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Bromido(2-[1-[2-(piperidin-1-yl)ethyl-imino]ethyl]phenolato)copper(II)

Xiao-Fan Zhao and Fang Li*

 College of Chemistry & Chemical Engineering, Shaoxing University, Shaoxing 312000, People's Republic of China
 Correspondence e-mail: xiaofan_zhao@126.com

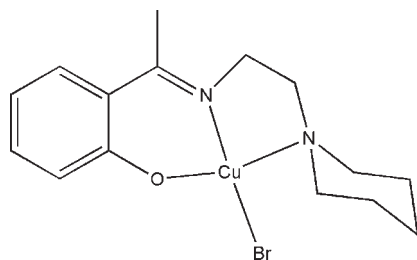
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.035; wR factor = 0.084; data-to-parameter ratio = 18.4.

In the title complex, $[\text{CuBr}(\text{C}_{15}\text{H}_{21}\text{N}_2\text{O})]$, the Cu^{II} atom is coordinated by one phenolate O, one imine N and one amine N atom of the tridentate Schiff base ligand and by one bromide ion, resulting in a distorted CuBrN_2O square-planar geometry for the metal ion, with the N atoms in a *cis* conformation.

Related literature

For a related structure and background references, see the preceding paper: Zhao & Li (2010).



Experimental

Crystal data

 $[\text{CuBr}(\text{C}_{15}\text{H}_{21}\text{N}_2\text{O})]$
 $M_r = 388.79$

 Monoclinic, $P2_1/c$
 $a = 10.988$ (3) Å
 $b = 17.181$ (5) Å
 $c = 8.173$ (2) Å
 $\beta = 92.366$ (3)°
 $V = 1541.6$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 4.01$ mm⁻¹
 $T = 298$ K
 $0.27 \times 0.23 \times 0.23$ mm

Data collection

 Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.411$, $T_{\text{max}} = 0.459$

 9503 measured reflections
 3357 independent reflections
 2373 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.084$
 $S = 1.06$
 3357 reflections

 182 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.872 (3)	Cu1—N2	2.034 (3)
Cu1—N1	1.954 (3)	Cu1—Br1	2.4030 (7)
O1—Cu1—N1	91.04 (11)	O1—Cu1—Br1	92.26 (8)
O1—Cu1—N2	162.99 (11)	N1—Cu1—Br1	159.19 (8)
N1—Cu1—N2	86.20 (11)	N2—Cu1—Br1	96.27 (8)

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); 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: HB5544).

References

- Bruker (1998). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
 Zhao, X.-F. & Li, F. (2010). Acta Cryst. E66, m912.

supporting information

Acta Cryst. (2010). E66, m913 [https://doi.org/10.1107/S1600536810026711]

Bromido(2-{1-[2-(piperidin-1-yl)ethylimino]ethyl}phenolato)copper(II)

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S1. Experimental

1-(2-Hydroxyphenyl)ethanone (1 mmol, 136 mg), 2-piperidin-1-ylethylamine (1 mmol, 128 mg), and copper(II) bromide (1 mmol, 223 mg) were dissolved in methanol (80 ml). The mixture was stirred at room temperature for 1 h to give a blue solution. The resulting solution was kept in air for a few days, and blue blocks of (I) were formed.

S2. Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$.

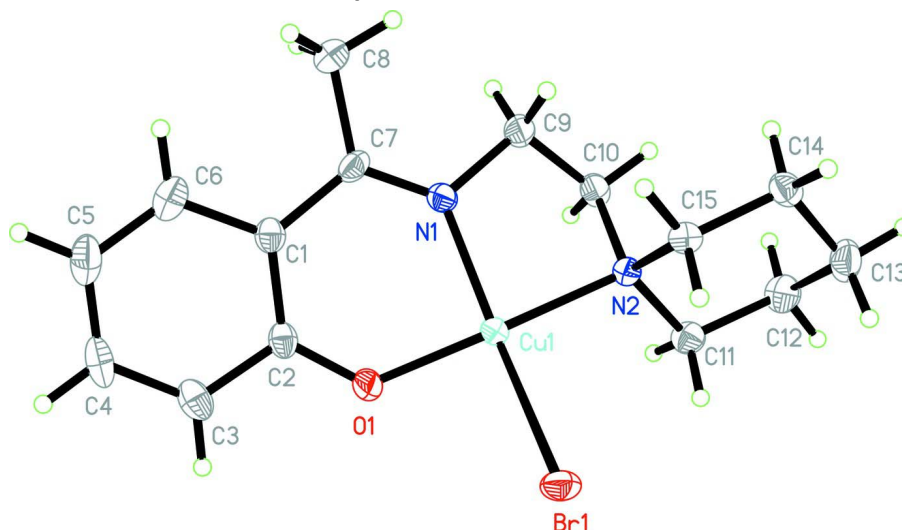


Figure 1

The structure of the title complex, showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

Bromido(2-{1-[2-(piperidin-1-yl)ethylimino]ethyl}phenolato)copper(II)

Crystal data

[CuBr(C₁₅H₂₁N₂O)]

$M_r = 388.79$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 10.988$ (3) Å

$b = 17.181$ (5) Å

$c = 8.173$ (2) Å

$\beta = 92.366$ (3)°

$V = 1541.6$ (7) Å³

$Z = 4$

$F(000) = 788$

$D_x = 1.675$ Mg m⁻³

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

Cell parameters from 2701 reflections

$\theta = 2.3$ – 26.3 °

$\mu = 4.01$ mm⁻¹

$T = 298$ K
Block, blue

$0.27 \times 0.23 \times 0.23$ mm

Data collection

Bruker SMART CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 ω scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\min} = 0.411$, $T_{\max} = 0.459$

9503 measured reflections
3357 independent reflections
2373 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
 $h = -12 \rightarrow 14$
 $k = -21 \rightarrow 21$
 $l = -7 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.084$
 $S = 1.06$
3357 reflections
182 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
 $w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 0.4765P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.40 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.49 \text{ e } \text{\AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.50444 (4)	0.13785 (2)	0.50364 (5)	0.02851 (12)
N1	0.6334 (3)	0.12175 (16)	0.3495 (3)	0.0315 (7)
N2	0.3861 (2)	0.12461 (14)	0.3077 (3)	0.0257 (6)
O1	0.6161 (2)	0.17983 (15)	0.6586 (3)	0.0441 (7)
Br1	0.36084 (4)	0.10855 (2)	0.70885 (4)	0.04276 (13)
C1	0.8014 (3)	0.13107 (19)	0.5452 (4)	0.0327 (8)
C2	0.7327 (3)	0.16805 (19)	0.6674 (4)	0.0318 (8)
C3	0.7973 (4)	0.1946 (2)	0.8102 (5)	0.0428 (9)
H3	0.7548	0.2208	0.8895	0.051*
C4	0.9194 (4)	0.1831 (2)	0.8359 (5)	0.0514 (11)
H4	0.9586	0.2013	0.9314	0.062*
C5	0.9849 (4)	0.1445 (3)	0.7204 (6)	0.0580 (12)
H5	1.0677	0.1355	0.7386	0.070*
C6	0.9266 (3)	0.1197 (2)	0.5789 (5)	0.0498 (11)

H6	0.9717	0.0942	0.5015	0.060*
C7	0.7472 (3)	0.1122 (2)	0.3834 (4)	0.0333 (8)
C8	0.8306 (4)	0.0842 (3)	0.2529 (5)	0.0555 (12)
H8A	0.7826	0.0659	0.1599	0.083*
H8B	0.8807	0.0426	0.2959	0.083*
H8C	0.8815	0.1264	0.2202	0.083*
C9	0.5824 (3)	0.1139 (2)	0.1796 (4)	0.0401 (9)
H9A	0.5748	0.0594	0.1503	0.048*
H9B	0.6357	0.1388	0.1038	0.048*
C10	0.4607 (3)	0.1519 (2)	0.1714 (4)	0.0354 (9)
H10A	0.4705	0.2079	0.1781	0.042*
H10B	0.4192	0.1397	0.0675	0.042*
C11	0.2726 (3)	0.1720 (2)	0.3175 (4)	0.0365 (9)
H11A	0.2943	0.2267	0.3228	0.044*
H11B	0.2327	0.1589	0.4174	0.044*
C12	0.1837 (4)	0.1588 (2)	0.1714 (5)	0.0478 (10)
H12A	0.1102	0.1888	0.1863	0.057*
H12B	0.2202	0.1769	0.0722	0.057*
C13	0.1513 (4)	0.0739 (3)	0.1531 (5)	0.0514 (11)
H13A	0.1009	0.0664	0.0542	0.062*
H13B	0.1050	0.0574	0.2455	0.062*
C14	0.2659 (3)	0.0248 (2)	0.1448 (4)	0.0368 (9)
H14A	0.2440	-0.0299	0.1429	0.044*
H14B	0.3066	0.0365	0.0446	0.044*
C15	0.3516 (3)	0.04072 (19)	0.2906 (4)	0.0300 (8)
H15A	0.3132	0.0240	0.3895	0.036*
H15B	0.4250	0.0100	0.2801	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0263 (2)	0.0346 (2)	0.0246 (2)	0.00112 (18)	0.00036 (16)	-0.00404 (17)
N1	0.0309 (18)	0.0366 (17)	0.0272 (16)	-0.0056 (12)	0.0035 (12)	-0.0042 (12)
N2	0.0262 (16)	0.0254 (15)	0.0255 (15)	0.0003 (11)	0.0006 (11)	0.0015 (11)
O1	0.0312 (15)	0.0577 (17)	0.0430 (16)	0.0065 (12)	-0.0044 (11)	-0.0243 (13)
Br1	0.0439 (3)	0.0565 (3)	0.0286 (2)	0.00307 (19)	0.00991 (16)	0.00076 (18)
C1	0.031 (2)	0.0294 (18)	0.037 (2)	-0.0027 (15)	-0.0023 (15)	0.0009 (15)
C2	0.032 (2)	0.0254 (17)	0.038 (2)	-0.0024 (15)	-0.0060 (15)	-0.0011 (16)
C3	0.053 (3)	0.033 (2)	0.041 (2)	-0.0026 (18)	-0.0108 (18)	-0.0011 (17)
C4	0.047 (3)	0.053 (3)	0.052 (3)	-0.011 (2)	-0.025 (2)	0.008 (2)
C5	0.038 (3)	0.072 (3)	0.062 (3)	-0.001 (2)	-0.016 (2)	0.011 (3)
C6	0.032 (2)	0.056 (3)	0.062 (3)	0.0000 (18)	0.001 (2)	0.006 (2)
C7	0.023 (2)	0.0343 (19)	0.044 (2)	-0.0033 (15)	0.0089 (16)	-0.0029 (16)
C8	0.032 (2)	0.083 (3)	0.052 (3)	0.000 (2)	0.0083 (19)	-0.019 (2)
C9	0.033 (2)	0.059 (2)	0.029 (2)	-0.0121 (18)	0.0057 (16)	-0.0005 (18)
C10	0.037 (2)	0.041 (2)	0.0274 (19)	-0.0124 (17)	0.0010 (15)	0.0044 (16)
C11	0.037 (2)	0.034 (2)	0.039 (2)	0.0100 (16)	0.0004 (16)	-0.0004 (17)
C12	0.038 (2)	0.058 (3)	0.047 (2)	0.018 (2)	-0.0096 (18)	0.003 (2)

C13	0.036 (2)	0.074 (3)	0.043 (2)	-0.011 (2)	-0.0067 (18)	0.005 (2)
C14	0.042 (2)	0.036 (2)	0.033 (2)	-0.0079 (17)	0.0008 (16)	-0.0017 (16)
C15	0.034 (2)	0.0250 (18)	0.0307 (19)	0.0006 (15)	0.0042 (15)	0.0024 (15)

Geometric parameters (Å, °)

Cu1—O1	1.872 (3)	C8—H8A	0.9600
Cu1—N1	1.954 (3)	C8—H8B	0.9600
Cu1—N2	2.034 (3)	C8—H8C	0.9600
Cu1—Br1	2.4030 (7)	C9—C10	1.487 (5)
N1—C7	1.281 (4)	C9—H9A	0.9700
N1—C9	1.482 (5)	C9—H9B	0.9700
N2—C10	1.485 (4)	C10—H10A	0.9700
N2—C11	1.493 (4)	C10—H10B	0.9700
N2—C15	1.495 (4)	C11—C12	1.528 (5)
O1—C2	1.296 (4)	C11—H11A	0.9700
C1—C6	1.405 (5)	C11—H11B	0.9700
C1—C2	1.425 (5)	C12—C13	1.508 (6)
C1—C7	1.464 (5)	C12—H12A	0.9700
C2—C3	1.417 (5)	C12—H12B	0.9700
C3—C4	1.364 (5)	C13—C14	1.520 (5)
C3—H3	0.9300	C13—H13A	0.9700
C4—C5	1.380 (6)	C13—H13B	0.9700
C4—H4	0.9300	C14—C15	1.513 (5)
C5—C6	1.366 (6)	C14—H14A	0.9700
C5—H5	0.9300	C14—H14B	0.9700
C6—H6	0.9300	C15—H15A	0.9700
C7—C8	1.512 (5)	C15—H15B	0.9700
O1—Cu1—N1	91.04 (11)	N1—C9—C10	107.9 (3)
O1—Cu1—N2	162.99 (11)	N1—C9—H9A	110.1
N1—Cu1—N2	86.20 (11)	C10—C9—H9A	110.1
O1—Cu1—Br1	92.26 (8)	N1—C9—H9B	110.1
N1—Cu1—Br1	159.19 (8)	C10—C9—H9B	110.1
N2—Cu1—Br1	96.27 (8)	H9A—C9—H9B	108.4
C7—N1—C9	121.3 (3)	N2—C10—C9	110.6 (3)
C7—N1—Cu1	127.4 (2)	N2—C10—H10A	109.5
C9—N1—Cu1	111.1 (2)	C9—C10—H10A	109.5
C10—N2—C11	110.8 (3)	N2—C10—H10B	109.5
C10—N2—C15	112.3 (2)	C9—C10—H10B	109.5
C11—N2—C15	108.8 (3)	H10A—C10—H10B	108.1
C10—N2—Cu1	101.6 (2)	N2—C11—C12	112.7 (3)
C11—N2—Cu1	113.9 (2)	N2—C11—H11A	109.1
C15—N2—Cu1	109.4 (2)	C12—C11—H11A	109.1
C2—O1—Cu1	126.6 (2)	N2—C11—H11B	109.1
C6—C1—C2	117.8 (3)	C12—C11—H11B	109.1
C6—C1—C7	120.3 (3)	H11A—C11—H11B	107.8
C2—C1—C7	121.6 (3)	C13—C12—C11	111.2 (3)

O1—C2—C3	117.1 (3)	C13—C12—H12A	109.4
O1—C2—C1	125.6 (3)	C11—C12—H12A	109.4
C3—C2—C1	117.4 (3)	C13—C12—H12B	109.4
C4—C3—C2	122.4 (4)	C11—C12—H12B	109.4
C4—C3—H3	118.8	H12A—C12—H12B	108.0
C2—C3—H3	118.8	C12—C13—C14	110.4 (3)
C3—C4—C5	120.1 (4)	C12—C13—H13A	109.6
C3—C4—H4	119.9	C14—C13—H13A	109.6
C5—C4—H4	119.9	C12—C13—H13B	109.6
C6—C5—C4	119.3 (4)	C14—C13—H13B	109.6
C6—C5—H5	120.4	H13A—C13—H13B	108.1
C4—C5—H5	120.4	C15—C14—C13	110.7 (3)
C5—C6—C1	122.9 (4)	C15—C14—H14A	109.5
C5—C6—H6	118.5	C13—C14—H14A	109.5
C1—C6—H6	118.5	C15—C14—H14B	109.5
N1—C7—C1	121.6 (3)	C13—C14—H14B	109.5
N1—C7—C8	120.2 (3)	H14A—C14—H14B	108.1
C1—C7—C8	118.2 (3)	N2—C15—C14	113.3 (3)
C7—C8—H8A	109.5	N2—C15—H15A	108.9
C7—C8—H8B	109.5	C14—C15—H15A	108.9
H8A—C8—H8B	109.5	N2—C15—H15B	108.9
C7—C8—H8C	109.5	C14—C15—H15B	108.9
H8A—C8—H8C	109.5	H15A—C15—H15B	107.7
H8B—C8—H8C	109.5		
