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

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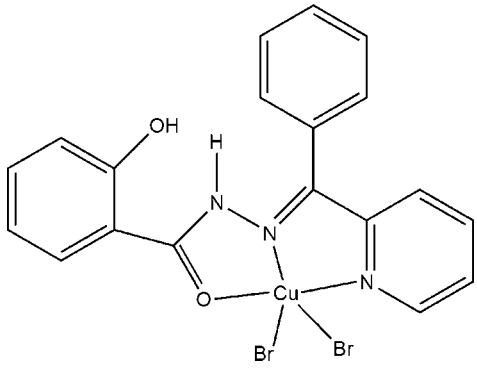
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.034; $wR$ factor = 0.082; data-to-parameter ratio = 14.1.

In the title complex, $[CuBr_2(C_{19}H_{15}N_3O_2)]$, 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 N—H···O hydrogen bond occurs in the ligand. In the crystal, molecules are connected by intermolecular C—H···O, C—H···Br and O—H···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

$[CuBr_2(C_{19}H_{15}N_3O_2)]$ $M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 5.20 mm$^{-1}$
$T$ = 298 K
0.23 × 0.19 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.94 e Å$^{-3}$
$\Delta\rho_{min}$ = −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, °).

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

We acknowledge the financial support of the National Natural Science Foundation of China (grant No. 20671048).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5107).

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Sur, H., Roychowdhuri, S. & Seth, S. (1993). *Acta Cryst.* C**49**, 870–873.

# supporting information

*Acta Cryst.* (2009). E**65**, m1251 [doi:10.1107/S1600536809038070]

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

**Ling-Qian Kong, Xiu-Ping Ju and Da-Cheng Li**

## S1. 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 $Cu(C_{19}H_{15}N_3O_2)Br_2$, which was 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), $Cu(C_{19}H_{15}N_3O_2)Br_2$ 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 $_{O}N_2Br_2$ set of donor atoms. The equatorial coordination sits are occupied by O1, N2, N3, Br1 and the axial coordination atom is Br2 with the distance of Cu1—Br2 2.5931 (8) A. In the structure, there are intramolecular N—H···O interactions. Except that, the complex is linked into one-dimensional chain by intermolecular C—H···Br interactions, and the neighboring chains form a two-dimensional network structure *via* C—H···Br and O—H···Br interactions. A three-dimensional network structure is connected *via* C—H···O and C—H···Br interactions between adjacent two-dimensional networks. So the complex is linked into a three-dimensional network structure *via* intermolecular C—H···O, C—H···Br and O—H···Br interactions.

## S2. Experimental

$CuBr_2.H_2O$ (0.25 mmol 0.065 g) was dissolved in 10 ml MeOH and a 10 ml 1,1-dichlorinemethane solution of 2-benzoyl-pyridine 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 resulted in dark green blocks of (I) at room temperature. m.p.>573 K. Elemental analysis for $_{C}19_{H}15_{Cu}N_3O_2Br_2$ calculated: C 42.21, H 2.80 N 7.77%; found: C 42.32, H 2.54, N 7.68%.

## S3. Refinement

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

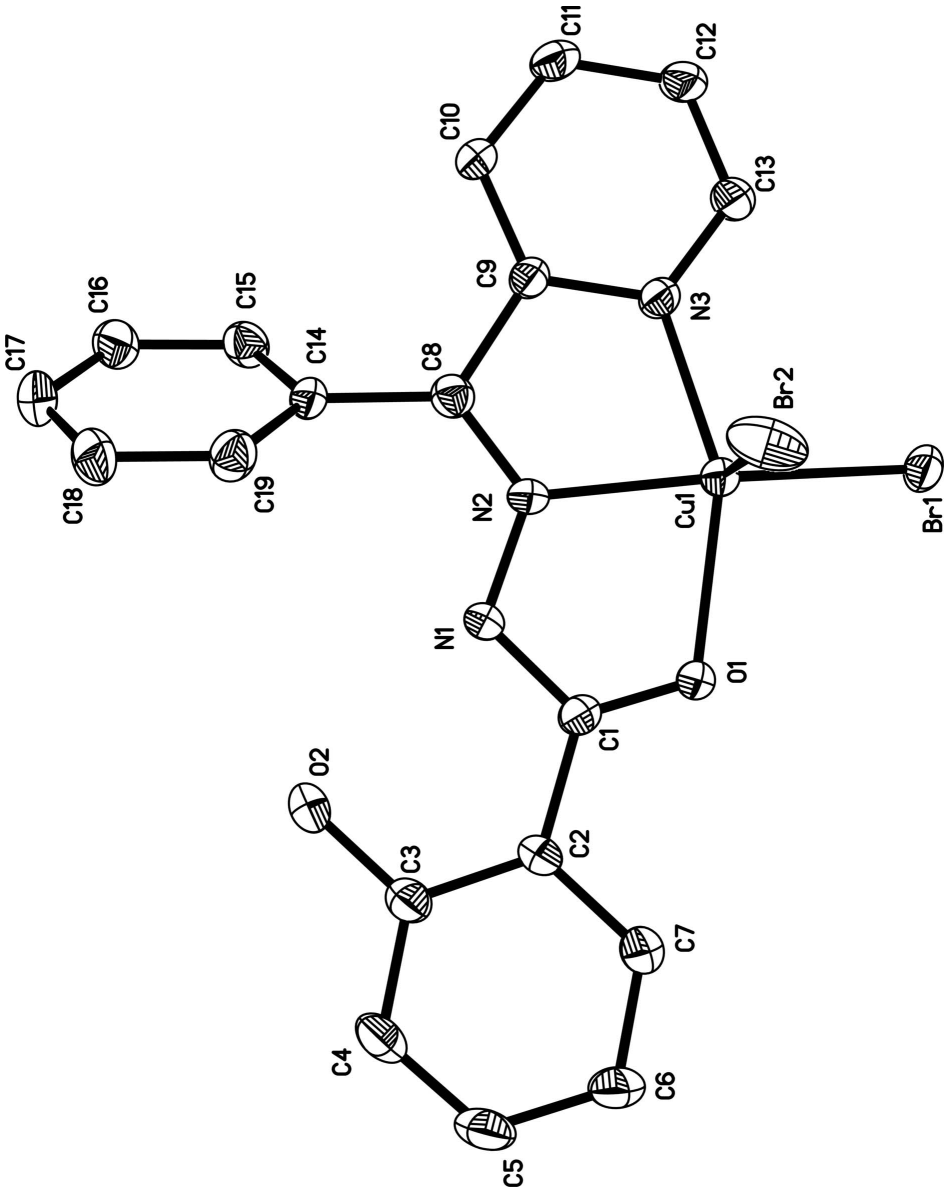


**Figure 1**

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*

$[CuBr_2(C_{19}H_{15}N_3O_2)]$
$M_r$ = 540.70
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 8.0779 (11) Å
$b$ = 16.302 (2) Å
$c$ = 15.0376 (18) Å
$\beta$ = 97.624 (2)°
$V$ = 1962.8 (4) Å$^3$
$Z$ = 4
$F(000)$ = 1060
$D_x$ = 1.830 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2246 reflections
$\theta$ = 2.5–25.1°
$\mu$ = 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
Graphite monochromator
$\omega$ 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 $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 19$
$l = -17 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
$S$ = 1.01
3446 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.94 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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* |
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |
| 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 |

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| 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) |

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|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2 | 0.86 | 1.92 | 2.574 (4) | 131 |
| O2—H2···Br2$^{i}$ | 0.82 | 2.35 | 3.153 (3) | 166 |
| C11—H11···O1$^{ii}$ | 0.93 | 2.58 | 3.503 (5) | 170 |
| C10—H10···Br1$^{ii}$ | 0.93 | 2.81 | 3.575 (4) | 141 |
| C15—H15···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) $x-1, y, z$.