (6)	0.70295 (3)	0.15437 (3)	0.03541 (16)
Br1	0.63665 (6)	0.81344 (2)	0.05459 (3)	0.04420 (15)
Br2	0.92790 (7)	0.70189 (3)	0.24686 (4)	0.06244 (18)
N1	0.5874 (4)	0.53300 (18)	0.1785 (2)	0.0390 (9)
H1	0.5667	0.4870	0.2027	0.047*
N2	0.5516 (4)	0.60651 (17)	0.2140 (2)	0.0349 (8)
N3	0.5009 (4)	0.75634 (19)	0.2434 (2)	0.0347 (8)
O1	0.6872 (4)	0.60672 (14)	0.07174 (18)	0.0389 (7)
O2	0.5854 (4)	0.37576 (16)	0.1626 (2)	0.0585 (10)
H2	0.5800	0.3273	0.1765	0.088*
C1	0.6586 (5)	0.5380 (2)	0.1020 (3)	0.0337 (10)
C2	0.7003 (5)	0.4611 (2)	0.0589 (3)	0.0341 (10)
C3	0.6649 (5)	0.3826 (2)	0.0886 (3)	0.0392 (11)
C4	0.7099 (6)	0.3140 (2)	0.0427 (3)	0.0481 (12)
H4	0.6868	0.2618	0.0625	0.058*
C5	0.7887 (6)	0.3237 (3)	-0.0321 (3)	0.0523 (13)
H5	0.8161	0.2774	-0.0631	0.063*
C6	0.8283 (6)	0.3997 (3)	-0.0622 (3)	0.0530 (13)
H6	0.8842	0.4053	-0.1121	0.064*
C7	0.7826 (6)	0.4679 (2)	-0.0164 (3)	0.0453 (12)
H7	0.8076	0.5198	-0.0365	0.054*
C8	0.4677 (5)	0.6152 (2)	0.2817 (3)	0.0347 (10)
C9	0.4411 (5)	0.7033 (2)	0.3016 (3)	0.0330 (10)
C10	0.3652 (5)	0.7305 (2)	0.3723 (3)	0.0382 (11)
H10	0.3305	0.6934	0.4131	0.046*

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C11	0.3407 (6)	0.8137 (2)	0.3823 (3)	0.0464 (12)
H11	0.2869	0.8332	0.4290	0.056*
C12	0.3965 (6)	0.8670 (2)	0.3226 (3)	0.0474 (12)
H12	0.3790	0.9232	0.3275	0.057*
C13	0.4786 (6)	0.8367 (2)	0.2553 (3)	0.0441 (12)
H13	0.5204	0.8735	0.2166	0.053*
C14	0.4049 (5)	0.5474 (2)	0.3330 (3)	0.0323 (10)
C15	0.2398 (5)	0.5486 (2)	0.3512 (3)	0.0410 (11)
H15	0.1692	0.5914	0.3300	0.049*
C16	0.1819 (6)	0.4863 (2)	0.4004 (3)	0.0466 (12)
H16	0.0725	0.4878	0.4133	0.056*
C17	0.2839 (6)	0.4219 (3)	0.4306 (3)	0.0530 (13)
H17	0.2435	0.3798	0.4634	0.064*
C18	0.4474 (6)	0.4201 (3)	0.4120 (3)	0.0520 (13)
H18	0.5165	0.3763	0.4319	0.062*
C19	0.5076 (5)	0.4825 (2)	0.3643 (3)	0.0428 (11)
H19	0.6180	0.4814	0.3529	0.051*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0471 (3)	0.0269 (3)	0.0353 (3)	0.0016 (2)	0.0168 (3)	0.0001 (2)
Br1	0.0552 (3)	0.0367 (2)	0.0453 (3)	0.0031 (2)	0.0238 (2)	0.0088 (2)
Br2	0.0575 (3)	0.0528 (3)	0.0716 (4)	0.0197 (2)	-0.0113 (3)	-0.0204 (3)
N1	0.057 (2)	0.0228 (17)	0.042 (2)	0.0029 (15)	0.0223 (19)	-0.0013 (15)
N2	0.048 (2)	0.0262 (18)	0.033 (2)	0.0023 (15)	0.0149 (18)	-0.0039 (15)
N3	0.041 (2)	0.0322 (19)	0.033 (2)	0.0046 (15)	0.0129 (17)	0.0022 (15)
O1	0.060 (2)	0.0265 (15)	0.0343 (18)	-0.0017 (13)	0.0203 (15)	-0.0002 (12)
O2	0.086 (3)	0.0286 (16)	0.068 (2)	-0.0033 (15)	0.038 (2)	0.0041 (15)
C1	0.038 (3)	0.034 (2)	0.031 (3)	0.0028 (18)	0.010 (2)	0.0000 (19)
C2	0.039 (3)	0.025 (2)	0.038 (3)	-0.0001 (17)	0.007 (2)	-0.0042 (18)
C3	0.042 (3)	0.031 (2)	0.046 (3)	-0.0022 (19)	0.009 (2)	-0.004 (2)
C4	0.053 (3)	0.026 (2)	0.066 (3)	-0.001 (2)	0.008 (3)	-0.004 (2)
C5	0.069 (4)	0.038 (3)	0.049 (3)	0.010 (2)	0.007 (3)	-0.014 (2)
C6	0.075 (4)	0.045 (3)	0.043 (3)	0.008 (2)	0.021 (3)	-0.009 (2)
C7	0.062 (3)	0.033 (2)	0.044 (3)	0.001 (2)	0.016 (3)	0.004 (2)
C8	0.034 (2)	0.034 (2)	0.036 (3)	-0.0020 (18)	0.005 (2)	-0.0017 (19)
C9	0.038 (3)	0.032 (2)	0.030 (2)	0.0024 (18)	0.009 (2)	0.0025 (18)
C10	0.049 (3)	0.036 (2)	0.033 (3)	-0.0011 (19)	0.016 (2)	-0.0008 (19)
C11	0.058 (3)	0.046 (3)	0.039 (3)	0.006 (2)	0.020 (2)	-0.006 (2)
C12	0.073 (4)	0.031 (2)	0.040 (3)	0.008 (2)	0.016 (3)	-0.002 (2)
C13	0.065 (3)	0.028 (2)	0.042 (3)	0.007 (2)	0.016 (3)	0.003 (2)
C14	0.040 (3)	0.030 (2)	0.029 (2)	0.0015 (18)	0.009 (2)	0.0044 (18)
C15	0.040 (3)	0.034 (2)	0.050 (3)	0.0055 (19)	0.009 (2)	0.001 (2)
C16	0.041 (3)	0.042 (3)	0.060 (3)	-0.009 (2)	0.020 (3)	-0.003 (2)
C17	0.071 (4)	0.039 (3)	0.052 (3)	-0.011 (2)	0.019 (3)	0.009 (2)
C18	0.066 (3)	0.037 (3)	0.054 (3)	0.011 (2)	0.014 (3)	0.015 (2)
C19	0.041 (3)	0.045 (3)	0.045 (3)	0.005 (2)	0.012 (2)	0.006 (2)

Geometric parameters (Å, °)

Cu1—N2	1.966 (3)	C6—H6	0.9300
Cu1—N3	2.018 (3)	C7—H7	0.9300
Cu1—O1	2.083 (2)	C8—C14	1.474 (5)
Cu1—Br1	2.3469 (6)	C8—C9	1.490 (5)
Cu1—Br2	2.5931 (8)	C9—C10	1.370 (5)
N1—C1	1.355 (5)	C10—C11	1.381 (5)
N1—N2	1.358 (4)	C10—H10	0.9300
N1—H1	0.8600	C11—C12	1.369 (6)
N2—C8	1.304 (5)	C11—H11	0.9300
N3—C13	1.338 (5)	C12—C13	1.373 (5)
N3—C9	1.363 (5)	C12—H12	0.9300
O1—C1	1.242 (4)	C13—H13	0.9300
O2—C3	1.361 (5)	C14—C19	1.388 (5)
O2—H2	0.8200	C14—C15	1.397 (5)
C1—C2	1.471 (5)	C15—C16	1.375 (5)
C2—C7	1.393 (5)	C15—H15	0.9300
C2—C3	1.396 (5)	C16—C17	1.374 (6)
C3—C4	1.388 (5)	C16—H16	0.9300
C4—C5	1.373 (6)	C17—C18	1.386 (6)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.373 (6)	C18—C19	1.371 (5)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.383 (5)	C19—H19	0.9300
N2—Cu1—N3	78.67 (12)	C6—C7—C2	121.9 (4)
N2—Cu1—O1	77.25 (11)	C6—C7—H7	119.0
N3—Cu1—O1	153.13 (12)	C2—C7—H7	119.0
N2—Cu1—Br1	159.76 (10)	N2—C8—C14	125.3 (3)
N3—Cu1—Br1	98.37 (9)	N2—C8—C9	111.4 (3)
O1—Cu1—Br1	100.10 (7)	C14—C8—C9	123.3 (3)
N2—Cu1—Br2	95.15 (10)	N3—C9—C10	121.8 (3)
N3—Cu1—Br2	100.15 (10)	N3—C9—C8	114.2 (3)
O1—Cu1—Br2	93.71 (8)	C10—C9—C8	124.0 (3)
Br1—Cu1—Br2	105.07 (2)	C9—C10—C11	119.2 (4)
C1—N1—N2	114.6 (3)	C9—C10—H10	120.4
C1—N1—H1	122.7	C11—C10—H10	120.4
N2—N1—H1	122.7	C12—C11—C10	119.2 (4)
C8—N2—N1	124.2 (3)	C12—C11—H11	120.4
C8—N2—Cu1	120.7 (2)	C10—C11—H11	120.4
N1—N2—Cu1	115.1 (2)	C11—C12—C13	119.2 (4)
C13—N3—C9	118.0 (3)	C11—C12—H12	120.4
C13—N3—Cu1	127.2 (3)	C13—C12—H12	120.4
C9—N3—Cu1	114.6 (2)	N3—C13—C12	122.6 (4)
C1—O1—Cu1	113.3 (2)	N3—C13—H13	118.7
C3—O2—H2	109.5	C12—C13—H13	118.7
O1—C1—N1	119.1 (3)	C19—C14—C15	119.2 (3)
O1—C1—C2	122.9 (4)	C19—C14—C8	121.1 (4)

supplementary materials

N1—C1—C2	118.0 (3)	C15—C14—C8	119.7 (3)
C7—C2—C3	118.3 (4)	C16—C15—C14	119.8 (4)
C7—C2—C1	116.9 (3)	C16—C15—H15	120.1
C3—C2—C1	124.9 (4)	C14—C15—H15	120.1
O2—C3—C4	121.6 (4)	C17—C16—C15	120.7 (4)
O2—C3—C2	118.4 (3)	C17—C16—H16	119.7
C4—C3—C2	120.0 (4)	C15—C16—H16	119.7
C5—C4—C3	119.7 (4)	C16—C17—C18	119.7 (4)
C5—C4—H4	120.1	C16—C17—H17	120.1
C3—C4—H4	120.1	C18—C17—H17	120.1
C4—C5—C6	121.9 (4)	C19—C18—C17	120.2 (4)
C4—C5—H5	119.1	C19—C18—H18	119.9
C6—C5—H5	119.1	C17—C18—H18	119.9
C5—C6—C7	118.2 (4)	C18—C19—C14	120.4 (4)
C5—C6—H6	120.9	C18—C19—H19	119.8
C7—C6—H6	120.9	C14—C19—H19	119.8
C1—N1—N2—C8	172.6 (4)	C3—C4—C5—C6	1.5 (8)
C1—N1—N2—Cu1	-6.5 (4)	C4—C5—C6—C7	-1.7 (8)
N3—Cu1—N2—C8	-4.6 (3)	C5—C6—C7—C2	0.7 (7)
O1—Cu1—N2—C8	-172.6 (3)	C3—C2—C7—C6	0.5 (7)
Br1—Cu1—N2—C8	-88.0 (4)	C1—C2—C7—C6	179.9 (4)
Br2—Cu1—N2—C8	94.8 (3)	N1—N2—C8—C14	2.8 (6)
N3—Cu1—N2—N1	174.6 (3)	Cu1—N2—C8—C14	-178.1 (3)
O1—Cu1—N2—N1	6.6 (3)	N1—N2—C8—C9	-176.9 (4)
Br1—Cu1—N2—N1	91.2 (4)	Cu1—N2—C8—C9	2.2 (5)
Br2—Cu1—N2—N1	-86.1 (3)	C13—N3—C9—C10	-2.2 (6)
N2—Cu1—N3—C13	-179.8 (4)	Cu1—N3—C9—C10	172.6 (3)
O1—Cu1—N3—C13	-153.1 (3)	C13—N3—C9—C8	178.5 (4)
Br1—Cu1—N3—C13	-20.1 (4)	Cu1—N3—C9—C8	-6.8 (4)
Br2—Cu1—N3—C13	87.0 (3)	N2—C8—C9—N3	3.1 (5)
N2—Cu1—N3—C9	6.0 (3)	C14—C8—C9—N3	-176.6 (4)
O1—Cu1—N3—C9	32.7 (5)	N2—C8—C9—C10	-176.2 (4)
Br1—Cu1—N3—C9	165.7 (3)	C14—C8—C9—C10	4.1 (7)
Br2—Cu1—N3—C9	-87.2 (3)	N3—C9—C10—C11	3.4 (7)
N2—Cu1—O1—C1	-6.0 (3)	C8—C9—C10—C11	-177.3 (4)
N3—Cu1—O1—C1	-32.8 (5)	C9—C10—C11—C12	-1.6 (7)
Br1—Cu1—O1—C1	-165.6 (3)	C10—C11—C12—C13	-1.4 (7)
Br2—Cu1—O1—C1	88.4 (3)	C9—N3—C13—C12	-0.9 (6)
Cu1—O1—C1—N1	4.5 (5)	Cu1—N3—C13—C12	-174.9 (3)
Cu1—O1—C1—C2	-174.8 (3)	C11—C12—C13—N3	2.7 (7)
N2—N1—C1—O1	1.1 (6)	N2—C8—C14—C19	48.2 (6)
N2—N1—C1—C2	-179.6 (3)	C9—C8—C14—C19	-132.1 (4)
O1—C1—C2—C7	3.1 (6)	N2—C8—C14—C15	-132.3 (4)
N1—C1—C2—C7	-176.1 (4)	C9—C8—C14—C15	47.4 (6)
O1—C1—C2—C3	-177.5 (4)	C19—C14—C15—C16	0.7 (6)
N1—C1—C2—C3	3.2 (6)	C8—C14—C15—C16	-178.8 (4)
C7—C2—C3—O2	179.6 (4)	C14—C15—C16—C17	-1.2 (7)
C1—C2—C3—O2	0.3 (6)	C15—C16—C17—C18	0.5 (7)
C7—C2—C3—C4	-0.7 (7)	C16—C17—C18—C19	0.6 (7)

C1—C2—C3—C4	180.0 (4)	C17—C18—C19—C14	-1.1 (7)
O2—C3—C4—C5	179.5 (4)	C15—C14—C19—C18	0.4 (7)
C2—C3—C4—C5	-0.2 (7)	C8—C14—C19—C18	179.9 (4)

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—H1 \cdots O2	0.86	1.92	2.574 (4)	131
O2—H2 \cdots Br2 ⁱ	0.82	2.35	3.153 (3)	166
C11—H11 \cdots O1 ⁱⁱ	0.93	2.58	3.503 (5)	170
C10—H10 \cdots Br1 ⁱⁱ	0.93	2.81	3.575 (4)	141
C15—H15 \cdots Br2 ⁱⁱⁱ	0.93	2.82	3.742 (4)	171

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

Fig. 1

