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Chlorido[2,4-dibromo-6-(2-pyridylmethylaminomethyl)phenolato]copper(II)

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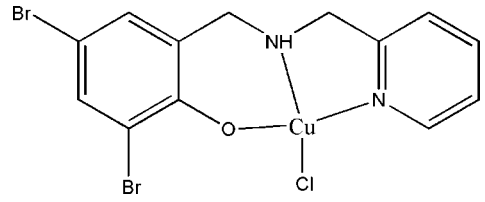
Key indicators: single-crystal X-ray study; T = 305 K; mean σ(C–C) = 0.009 Å; R factor = 0.051; wR factor = 0.137; data-to-parameter ratio = 18.8.

In the title compound, [Cu($C_{13}H_{11}Br_2N_2O$)Cl], the Cu^{II} atom is four-coordinated by an *N*,*N*,*O*-tridentate 2,4-dibromo-6-(2-pyridylmethylaminomethyl)phenolate ligand and a chloride ion in a distorted square-planar arrangement. An N—H···O hydrogen bond helps to stabilize the struture.

Related literature

For background, see: Solomon *et al.* (1996); Ma *et al.* (2007).



Experimental

Crystal data

[Cu($C_{13}H_{11}Br_2N_2O$)Cl]
M_r = 470.05
Monoclinic, $P2_1/c$
a = 13.447 (4) Å
b = 16.628 (5) Å
c = 6.881 (2) Å
β = 99.179 (4)°
V = 1518.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.87 mm^{-1}
T = 305 (2) K
0.32 × 0.26 × 0.20 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.133, T_{max} = 0.251
8786 measured reflections
3459 independent reflections
2044 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.137
S = 0.94
3459 reflections
184 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.923 (4)	Cu1—N1	2.011 (5)
Cu1—N2	2.001 (4)	Cu1—Cl1	2.2517 (16)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O1^{i}	0.94 (4)	2.14 (5)	2.918 (6)	139 (5)

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2515).

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supplementary materials

Acta Cryst. (2007). E**63**, m2431 [**doi:10.1107/S1600536807041669**]

Chlorido[2,4-dibromo-6-(2-pyridylmethylaminomethyl)phenolato]copper(II)

J.-C. Ma, J. Yang and J.-F. Ma

Comment

Copper(II) complexes with various organic ligands have been a subject of intense study because of their important biological properties (Solomon *et al.*, 1996). Here, we report the synthesis and structure of the new title complex, Cu(dmp)Cl, (I), where dmp is 2,4-dibromo-6((pyridine-2-ylmethylamino)methy)phenol.

Selected bond lengths are listed in Table 1. The Cu^{II} atom is four-coordinated by one pyridine N atom, one amine N atom and one phenolate O atom from the ligand and one chloride ion in a distorted square-planar arangement (Fig. 1). The metal to ligand-atom distances in (I) are similar to the ones found in bis[2,4-dibromo-6((pyridnine-2-ylmethylamino)methy) phenolato]bis[nitratocopper(II)] (Ma *et al.*, 2007).

An N—H···O hydrogen bond (Table 2) helps to stabilize the packing in (I).

Experimental

2,4-Dibromo-6-((pyridine-2-ylmethylamino)methyl)phenol (0.372 g, 1 mmol) was added to a methanol solution (20 ml) of $CuCl_2{\cdot}2H_2O$ (0.170 g, 1 mmol) with stirring. The resulting solution was left to stand at room temperture and blue blocks of (I) were obtained after several days.

Refinement

All H-atoms bound to carbon were refined using a riding model [C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C)]. The amino H atom was located in a difference map and it sposition was freely refined with U_{iso}(H) = 1.2 U_{eq}(N).

Figures

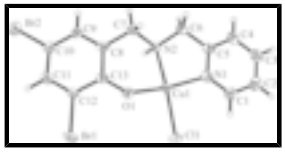

Fig. 1. A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms).

Chlorido[2,4-dibromo-6-(2-pyridylmethylaminomethyl)phenolato]copper(II)

Crystal data

$[Cu(C_{13}H_{11}Br_2N_2O)Cl]$	F_{000} = 908
M_r = 470.05	D_x = 2.056 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8947 reflections
a = 13.447 (4) Å	θ = 2.0–28.2º
b = 16.628 (5) Å	μ = 6.87 mm^{-1}
c = 6.881 (2) Å	T = 305 (2) K
β = 99.179 (4)º	Block, blue
V = 1518.8 (8) $Å^3$	0.32 × 0.26 × 0.20 mm
Z = 4	

Data collection

Bruker APEX CCD diffractometer	3459 independent reflections
Radiation source: fine-focus sealed tube	2044 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 305(2) K	θ_{max} = 28.2º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -17 \rightarrow 11$
T_{min} = 0.133, T_{max} = 0.251	$k = -21 \rightarrow 20$
8786 measured reflections	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.137	$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.94	$(\Delta/\sigma)_{max} < 0.001$
3459 reflections	$\Delta\rho_{max}$ = 1.04 e $Å^{-3}$
184 parameters	$\Delta\rho_{min}$ = −0.83 e $Å^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	−0.0249 (5)	0.1997 (4)	0.2698 (10)	0.0567 (18)
H1	−0.0348	0.2549	0.2769	0.068*
C2	−0.1045 (5)	0.1518 (5)	0.1881 (12)	0.071 (2)
H2	−0.1667	0.1746	0.1402	0.085*
C3	−0.0908 (5)	0.0702 (4)	0.1784 (10)	0.064 (2)
H3	−0.1436	0.0370	0.1239	0.077*
C4	0.0020 (5)	0.0386 (4)	0.2504 (10)	0.0555 (17)
H4	0.0131	−0.0165	0.2453	0.067*
C5	0.0794 (4)	0.0900 (3)	0.3312 (9)	0.0433 (14)
C6	0.1807 (4)	0.0582 (3)	0.4151 (10)	0.0517 (16)
H6A	0.1775	0.0324	0.5405	0.062*
H6B	0.2010	0.0180	0.3269	0.062*
C7	0.3373 (4)	0.1065 (3)	0.6124 (9)	0.0423 (14)
H7A	0.3642	0.0530	0.5977	0.051*
H7B	0.3093	0.1074	0.7338	0.051*
C8	0.4210 (4)	0.1665 (3)	0.6255 (8)	0.0376 (13)
C9	0.5188 (4)	0.1412 (3)	0.6364 (8)	0.0388 (13)
H9	0.5326	0.0864	0.6338	0.047*
C10	0.5971 (4)	0.1957 (4)	0.6513 (9)	0.0442 (14)
C11	0.5778 (4)	0.2781 (4)	0.6515 (9)	0.0460 (15)
H11	0.6303	0.3150	0.6598	0.055*
C12	0.4791 (4)	0.3039 (3)	0.6390 (8)	0.0381 (13)
C13	0.3969 (4)	0.2501 (3)	0.6281 (8)	0.0358 (13)
N1	0.0656 (3)	0.1695 (3)	0.3389 (7)	0.0453 (12)
N2	0.2557 (3)	0.1231 (3)	0.4435 (7)	0.0372 (11)
O1	0.3038 (3)	0.2762 (2)	0.6237 (6)	0.0431 (10)
Cu1	0.19000 (5)	0.23063 (4)	0.45485 (11)	0.0392 (2)
Br1	0.45266 (5)	0.41577 (3)	0.63413 (9)	0.0508 (2)
Br2	0.73138 (5)	0.15965 (5)	0.66154 (15)	0.0798 (3)
Cl1	0.12562 (12)	0.35288 (9)	0.3686 (3)	0.0528 (4)
H2N	0.291 (4)	0.133 (4)	0.337 (8)	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.045 (4)	0.049 (4)	0.073 (5)	0.002 (3)	−0.002 (3)	−0.009 (3)
C2	0.043 (4)	0.069 (6)	0.093 (6)	0.002 (3)	−0.009 (4)	0.003 (4)
C3	0.061 (4)	0.055 (5)	0.072 (5)	−0.019 (3)	−0.003 (4)	0.002 (4)
C4	0.053 (4)	0.045 (4)	0.066 (5)	−0.012 (3)	0.002 (3)	−0.005 (3)
C5	0.056 (4)	0.032 (3)	0.041 (4)	−0.005 (3)	0.005 (3)	−0.004 (3)
C6	0.054 (4)	0.024 (3)	0.075 (5)	−0.008 (3)	0.004 (3)	−0.005 (3)
C7	0.050 (3)	0.027 (3)	0.050 (4)	0.003 (2)	0.007 (3)	0.002 (3)
C8	0.055 (3)	0.022 (3)	0.034 (3)	0.002 (2)	0.000 (3)	−0.001 (2)
C9	0.041 (3)	0.033 (3)	0.038 (3)	0.004 (2)	−0.007 (2)	−0.001 (2)

C10	0.046 (3)	0.039 (4)	0.046 (4)	0.008 (3)	0.000 (3)	−0.001 (3)
C11	0.050 (4)	0.042 (4)	0.045 (4)	−0.010 (3)	0.003 (3)	−0.005 (3)
C12	0.049 (3)	0.024 (3)	0.039 (3)	0.001 (2)	0.002 (3)	0.001 (2)
C13	0.045 (3)	0.029 (3)	0.032 (3)	0.002 (2)	0.004 (2)	−0.004 (2)
N1	0.046 (3)	0.039 (3)	0.050 (3)	−0.003 (2)	0.006 (2)	−0.006 (2)
N2	0.038 (3)	0.023 (2)	0.049 (3)	−0.0042 (19)	0.002 (2)	0.002 (2)
O1	0.045 (2)	0.028 (2)	0.053 (3)	0.0031 (16)	−0.0033 (18)	−0.0094 (18)
Cu1	0.0457 (4)	0.0235 (4)	0.0461 (5)	0.0024 (3)	0.0001 (3)	−0.0024 (3)
Br1	0.0744 (5)	0.0233 (3)	0.0519 (4)	−0.0046 (3)	0.0015 (3)	−0.0005 (3)
Br2	0.0459 (4)	0.0605 (5)	0.1286 (8)	0.0074 (3)	0.0000 (4)	−0.0052 (5)
Cl1	0.0572 (9)	0.0307 (8)	0.0698 (11)	0.0100 (6)	0.0079 (8)	0.0083 (7)

Geometric parameters (Å, °)

C1—N1	1.331 (7)	C7—H7B	0.9700
C1—C2	1.379 (9)	C8—C9	1.372 (7)
C1—H1	0.9300	C8—C13	1.428 (7)
C2—C3	1.372 (9)	C9—C10	1.380 (8)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.373 (9)	C10—C11	1.395 (8)
C3—H3	0.9300	C10—Br2	1.893 (6)
C4—C5	1.392 (8)	C11—C12	1.385 (8)
C4—H4	0.9300	C11—H11	0.9300
C5—N1	1.338 (7)	C12—C13	1.414 (8)
C5—C6	1.490 (8)	C12—Br1	1.893 (5)
C6—N2	1.469 (7)	C13—O1	1.321 (6)
C6—H6A	0.9700	N2—H2N	0.94 (4)
C6—H6B	0.9700	Cu1—O1	1.923 (4)
C7—N2	1.492 (7)	Cu1—N2	2.001 (4)
C7—C8	1.496 (7)	Cu1—N1	2.011 (5)
C7—H7A	0.9700	Cu1—Cl1	2.2517 (16)
N1—C1—C2	122.3 (6)	C8—C9—H9	119.5
N1—C1—H1	118.9	C10—C9—H9	119.5
C2—C1—H1	118.9	C9—C10—C11	120.4 (5)
C3—C2—C1	119.3 (6)	C9—C10—Br2	120.5 (4)
C3—C2—H2	120.4	C11—C10—Br2	119.1 (4)
C1—C2—H2	120.4	C12—C11—C10	118.8 (5)
C2—C3—C4	118.9 (6)	C12—C11—H11	120.6
C2—C3—H3	120.6	C10—C11—H11	120.6
C4—C3—H3	120.6	C11—C12—C13	122.7 (5)
C3—C4—C5	119.2 (6)	C11—C12—Br1	118.8 (4)
C3—C4—H4	120.4	C13—C12—Br1	118.6 (4)
C5—C4—H4	120.4	O1—C13—C12	121.5 (5)
N1—C5—C4	121.6 (6)	O1—C13—C8	122.4 (5)
N1—C5—C6	117.4 (5)	C12—C13—C8	116.1 (5)
C4—C5—C6	121.0 (6)	C1—N1—C5	118.9 (5)
N2—C6—C5	110.9 (5)	C1—N1—Cu1	127.4 (4)
N2—C6—H6A	109.5	C5—N1—Cu1	113.8 (4)
C5—C6—H6A	109.5	C6—N2—C7	111.8 (4)

N2—C6—H6B	109.5	C6—N2—Cu1	111.3 (4)
C5—C6—H6B	109.5	C7—N2—Cu1	114.2 (3)
H6A—C6—H6B	108.1	C6—N2—H2N	116 (4)
N2—C7—C8	112.1 (5)	C7—N2—H2N	104 (4)
N2—C7—H7A	109.2	Cu1—N2—H2N	99 (4)
C8—C7—H7A	109.2	C13—O1—Cu1	123.0 (3)
N2—C7—H7B	109.2	O1—Cu1—N2	93.56 (16)
C8—C7—H7B	109.2	O1—Cu1—N1	166.0 (2)
H7A—C7—H7B	107.9	N2—Cu1—N1	82.99 (19)
C9—C8—C13	121.0 (5)	O1—Cu1—Cl1	92.22 (12)
C9—C8—C7	120.2 (5)	N2—Cu1—Cl1	161.76 (15)
C13—C8—C7	118.8 (5)	N1—Cu1—Cl1	95.21 (15)
C8—C9—C10	121.1 (5)		
N1—C1—C2—C3	0.5 (12)	C2—C1—N1—Cu1	178.1 (6)
C1—C2—C3—C4	0.0 (12)	C4—C5—N1—C1	0.9 (10)
C2—C3—C4—C5	0.1 (11)	C6—C5—N1—C1	−178.3 (6)
C3—C4—C5—N1	−0.5 (10)	C4—C5—N1—Cu1	−178.2 (5)
C3—C4—C5—C6	178.6 (6)	C6—C5—N1—Cu1	2.6 (7)
N1—C5—C6—N2	−15.6 (8)	C5—C6—N2—C7	149.8 (5)
C4—C5—C6—N2	165.2 (6)	C5—C6—N2—Cu1	20.7 (7)
N2—C7—C8—C9	−127.8 (6)	C8—C7—N2—C6	172.3 (5)
N2—C7—C8—C13	52.8 (7)	C8—C7—N2—Cu1	−60.2 (5)
C13—C8—C9—C10	0.3 (9)	C12—C13—O1—Cu1	138.6 (4)
C7—C8—C9—C10	−179.1 (5)	C8—C13—O1—Cu1	−42.4 (7)
C8—C9—C10—C11	−1.3 (9)	C13—O1—Cu1—N2	26.5 (4)
C8—C9—C10—Br2	−178.9 (4)	C13—O1—Cu1—N1	101.6 (8)
C9—C10—C11—C12	0.8 (9)	C13—O1—Cu1—Cl1	−136.2 (4)
Br2—C10—C11—C12	178.4 (4)	C6—N2—Cu1—O1	150.7 (4)
C10—C11—C12—C13	0.7 (9)	C7—N2—Cu1—O1	22.9 (4)
C10—C11—C12—Br1	−178.8 (4)	C6—N2—Cu1—N1	−15.7 (4)
C11—C12—C13—O1	177.4 (5)	C7—N2—Cu1—N1	−143.5 (4)
Br1—C12—C13—O1	−3.1 (7)	C6—N2—Cu1—Cl1	−101.1 (5)
C11—C12—C13—C8	−1.6 (8)	C7—N2—Cu1—Cl1	131.1 (4)
Br1—C12—C13—C8	177.9 (4)	C1—N1—Cu1—O1	112.1 (8)
C9—C8—C13—O1	−177.9 (5)	C5—N1—Cu1—O1	−68.8 (9)
C7—C8—C13—O1	1.5 (8)	C1—N1—Cu1—N2	−171.6 (6)
C9—C8—C13—C12	1.1 (8)	C5—N1—Cu1—N2	7.5 (4)
C7—C8—C13—C12	−179.5 (5)	C1—N1—Cu1—Cl1	−9.8 (6)
C2—C1—N1—C5	−0.9 (10)	C5—N1—Cu1—Cl1	169.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O1^{i}	0.94 (4)	2.14 (5)	2.918 (6)	139 (5)

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

Fig. 1