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# Bis{2,4-dibromo-6-[(naphthalen-1-ylimino)methyl]phenolato-$\kappa^2N,O$}(1,10-phenanthroline-$\kappa^2N,N'$)copper(II)

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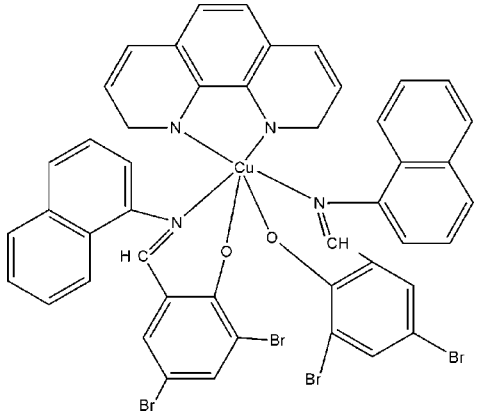
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.013 Å; $R$ factor = 0.059; $wR$ factor = 0.165; data-to-parameter ratio = 13.6.

In the title compound, $C_{46}H_{28}Br_4CuN_4O_2$ or $[Cu(L)_2(phen)]$ {$L$ = 2,4-dibromo-6-[(naphthalen-1-ylimino)methyl]phenolate, $C_{17}H_{10}Br_2NO$; phen = 1,10-phenanthroline, $C_{12}H_8N_2$}, the central $Cu^{II}$, which lies on a twofold axis, binds two N and two O atoms from the two Schiff base ligands and two N atoms from 1,10-phenanthroline in a distorted octahedral arrangement. In the crystal structure, C—H···Br hydrogen bonds link the molecules into rows along $c$.

## Related literature

For related complexes of Schiff bases with transition metal ions, see: Mostafa & Haifaa (2007); Musie *et al.* (2003); Patel *et al.* (2006). For related literature, see: Mehmet *et al.* (2007).




## Experimental

### Crystal data

$[Cu(C_{17}H_{10}Br_2NO)_2(C_{12}H_8N_2)]$
$M_r$ = 1051.90
Monoclinic, $C2/c$
$a$ = 20.288 (2) Å
$b$ = 14.5052 (18) Å
$c$ = 15.227 (2) Å
$\beta$ = 116.977 (2)°
$V$ = 3993.5 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 4.59 mm$^{-1}$
$T$ = 298 (2) K
0.38 × 0.19 × 0.17 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.274, $T_{max}$ = 0.509
(expected range = 0.247–0.458)
10067 measured reflections
3513 independent reflections
1877 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.086

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.165
$S$ = 0.97
3513 reflections
258 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.73 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C15—H15···Br1$^{i}$ | 0.93 | 2.93 | 3.773 (13) | 152 |

Symmetry code: (i) $x+\frac{3}{2}, y+\frac{5}{2}, z$.

Data collection: *SMART* (Bruker 2001); cell refinement: *SAINT* (Bruker 2001); 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: SJ2345).

## References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART* (Version 5.0) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Mehmet, T., Duygu, E. & Ferhan, T. (2007). *Spectrochim. Acta Part A*, **67**, 916–929.
Mostafa, E. B. & Haifaa, E. T. (2007). *Spectrochim. Acta Part A*, **66**, 28–36.
Musie, G. T., Li, X. B. & Powell, D. R. (2003). *Inorg. Chim. Acta*, **348**, 69–74.
Patel, R. N., Nripendra Singh, V. L. N. & Gundla, R. N. (2006). *Polyhedron*, **25**, 3312–3318.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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# supplementary materials

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# Bis{2,4-dibromo-6-[(naphthalen-1-ylimino)methyl]phenolato-$\kappa^2N,O$}(1,10-phenanthroline-$\kappa^2N,N'$)copper(II)

**Z. Liu, L. X. Jin, J. H. Xia and G. Z. Li**

## Comment

Schiff bases play an important role in inorganic chemistry as they easily form stable complexes with most transition metal ions (Mostafa & Haifaa, 2007, Musie *et al.*, 2003, Patel *et al.*, 2006). We report herein the synthesis and crystal structure of (I), Fig 1, a mononuclear Cu(II) complex of the new Schiff base ligand 2,4-dibromo-6-((naphthalen-1-ylimino)methyl)phenolate and 1,10-phenanthroline. The copper$^{II}$ cation lies on a twofold axis and is coordinated by two N and two O atoms from the Schiff base and two N atoms from 1,10-phenanthroline, in a slightly distorted octahedral geometry.

In the crystal weak, non-classical C—H···Br hydrogen bonds link the molecules in rows along c, Fig 2.

## Experimental

1-naphthylamine (0.286 g, 2 mmol) and 3,5-Bibromo-2-hydroxy-benzaldehyde (0.560 g, 2 mmol) were mixed in ethanol and stirred for 30 min at room temperature to yield the Schiff base 2,4-dibromo-6-((naphthalen-1-ylimino)methyl)phenol. A mixture of this Schiff base (0.201 g, 0.5 mmol), $CuSO_4{\cdot}5H_2O_2$ (0.125 g, 0.5 mmol), phen (0.198 g 0.1 mmol,) and 6 drops of triethylamine in 5 ml e thanol and 5 ml acetonitrile was sealed in a 30 ml Teflon-lined stainless steel vessel, which was heated at 333 K for 7 days under autogenous pressure. On cooling to room temperature blue crystals of the title compound (I) were produced (yield: 53%, based on Cu).

## Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, $U_{iso}$=1.2$U_{eq}$ (C).

## Figures

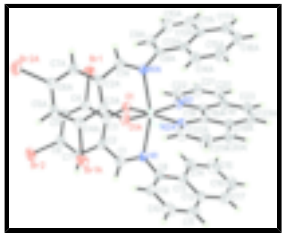

Fig. 1. A view of (I), showing 30% probability displacement ellipsoids.

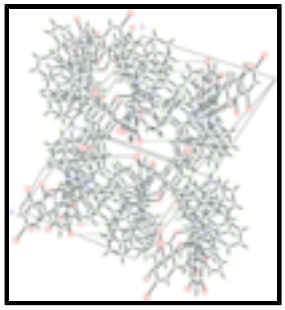

Fig. 2. Crystal packing of (I) with H-bonds drawn as dashed lines.

**Bis{2,4-dibromo-6-[(naphthalen-1-ylimino)methyl]phenolato-κ$^2$*N*, O}(1,10-phenanthroline-κ$^2$*N*,*N*')copper(II)**

*Crystal data*

| | |
|---|---|
| $[Cu(C_{17}H_{10}Br_2NO)_2(C_{12}H_8N_2)]$ | $F_{000}$ = 2068 |
| $M_r$ = 1051.90 | $D_x$ = 1.750 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 1985 reflections |
| *a* = 20.288 (2) Å | θ = 2.8–20.6º |
| *b* = 14.5052 (18) Å | μ = 4.59 mm$^{-1}$ |
| *c* = 15.227 (2) Å | *T* = 298 (2) K |
| β = 116.977 (2)º | Block, blue |
| *V* = 3993.5 (9) Å$^3$ | 0.38 × 0.19 × 0.17 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3513 independent reflections |
| Radiation source: fine-focus sealed tube | 1877 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.086 |
| *T* = 298(2) K | $\theta_{max}$ = 25.0º |
| φ and ω scans | $\theta_{min}$ = 1.8º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −14→24 |
| $T_{min}$ = 0.274, $T_{max}$ = 0.509 | *k* = −16→17 |
| 10067 measured reflections | *l* = −17→18 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.059 | H-atom parameters constrained |
| $wR(F^2)$ = 0.165 | $w = 1/[\sigma^2(F_o^2) + (0.0811P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| $S$ = 0.97 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 3513 reflections | $\Delta\rho_{max}$ = 0.95 e Å$^{-3}$ |
| 258 parameters | $\Delta\rho_{min}$ = −0.73 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.5000 | 0.93455 (7) | 0.2500 | 0.0392 (4) |
| Br1 | 0.37169 (5) | 0.70105 (6) | 0.02414 (6) | 0.0636 (3) |
| Br2 | 0.62496 (6) | 0.47645 (6) | 0.17224 (8) | 0.0864 (4) |
| N1 | 0.6262 (3) | 0.9081 (4) | 0.2840 (4) | 0.0421 (15) |
| N2 | 0.4717 (3) | 1.0413 (4) | 0.1537 (4) | 0.0404 (15) |
| O1 | 0.4819 (3) | 0.8458 (3) | 0.1455 (3) | 0.0430 (12) |
| C1 | 0.6420 (4) | 0.8241 (5) | 0.2785 (5) | 0.0437 (19) |
| H1 | 0.6907 | 0.8064 | 0.3181 | 0.052* |
| C2 | 0.5920 (4) | 0.7527 (5) | 0.2168 (5) | 0.0398 (18) |
| C3 | 0.5152 (4) | 0.7679 (5) | 0.1568 (5) | 0.0404 (18) |
| C4 | 0.4749 (4) | 0.6892 (5) | 0.1040 (5) | 0.0435 (19) |
| C5 | 0.5061 (5) | 0.6039 (5) | 0.1086 (5) | 0.052 (2) |
| H5 | 0.4772 | 0.5543 | 0.0731 | 0.063* |
| C6 | 0.5824 (5) | 0.5933 (5) | 0.1682 (6) | 0.051 (2) |
| C7 | 0.6236 (5) | 0.6661 (5) | 0.2209 (5) | 0.049 (2) |
| H7 | 0.6741 | 0.6582 | 0.2605 | 0.058* |
| C8 | 0.6805 (4) | 0.9648 (5) | 0.3581 (6) | 0.0457 (19) |
| C9 | 0.7164 (5) | 0.9372 (5) | 0.4543 (6) | 0.061 (2) |
| H9 | 0.7083 | 0.8785 | 0.4719 | 0.073* |
| C10 | 0.7658 (6) | 0.9981 (7) | 0.5273 (7) | 0.085 (3) |
| H10 | 0.7919 | 0.9781 | 0.5921 | 0.101* |
| C11 | 0.7751 (5) | 1.0838 (7) | 0.5035 (8) | 0.087 (3) |
| H11 | 0.8062 | 1.1236 | 0.5528 | 0.104* |
| C12 | 0.7393 (5) | 1.1154 (5) | 0.4061 (8) | 0.066 (3) |
| C13 | 0.6910 (4) | 1.0555 (5) | 0.3300 (7) | 0.053 (2) |
| C14 | 0.6534 (5) | 1.0870 (6) | 0.2316 (7) | 0.066 (2) |
| H14 | 0.6228 | 1.0475 | 0.1816 | 0.079* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.6629 (7) | 1.1759 (8) | 0.2112 (10) | 0.097 (4) |
| H15 | 0.6373 | 1.1969 | 0.1467 | 0.116* |
| C16 | 0.7096 (7) | 1.2367 (7) | 0.2837 (12) | 0.102 (4) |
| H16 | 0.7158 | 1.2966 | 0.2669 | 0.122* |
| C17 | 0.7461 (6) | 1.2080 (7) | 0.3789 (10) | 0.088 (3) |
| H17 | 0.7760 | 1.2494 | 0.4272 | 0.105* |
| C18 | 0.4844 (4) | 1.1253 (4) | 0.1971 (5) | 0.0370 (17) |
| C19 | 0.4695 (4) | 1.2085 (5) | 0.1460 (6) | 0.049 (2) |
| C20 | 0.4396 (5) | 1.2025 (6) | 0.0433 (6) | 0.060 (2) |
| H20 | 0.4288 | 1.2559 | 0.0056 | 0.072* |
| C21 | 0.4263 (5) | 1.1177 (6) | −0.0020 (6) | 0.067 (3) |
| H21 | 0.4063 | 1.1134 | −0.0702 | 0.080* |
| C22 | 0.4434 (4) | 1.0386 (5) | 0.0560 (5) | 0.050 (2) |
| H22 | 0.4346 | 0.9814 | 0.0251 | 0.060* |
| C23 | 0.4850 (5) | 1.2925 (5) | 0.2001 (6) | 0.067 (3) |
| H23 | 0.4742 | 1.3484 | 0.1664 | 0.080* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0522 (8) | 0.0356 (7) | 0.0274 (7) | 0.000 | 0.0161 (6) | 0.000 |
| Br1 | 0.0580 (6) | 0.0703 (6) | 0.0482 (5) | −0.0060 (5) | 0.0115 (4) | −0.0159 (4) |
| Br2 | 0.0961 (9) | 0.0469 (6) | 0.0961 (8) | 0.0138 (5) | 0.0260 (7) | −0.0145 (5) |
| N1 | 0.044 (4) | 0.039 (3) | 0.041 (4) | −0.002 (3) | 0.018 (3) | −0.005 (3) |
| N2 | 0.042 (4) | 0.047 (4) | 0.032 (4) | −0.001 (3) | 0.017 (3) | 0.000 (3) |
| O1 | 0.052 (3) | 0.042 (3) | 0.030 (3) | 0.003 (3) | 0.014 (2) | −0.002 (2) |
| C1 | 0.046 (5) | 0.050 (5) | 0.035 (4) | −0.003 (4) | 0.018 (4) | −0.006 (3) |
| C2 | 0.048 (5) | 0.041 (4) | 0.030 (4) | −0.006 (4) | 0.017 (4) | −0.006 (3) |
| C3 | 0.058 (5) | 0.040 (4) | 0.027 (4) | −0.004 (4) | 0.023 (4) | −0.002 (3) |
| C4 | 0.053 (5) | 0.048 (4) | 0.030 (4) | −0.002 (4) | 0.019 (4) | −0.001 (3) |
| C5 | 0.078 (7) | 0.041 (4) | 0.035 (4) | −0.008 (5) | 0.023 (5) | −0.009 (3) |
| C6 | 0.063 (6) | 0.041 (4) | 0.047 (5) | 0.004 (4) | 0.022 (4) | −0.001 (4) |
| C7 | 0.056 (5) | 0.043 (4) | 0.042 (5) | 0.003 (4) | 0.019 (4) | 0.002 (3) |
| C8 | 0.041 (5) | 0.046 (4) | 0.048 (5) | −0.003 (4) | 0.017 (4) | −0.007 (4) |
| C9 | 0.064 (6) | 0.056 (5) | 0.047 (5) | 0.003 (5) | 0.011 (4) | −0.012 (4) |
| C10 | 0.089 (8) | 0.077 (6) | 0.044 (6) | 0.012 (6) | −0.008 (5) | −0.021 (5) |
| C11 | 0.059 (7) | 0.085 (7) | 0.087 (8) | 0.004 (6) | 0.008 (6) | −0.048 (6) |
| C12 | 0.051 (6) | 0.045 (5) | 0.093 (8) | 0.005 (5) | 0.025 (6) | −0.026 (5) |
| C13 | 0.041 (5) | 0.048 (5) | 0.074 (6) | −0.001 (4) | 0.028 (5) | −0.011 (4) |
| C14 | 0.061 (6) | 0.066 (6) | 0.073 (7) | 0.003 (5) | 0.034 (5) | 0.008 (5) |
| C15 | 0.098 (9) | 0.083 (8) | 0.141 (11) | 0.017 (7) | 0.083 (9) | 0.041 (8) |
| C16 | 0.093 (10) | 0.056 (7) | 0.193 (15) | −0.004 (7) | 0.096 (11) | 0.016 (8) |
| C17 | 0.066 (7) | 0.060 (7) | 0.145 (11) | −0.010 (6) | 0.056 (8) | −0.025 (7) |
| C18 | 0.034 (4) | 0.035 (4) | 0.042 (4) | −0.002 (3) | 0.017 (4) | 0.001 (3) |
| C19 | 0.048 (5) | 0.041 (4) | 0.059 (5) | 0.000 (4) | 0.026 (4) | 0.008 (4) |
| C20 | 0.074 (6) | 0.060 (5) | 0.051 (5) | 0.011 (5) | 0.032 (5) | 0.022 (4) |
| C21 | 0.091 (7) | 0.069 (6) | 0.035 (5) | 0.011 (5) | 0.024 (5) | 0.020 (4) |
| C22 | 0.064 (5) | 0.054 (5) | 0.033 (4) | −0.001 (4) | 0.023 (4) | −0.001 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.076 (7) | 0.044 (4) | 0.081 (6) | 0.009 (5) | 0.036 (6) | 0.019 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.948 (4) | C9—H9 | 0.9300 |
| Cu1—O1$^{i}$ | 1.948 (4) | C10—C11 | 1.332 (13) |
| Cu1—N2$^{i}$ | 2.029 (5) | C10—H10 | 0.9300 |
| Cu1—N2 | 2.029 (5) | C11—C12 | 1.400 (13) |
| Cu1—N1$^{i}$ | 2.402 (6) | C11—H11 | 0.9300 |
| Cu1—N1 | 2.402 (6) | C12—C13 | 1.424 (11) |
| Br1—C4 | 1.893 (8) | C12—C17 | 1.431 (13) |
| Br2—C6 | 1.890 (7) | C13—C14 | 1.413 (11) |
| N1—C1 | 1.273 (8) | C14—C15 | 1.361 (12) |
| N1—C8 | 1.426 (9) | C14—H14 | 0.9300 |
| N2—C22 | 1.330 (8) | C15—C16 | 1.394 (16) |
| N2—C18 | 1.355 (8) | C15—H15 | 0.9300 |
| O1—C3 | 1.288 (8) | C16—C17 | 1.360 (15) |
| C1—C2 | 1.455 (9) | C16—H16 | 0.9300 |
| C1—H1 | 0.9300 | C17—H17 | 0.9300 |
| C2—C7 | 1.399 (9) | C18—C19 | 1.393 (9) |
| C2—C3 | 1.421 (10) | C18—C18$^{i}$ | 1.438 (13) |
| C3—C4 | 1.421 (9) | C19—C20 | 1.401 (10) |
| C4—C5 | 1.377 (9) | C19—C23 | 1.424 (10) |
| C5—C6 | 1.403 (11) | C20—C21 | 1.375 (10) |
| C5—H5 | 0.9300 | C20—H20 | 0.9300 |
| C6—C7 | 1.360 (10) | C21—C22 | 1.393 (10) |
| C7—H7 | 0.9300 | C21—H21 | 0.9300 |
| C8—C9 | 1.368 (10) | C22—H22 | 0.9300 |
| C8—C13 | 1.429 (10) | C23—C23$^{i}$ | 1.357 (16) |
| C9—C10 | 1.417 (11) | C23—H23 | 0.9300 |
| O1—Cu1—O1$^{i}$ | 97.3 (3) | C8—C9—C10 | 120.0 (8) |
| O1—Cu1—N2$^{i}$ | 169.1 (2) | C8—C9—H9 | 120.0 |
| O1$^{i}$—Cu1—N2$^{i}$ | 91.5 (2) | C10—C9—H9 | 120.0 |
| O1—Cu1—N2 | 91.5 (2) | C11—C10—C9 | 120.4 (9) |
| O1$^{i}$—Cu1—N2 | 169.1 (2) | C11—C10—H10 | 119.8 |
| N2$^{i}$—Cu1—N2 | 80.5 (3) | C9—C10—H10 | 119.8 |
| O1—Cu1—N1$^{i}$ | 86.0 (2) | C10—C11—C12 | 121.6 (8) |
| O1$^{i}$—Cu1—N1$^{i}$ | 81.9 (2) | C10—C11—H11 | 119.2 |
| N2$^{i}$—Cu1—N1$^{i}$ | 101.7 (2) | C12—C11—H11 | 119.2 |
| N2—Cu1—N1$^{i}$ | 92.4 (2) | C11—C12—C13 | 119.8 (8) |
| O1—Cu1—N1 | 81.9 (2) | C11—C12—C17 | 122.8 (10) |
| O1$^{i}$—Cu1—N1 | 86.0 (2) | C13—C12—C17 | 117.3 (10) |
| N2$^{i}$—Cu1—N1 | 92.4 (2) | C14—C13—C12 | 120.5 (8) |
| N2—Cu1—N1 | 101.7 (2) | C14—C13—C8 | 122.2 (7) |
| N1$^{i}$—Cu1—N1 | 161.6 (3) | C12—C13—C8 | 117.3 (8) |

| | | | |
|---|---|---|---|
| C1—N1—C8 | 118.5 (6) | C15—C14—C13 | 118.9 (10) |
| C1—N1—Cu1 | 114.5 (5) | C15—C14—H14 | 120.5 |
| C8—N1—Cu1 | 116.4 (4) | C13—C14—H14 | 120.5 |
| C22—N2—C18 | 117.6 (6) | C14—C15—C16 | 122.3 (12) |
| C22—N2—Cu1 | 128.5 (5) | C14—C15—H15 | 118.8 |
| C18—N2—Cu1 | 113.9 (4) | C16—C15—H15 | 118.8 |
| C3—O1—Cu1 | 125.3 (4) | C17—C16—C15 | 119.7 (10) |
| N1—C1—C2 | 126.9 (7) | C17—C16—H16 | 120.1 |
| N1—C1—H1 | 116.5 | C15—C16—H16 | 120.1 |
| C2—C1—H1 | 116.5 | C16—C17—C12 | 121.2 (10) |
| C7—C2—C3 | 120.9 (6) | C16—C17—H17 | 119.4 |
| C7—C2—C1 | 116.0 (7) | C12—C17—H17 | 119.4 |
| C3—C2—C1 | 123.1 (6) | N2—C18—C19 | 124.2 (6) |
| O1—C3—C2 | 125.3 (6) | N2—C18—C18$^{i}$ | 115.9 (4) |
| O1—C3—C4 | 119.8 (7) | C19—C18—C18$^{i}$ | 120.0 (4) |
| C2—C3—C4 | 114.9 (7) | C18—C19—C20 | 116.4 (7) |
| C5—C4—C3 | 124.1 (7) | C18—C19—C23 | 118.9 (7) |
| C5—C4—Br1 | 117.6 (6) | C20—C19—C23 | 124.7 (7) |
| C3—C4—Br1 | 118.4 (5) | C21—C20—C19 | 120.2 (7) |
| C4—C5—C6 | 118.5 (7) | C21—C20—H20 | 119.9 |
| C4—C5—H5 | 120.7 | C19—C20—H20 | 119.9 |
| C6—C5—H5 | 120.7 | C20—C21—C22 | 118.9 (7) |
| C7—C6—C5 | 119.9 (7) | C20—C21—H21 | 120.5 |
| C7—C6—Br2 | 121.9 (6) | C22—C21—H21 | 120.5 |
| C5—C6—Br2 | 118.2 (6) | N2—C22—C21 | 122.8 (7) |
| C6—C7—C2 | 121.7 (7) | N2—C22—H22 | 118.6 |
| C6—C7—H7 | 119.2 | C21—C22—H22 | 118.6 |
| C2—C7—H7 | 119.2 | C23$^{i}$—C23—C19 | 121.1 (4) |
| C9—C8—N1 | 121.5 (7) | C23$^{i}$—C23—H23 | 119.4 |
| C9—C8—C13 | 120.8 (7) | C19—C23—H23 | 119.4 |
| N1—C8—C13 | 117.4 (7) | | |
| O1—Cu1—N1—C1 | −42.1 (5) | Br2—C6—C7—C2 | 179.3 (5) |
| O1$^{i}$—Cu1—N1—C1 | 55.8 (5) | C3—C2—C7—C6 | −0.3 (11) |
| N2$^{i}$—Cu1—N1—C1 | 147.2 (5) | C1—C2—C7—C6 | 178.7 (6) |
| N2—Cu1—N1—C1 | −132.0 (5) | C1—N1—C8—C9 | −49.5 (10) |
| N1$^{i}$—Cu1—N1—C1 | 7.1 (5) | Cu1—N1—C8—C9 | 93.2 (8) |
| O1—Cu1—N1—C8 | 173.7 (5) | C1—N1—C8—C13 | 136.6 (7) |
| O1$^{i}$—Cu1—N1—C8 | −88.4 (5) | Cu1—N1—C8—C13 | −80.8 (7) |
| N2$^{i}$—Cu1—N1—C8 | 3.0 (5) | N1—C8—C9—C10 | −175.2 (8) |
| N2—Cu1—N1—C8 | 83.8 (5) | C13—C8—C9—C10 | −1.4 (12) |
| N1$^{i}$—Cu1—N1—C8 | −137.1 (5) | C8—C9—C10—C11 | 3.1 (15) |
| O1—Cu1—N2—C22 | 7.0 (6) | C9—C10—C11—C12 | −2.7 (16) |
| O1$^{i}$—Cu1—N2—C22 | −136.8 (10) | C10—C11—C12—C13 | 0.6 (15) |
| N2$^{i}$—Cu1—N2—C22 | 179.5 (8) | C10—C11—C12—C17 | 177.6 (10) |
| N1$^{i}$—Cu1—N2—C22 | −79.0 (6) | C11—C12—C13—C14 | 178.9 (8) |
| N1—Cu1—N2—C22 | 89.1 (6) | C17—C12—C13—C14 | 1.8 (12) |

| | | | |
|---|---|---|---|
| O1—Cu1—N2—C18 | −172.5 (5) | C11—C12—C13—C8 | 1.0 (12) |
| O1$^{i}$—Cu1—N2—C18 | 43.7 (14) | C17—C12—C13—C8 | −176.1 (8) |
| N2$^{i}$—Cu1—N2—C18 | −0.1 (4) | C9—C8—C13—C14 | −178.4 (8) |
| N1$^{i}$—Cu1—N2—C18 | 101.4 (5) | N1—C8—C13—C14 | −4.5 (11) |
| N1—Cu1—N2—C18 | −90.5 (5) | C9—C8—C13—C12 | −0.6 (11) |
| O1$^{i}$—Cu1—O1—C3 | −35.9 (5) | N1—C8—C13—C12 | 173.4 (7) |
| N2$^{i}$—Cu1—O1—C3 | 107.5 (12) | C12—C13—C14—C15 | −1.5 (13) |
| N2—Cu1—O1—C3 | 150.6 (6) | C8—C13—C14—C15 | 176.3 (8) |
| N1$^{i}$—Cu1—O1—C3 | −117.2 (6) | C13—C14—C15—C16 | 1.5 (15) |
| N1—Cu1—O1—C3 | 49.0 (5) | C14—C15—C16—C17 | −1.7 (17) |
| C8—N1—C1—C2 | 172.1 (7) | C15—C16—C17—C12 | 2.0 (17) |
| Cu1—N1—C1—C2 | 28.7 (9) | C11—C12—C17—C16 | −179.1 (10) |
| N1—C1—C2—C7 | 177.3 (7) | C13—C12—C17—C16 | −2.1 (15) |
| N1—C1—C2—C3 | −3.7 (11) | C22—N2—C18—C19 | 0.2 (11) |
| Cu1—O1—C3—C2 | −41.1 (9) | Cu1—N2—C18—C19 | 179.8 (6) |
| Cu1—O1—C3—C4 | 141.3 (5) | C22—N2—C18—C18$^{i}$ | −179.4 (7) |
| C7—C2—C3—O1 | −177.1 (6) | Cu1—N2—C18—C18$^{i}$ | 0.2 (10) |
| C1—C2—C3—O1 | 4.0 (10) | N2—C18—C19—C20 | −0.1 (11) |
| C7—C2—C3—C4 | 0.6 (9) | C18$^{i}$—C18—C19—C20 | 179.5 (8) |
| C1—C2—C3—C4 | −178.3 (6) | N2—C18—C19—C23 | 179.7 (7) |
| O1—C3—C4—C5 | 177.7 (6) | C18$^{i}$—C18—C19—C23 | −0.7 (13) |
| C2—C3—C4—C5 | −0.1 (10) | C18—C19—C20—C21 | 0.1 (12) |
| O1—C3—C4—Br1 | −3.7 (9) | C23—C19—C20—C21 | −179.6 (9) |
| C2—C3—C4—Br1 | 178.5 (5) | C19—C20—C21—C22 | −0.3 (13) |
| C3—C4—C5—C6 | −0.7 (11) | C18—N2—C22—C21 | −0.4 (11) |
| Br1—C4—C5—C6 | −179.3 (5) | Cu1—N2—C22—C21 | −179.9 (6) |
| C4—C5—C6—C7 | 1.0 (11) | C20—C21—C22—N2 | 0.4 (13) |
| C4—C5—C6—Br2 | −178.9 (5) | C18—C19—C23—C23$^{i}$ | 1.3 (16) |
| C5—C6—C7—C2 | −0.6 (12) | C20—C19—C23—C23$^{i}$ | −179.0 (10) |

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C15—H15···Br1$^{ii}$ | 0.93 | 2.93 | 3.773 (13) | 152 |

Symmetry codes: (ii) *x*+3/2, *y*+5/2, *z*.

**Fig. 1**

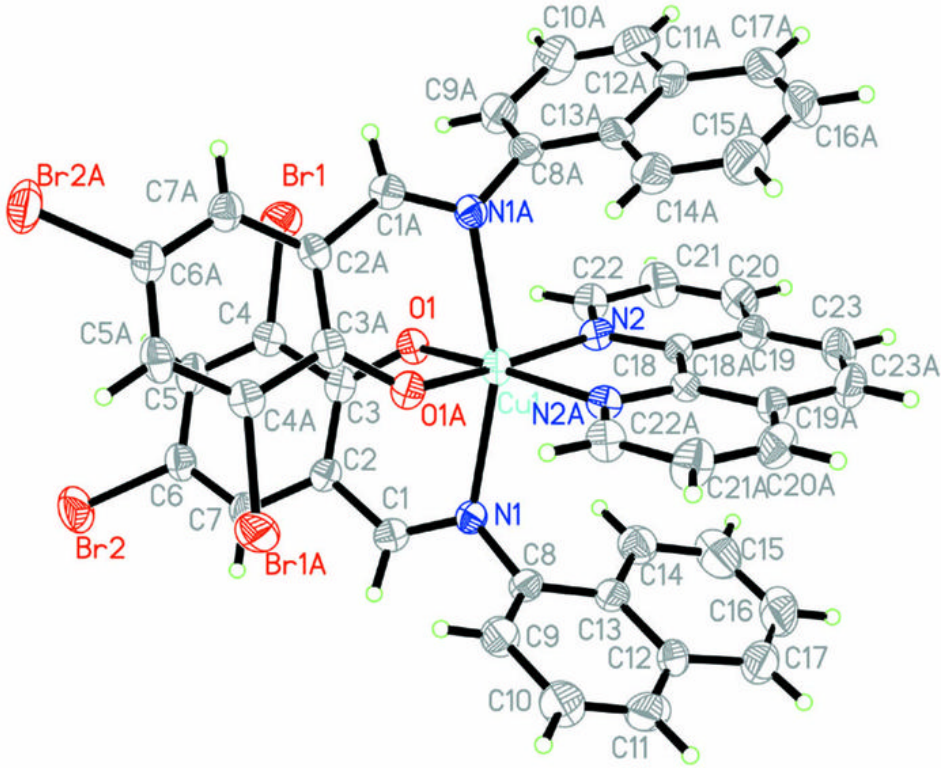
C10A
C11A
C17A
C9A
C12A
C13A
C15A
C16A
Br2A
C7A
Br1
C8A
C1A
N1A
C14A
C6A
C2A
C22
C21
C20
C4
C3A
O1
N2
C23
C5A
C18
C18A
C19
C23A
C5
C4A
C3
O1A
Cu1
N2A
C22A
C19A
C2
C21A
C20A
C6
C1
N1
C7
C8
C15
Br2
Br1A
C14
C16
C9
C13
C12
C17
C10
C11

**Fig. 2**