Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bromido(2-{1-[2-(morpholin-4-yl)ethylimino]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

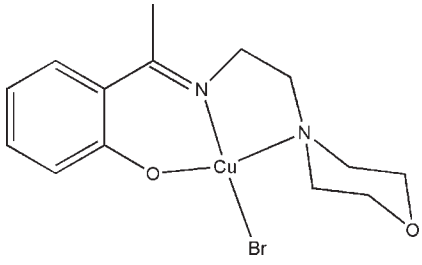
Received 5 July 2010; accepted 6 July 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; R factor = 0.074; wR factor = 0.171; data-to-parameter ratio = 17.6.

In the title complex, [$CuBr(C_{14}H_{19}N_2O_2)$], 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, with the N atoms in a *cis* arrangement. The morpholine ring adopts a chair conformation.

Related literature

For background to Schiff base complexes and a related structure, see: Zhao (2008). For similar copper(II) complexes with Schiff bases, see: Zhu *et al.* (2005); Ni *et al.* (2005); Zhu (2010); Suleiman Gwaram *et al.* (2010).



Experimental

Crystal data

[$CuBr(C_{14}H_{19}N_2O_2)$]
M_r = 390.76
Monoclinic, $P2_1/c$
a = 10.808 (2) Å
b = 17.152 (3) Å
c = 8.107 (2) Å
β = 90.059 (1)°
V = 1502.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.11 mm^{-1}
T = 298 K
0.32 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.353, T_{max} = 0.372
9814 measured reflections
3211 independent reflections
2506 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.171
S = 1.13
3211 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.877 (6)	Cu1—N2	2.095 (6)
Cu1—N1	1.917 (7)	Cu1—Br1	2.4006 (14)
O1—Cu1—N1	91.1 (3)	O1—Cu1—Br1	92.2 (2)
O1—Cu1—N2	161.7 (3)	N1—Cu1—Br1	157.9 (2)
N1—Cu1—N2	87.5 (2)	N2—Cu1—Br1	95.99 (16)

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*.

Financial support from the Shaoxing University research fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5543).

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supporting information

Acta Cryst. (2010). E**66**, m912 [https://doi.org/10.1107/S160053681002670X]

Bromido(2-{1-[2-(morpholin-4-yl)ethylimino]ethyl}phenolato)copper(II)

Xiao-Fan Zhao and Fang Li

S1. Comment

As part of our ongoing studies of Schiff base complexes (e.g. Zhao, 2008), the title mononuclear copper(II) complex, (I), is reported here.

In the title complex, the Cu atom is four-coordinated by one phenolate O, one imine N, and one amine N atoms of 2-[1-(2-morpholin-4-ylethylimino)ethyl]phenolate, and by one bromide atom, forming a square planar geometry (Fig. 1). The bond lengths (Table 1) in the square planar coordination are comparable with those reported in similar copper structures with Schiff bases (Zhu *et al.*, 2005; Ni *et al.*, 2005; Zhu, 2010; Suleiman Gwaram *et al.*, 2010).

S2. Experimental

1-(2-Hydroxyphenyl)ethanone (1 mmol, 136 mg), 2-morpholin-4-ylethylamine (1 mmol, 130 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 week, and blue blocks of (I) were formed.

S3. 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_{iso}(H) = 1.2 or 1.5U_{eq}(C).

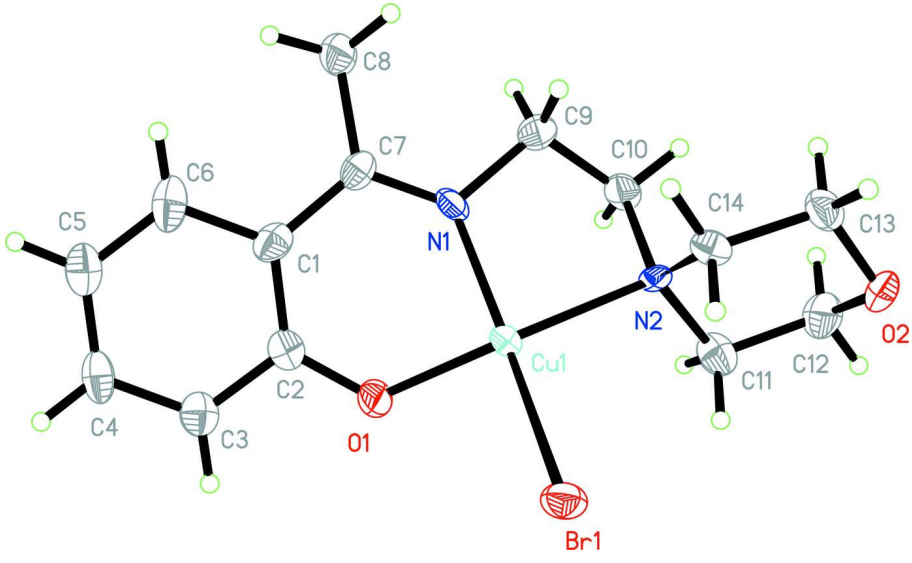

Figure 1

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

Bromido(2-{1-[2-(morpholin-4-yl)ethylimino]ethyl}phenolato)copper(II)

Crystal data

[CuBr($C_{14}H_{19}N_2O_2$)]
M_r = 390.76
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.808 (2) Å
b = 17.152 (3) Å
c = 8.107 (2) Å
β = 90.059 (1)°
V = 1502.9 (5) Å^3
Z = 4
$F(000)$ = 788
D_x = 1.727 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3491 reflections
θ = 2.7–26.4°
μ = 4.11 mm^{-1}
T = 298 K
Block, blue
0.32 × 0.30 × 0.30 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} = 0.353, T_{max} = 0.372
9814 measured reflections
3211 independent reflections
2506 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.0°, θ_{min} = 2.2°
h = −13→12
k = −21→21
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.171
S = 1.13
3211 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
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 17.4414P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.98896 (9)	0.13655 (6)	0.00058 (11)	0.0314 (3)
Br1	1.13378 (9)	0.10662 (6)	−0.21461 (11)	0.0482 (3)
N1	0.8594 (6)	0.1190 (4)	0.1576 (8)	0.0364 (16)
N2	1.1147 (5)	0.1243 (4)	0.1957 (7)	0.0268 (13)

O1	0.8763 (6)	0.1804 (4)	−0.1494 (8)	0.0513 (17)
O2	1.3588 (5)	0.0900 (4)	0.3093 (9)	0.0535 (17)
C1	0.6903 (8)	0.1273 (5)	−0.0276 (12)	0.042 (2)
C2	0.7578 (8)	0.1655 (5)	−0.1526 (11)	0.0408 (19)
C3	0.6965 (9)	0.1916 (5)	−0.2956 (12)	0.045 (2)
H3	0.7402	0.2196	−0.3746	0.054*
C4	0.5723 (9)	0.1763 (6)	−0.3203 (13)	0.055 (3)
H4	0.5337	0.1924	−0.4171	0.066*
C5	0.5052 (10)	0.1369 (7)	−0.2008 (14)	0.062 (3)
H5	0.4218	0.1262	−0.2180	0.075*
C6	0.5630 (9)	0.1130 (6)	−0.0536 (14)	0.055 (3)
H6	0.5170	0.0877	0.0272	0.066*
C7	0.7411 (7)	0.1089 (5)	0.1327 (11)	0.0368 (18)
C8	0.6584 (9)	0.0816 (7)	0.2725 (13)	0.060 (3)
H8A	0.7001	0.0418	0.3345	0.090*
H8B	0.5829	0.0609	0.2279	0.090*
H8C	0.6398	0.1248	0.3436	0.090*
C9	0.9094 (8)	0.1095 (6)	0.3272 (11)	0.046 (2)
H9A	0.8534	0.1327	0.4068	0.055*
H9B	0.9184	0.0546	0.3532	0.055*
C10	1.0320 (8)	0.1490 (5)	0.3342 (10)	0.041 (2)
H10A	1.0717	0.1369	0.4385	0.050*
H10B	1.0199	0.2050	0.3292	0.050*
C11	1.2203 (9)	0.1793 (5)	0.1721 (12)	0.049 (2)
H11A	1.1904	0.2326	0.1744	0.058*
H11B	1.2586	0.1701	0.0657	0.058*
C12	1.3139 (9)	0.1672 (7)	0.3076 (14)	0.059 (3)
H12A	1.3826	0.2029	0.2920	0.070*
H12B	1.2760	0.1789	0.4132	0.070*
C13	1.2577 (9)	0.0373 (6)	0.3351 (11)	0.048 (2)
H13A	1.2214	0.0473	0.4423	0.057*
H13B	1.2888	−0.0158	0.3352	0.057*
C14	1.1597 (8)	0.0450 (5)	0.2050 (10)	0.0362 (18)
H14A	1.1934	0.0298	0.0990	0.043*
H14B	1.0914	0.0102	0.2304	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0325 (5)	0.0353 (5)	0.0264 (5)	−0.0002 (4)	−0.0019 (4)	0.0039 (4)
Br1	0.0548 (6)	0.0576 (6)	0.0322 (5)	−0.0018 (4)	0.0064 (4)	0.0000 (4)
N1	0.038 (4)	0.044 (4)	0.027 (3)	0.008 (3)	−0.006 (3)	0.008 (3)
N2	0.026 (3)	0.038 (4)	0.017 (3)	−0.008 (3)	0.006 (2)	−0.010 (2)
O1	0.039 (3)	0.060 (4)	0.055 (4)	−0.004 (3)	−0.009 (3)	0.030 (3)
O2	0.028 (3)	0.068 (5)	0.064 (4)	0.005 (3)	0.003 (3)	0.014 (4)
C1	0.039 (5)	0.029 (4)	0.058 (6)	−0.002 (3)	−0.001 (4)	0.009 (4)
C2	0.046 (5)	0.036 (5)	0.040 (5)	0.006 (4)	−0.005 (4)	−0.004 (4)
C3	0.049 (5)	0.038 (5)	0.048 (5)	0.006 (4)	−0.008 (4)	0.001 (4)

C4	0.046 (6)	0.058 (6)	0.061 (6)	0.013 (5)	−0.024 (5)	−0.003 (5)
C5	0.052 (6)	0.068 (7)	0.068 (7)	−0.002 (5)	−0.024 (5)	−0.012 (6)
C6	0.039 (5)	0.058 (6)	0.068 (7)	0.005 (4)	−0.012 (5)	−0.007 (5)
C7	0.029 (4)	0.035 (4)	0.046 (5)	0.006 (3)	0.006 (3)	−0.005 (4)
C8	0.036 (5)	0.091 (8)	0.054 (6)	0.013 (5)	0.003 (4)	0.018 (6)
C9	0.038 (5)	0.065 (6)	0.035 (5)	0.005 (4)	0.011 (4)	−0.001 (4)
C10	0.043 (5)	0.052 (5)	0.029 (4)	0.007 (4)	0.002 (3)	−0.006 (4)
C11	0.061 (6)	0.034 (5)	0.051 (6)	−0.004 (4)	−0.012 (5)	0.003 (4)
C12	0.041 (5)	0.069 (7)	0.066 (7)	−0.014 (5)	−0.011 (5)	−0.009 (6)
C13	0.053 (6)	0.049 (6)	0.041 (5)	0.014 (4)	−0.004 (4)	0.008 (4)
C14	0.045 (5)	0.030 (4)	0.035 (4)	0.002 (3)	0.003 (4)	−0.001 (3)

Geometric parameters (Å, º)

Cu1—O1	1.877 (6)	C5—H5	0.9300
Cu1—N1	1.917 (7)	C6—H6	0.9300
Cu1—N2	2.095 (6)	C7—C8	1.518 (12)
Cu1—Br1	2.4006 (14)	C8—H8A	0.9600
N1—C7	1.306 (11)	C8—H8B	0.9600
N1—C9	1.486 (11)	C8—H8C	0.9600
N2—C14	1.447 (10)	C9—C10	1.489 (13)
N2—C11	1.494 (11)	C9—H9A	0.9700
N2—C10	1.497 (9)	C9—H9B	0.9700
O1—C2	1.306 (11)	C10—H10A	0.9700
O2—C12	1.411 (13)	C10—H10B	0.9700
O2—C13	1.434 (12)	C11—C12	1.508 (13)
C1—C6	1.413 (12)	C11—H11A	0.9700
C1—C2	1.411 (12)	C11—H11B	0.9700
C1—C7	1.445 (12)	C12—H12A	0.9700
C2—C3	1.408 (12)	C12—H12B	0.9700
C3—C4	1.382 (13)	C13—C14	1.500 (12)
C3—H3	0.9300	C13—H13A	0.9700
C4—C5	1.387 (16)	C13—H13B	0.9700
C4—H4	0.9300	C14—H14A	0.9700
C5—C6	1.407 (14)	C14—H14B	0.9700
O1—Cu1—N1	91.1 (3)	H8A—C8—H8B	109.5
O1—Cu1—N2	161.7 (3)	C7—C8—H8C	109.5
N1—Cu1—N2	87.5 (2)	H8A—C8—H8C	109.5
O1—Cu1—Br1	92.2 (2)	H8B—C8—H8C	109.5
N1—Cu1—Br1	157.9 (2)	C10—C9—N1	108.0 (7)
N2—Cu1—Br1	95.99 (16)	C10—C9—H9A	110.1
C7—N1—C9	118.9 (7)	N1—C9—H9A	110.1
C7—N1—Cu1	129.3 (6)	C10—C9—H9B	110.1
C9—N1—Cu1	111.5 (5)	N1—C9—H9B	110.1
C14—N2—C11	110.1 (6)	H9A—C9—H9B	108.4
C14—N2—C10	115.3 (6)	C9—C10—N2	112.0 (7)
C11—N2—C10	112.0 (6)	C9—C10—H10A	109.2

C14—N2—Cu1	110.6 (5)	N2—C10—H10A	109.2
C11—N2—Cu1	109.6 (5)	C9—C10—H10B	109.2
C10—N2—Cu1	98.7 (5)	N2—C10—H10B	109.2
C2—O1—Cu1	124.8 (6)	H10A—C10—H10B	107.9
C12—O2—C13	109.3 (7)	N2—C11—C12	109.4 (7)
C6—C1—C2	118.5 (9)	N2—C11—H11A	109.8
C6—C1—C7	117.7 (8)	C12—C11—H11A	109.8
C2—C1—C7	123.4 (8)	N2—C11—H11B	109.8
O1—C2—C3	114.5 (8)	C12—C11—H11B	109.8
O1—C2—C1	125.8 (8)	H11A—C11—H11B	108.2
C3—C2—C1	119.7 (8)	O2—C12—C11	111.5 (8)
C4—C3—C2	121.0 (9)	O2—C12—H12A	109.3
C4—C3—H3	119.5	C11—C12—H12A	109.3
C2—C3—H3	119.5	O2—C12—H12B	109.3
C5—C4—C3	120.0 (9)	C11—C12—H12B	109.3
C5—C4—H4	120.0	H12A—C12—H12B	108.0
C3—C4—H4	120.0	O2—C13—C14	112.3 (7)
C4—C5—C6	120.2 (10)	O2—C13—H13A	109.1
C4—C5—H5	119.9	C14—C13—H13A	109.1
C6—C5—H5	119.9	O2—C13—H13B	109.1
C5—C6—C1	120.5 (10)	C14—C13—H13B	109.1
C5—C6—H6	119.7	H13A—C13—H13B	107.9
C1—C6—H6	119.7	N2—C14—C13	110.9 (7)
N1—C7—C1	118.8 (8)	N2—C14—H14A	109.5
N1—C7—C8	120.2 (8)	C13—C14—H14A	109.5
C1—C7—C8	121.0 (8)	N2—C14—H14B	109.5
C7—C8—H8A	109.5	C13—C14—H14B	109.5
C7—C8—H8B	109.5	H14A—C14—H14B	108.1