Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{4,4′,6,6′-Tetrabromo-2,2′-[(2,2-dimethylpropane-1,3-diyl)bis(nitrilomethanylylidene)]diphenolato}copper(II)

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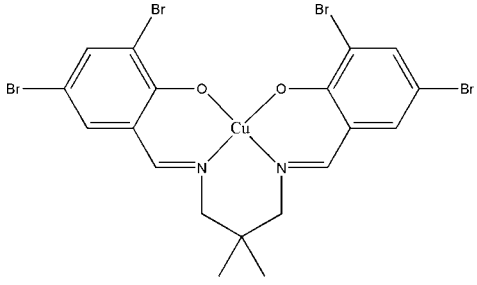
Received 6 January 2012; accepted 2 March 2012

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.078; data-to-parameter ratio = 19.8.

In the title compound, $[Cu(C_{19}H_{16}Br_4N_2O_2)]$, the Cu^{II} ion and the substituted C atom of the diamine fragment lie on a crystallographic twofold rotation axis. The geometry around the Cu^{II} ion is distorted square-planar, which is defined by the N_2O_2 donor atoms of the coordinated Schiff base ligand. The dihedral angle between the symmetry-related substituted benzene rings is 25.33 (14)°. The crystal structure is stabilized by an intermolecular π–π interaction [centroid–centroid distance = 3.8891 (18) Å].

Related literature

For standard bond lengths, see: Allen *et al.* (1987). For applications of Schiff base ligands in coordination chemistry, see: Granovski *et al.* (1993); Blower (1998). For a related structure, see: Kargar *et al.* (2008).



Experimental

Crystal data

$[Cu(C_{19}H_{16}Br_4N_2O_2)]$
M_r = 687.52
Orthorhombic, *Pbcn*
a = 16.3594 (8) Å
b = 15.5106 (8) Å
c = 8.4686 (4) Å
V = 2148.86 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.47 mm^{-1}
T = 291 K
0.21 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.269, T_{max} = 0.551
9913 measured reflections
2537 independent reflections
1625 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.078
S = 1.00
2537 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HK and MH thank PNU for financial support. MNT thanks GC University of Sargodha, Pakistan, for the research facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2199).

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supporting information

Acta Cryst. (2012). E**68**, m392 [https://doi.org/10.1107/S1600536812009397]

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S1. Comment

Schiff base complexes are one of the most important stereochemical models in transition metal coordination chemistry, with the ease of preparation and structural variations (Granovski *et al.*, 1993; Blower (1998)).

The asymmetric unit of the title compound, Fig. 1, comprises half of a potentially tetradentate Schiff base ligand. The bond lengths (Allen *et al.*, 1987) and angles are within the normal ranges. The Cu1 and C9 atoms lie on crystallographic two-fold rotation axis. The crystal structure is further stabilized by the intermolecular π-π interaction, (Fig. 2), [$Cg1\cdots Cg1^{i}$ = 3.8891 (18)Å; (i) 1 - *X*, 1 - *Y*, -*Z*; *Cg*1 is the centroid of Cu(1)/O(1)/C(1)/C(6)/C(7)/N(1) ring].

S2. Experimental

The title compound was synthesized by adding 3,5-dibromo-salicylaldehyde-2,2-dimethyl-1,3- propanediamine (2 mmol) to a solution of $CuCl_2$. $4H_2O$ (2.1 mmol) in ethanol (30 ml). The mixture was refluxed with stirring for half an hour. The resultant solution was filtered. Green single crystals of the title compound suitable for *X*-ray structure determination were recrystallized from ethanol by slow evaporation of the solvents at room temperature over several days.

S3. Refinement

All hydrogen atoms were positioned geometrically with C—H = 0.93-0.97 Å and included in a riding model and treated as riding atoms: C—H = 0.93, 0.96 and 0.97 Å for CH, CH_3 and CH_2 H-atoms, respectively, with U_{iso} (H) = k x U_{eq}(C), where k = 1.5 for CH_3 H-atoms, and k = 1.2 for all other H-atoms..

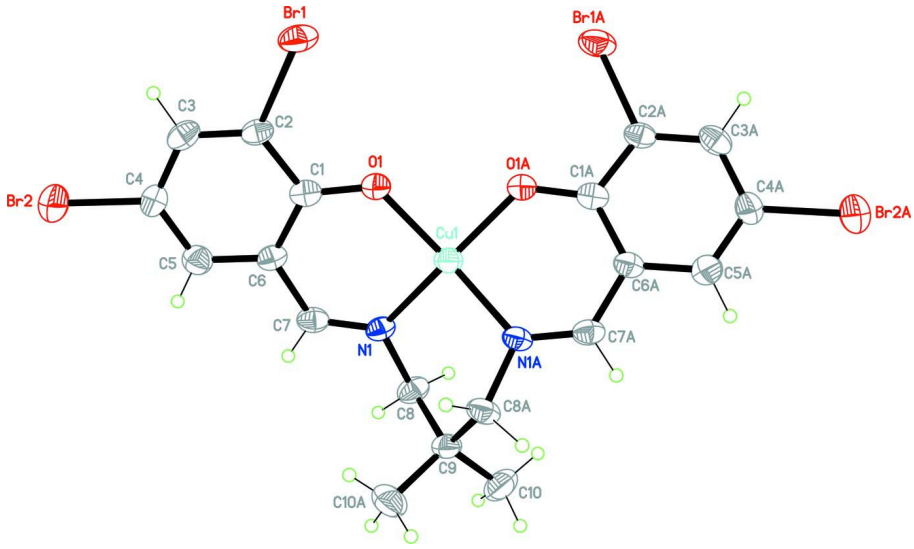

Figure 1

The ORTEP plot of the title compound, showing 40% probability displacement ellipsoids and the atomic numbering.

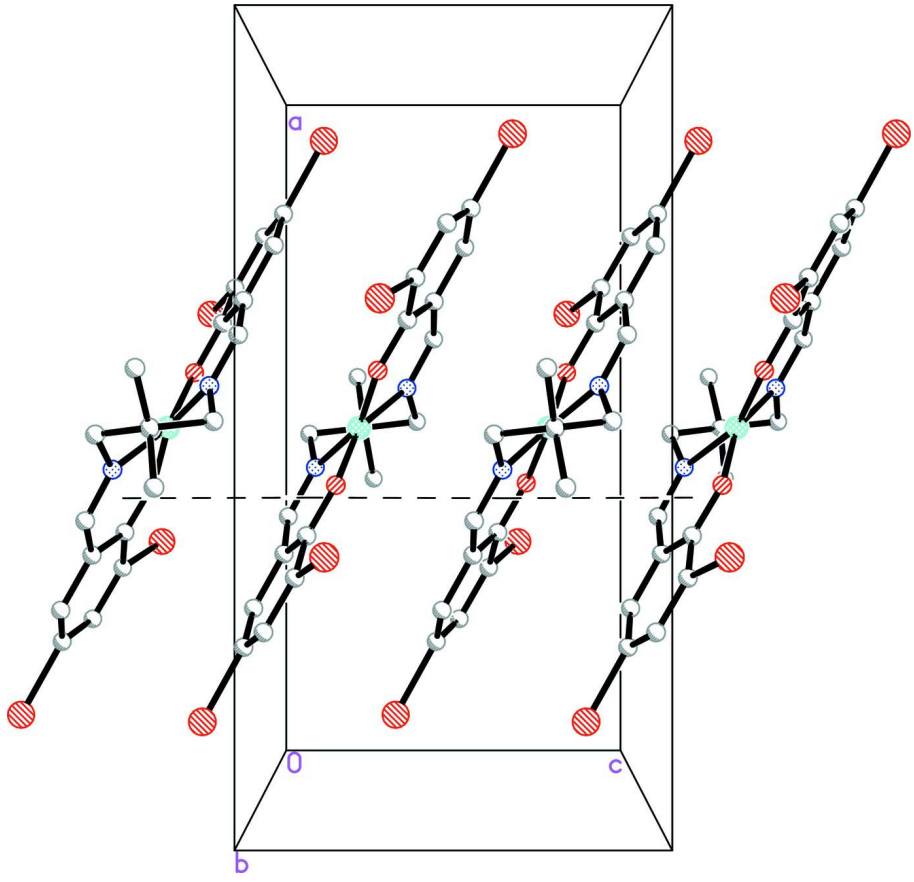

Figure 2

The packing diagram of the title compound viewed down the *b*-axis showing linking of molecules through the intermolecular π-π intearctions (dashed lines). The hydrogen atoms omitted for clarity.

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Hall symbol: -P 2n 2ab
a = 16.3594 (8) Å
b = 15.5106 (8) Å
c = 8.4686 (4) Å
V = 2148.86 (18) Å^3
Z = 4
$F(000)$ = 1316
D_x = 2.125 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1535 reflections
θ = 2.5–27.5°
μ = 8.47 mm^{-1}
T = 291 K
Block, green
0.21 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.269, T_{max} = 0.551
9913 measured reflections
2537 independent reflections
1625 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 28.0°, θ_{min} = 1.8°
h = −21→18
k = −20→13
l = −10→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.078
S = 1.00
2537 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0202P)^2 + 1.7635P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
Br1	0.33450 (3)	0.74146 (3)	0.18143 (5)	0.05098 (16)
Br2	0.10313 (3)	0.54552 (4)	−0.15415 (7)	0.0733 (2)
Cu1	0.5000	0.48415 (4)	0.2500	0.03410 (18)
N1	0.4444 (2)	0.39656 (19)	0.1258 (3)	0.0332 (7)
O1	0.42323 (17)	0.57112 (16)	0.1958 (3)	0.0395 (7)

C1	0.3547 (2)	0.5618 (2)	0.1192 (4)	0.0341 (9)
C2	0.3023 (2)	0.6335 (2)	0.0965 (4)	0.0341 (9)
C3	0.2301 (2)	0.6285 (3)	0.0162 (4)	0.0406 (10)
H3	0.1982	0.6776	0.0030	0.049*
C4	0.2042 (2)	0.5504 (3)	−0.0458 (5)	0.0417 (10)
C5	0.2520 (3)	0.4788 (3)	−0.0299 (4)	0.0425 (10)
H5	0.2348	0.4267	−0.0730	0.051*
C6	0.3270 (2)	0.4831 (2)	0.0511 (4)	0.0342 (9)
C7	0.3757 (3)	0.4058 (2)	0.0534 (4)	0.0368 (10)
H7	0.3560	0.3585	−0.0022	0.044*
C8	0.4911 (3)	0.3163 (2)	0.1017 (4)	0.0404 (10)
H8A	0.5453	0.3310	0.0635	0.048*
H8B	0.4644	0.2825	0.0204	0.048*
C9	0.5000	0.2606 (3)	0.2500	0.0390 (14)
C10	0.5749 (3)	0.2038 (3)	0.2270 (5)	0.0574 (13)
H10A	0.6231	0.2391	0.2253	0.086*
H10B	0.5703	0.1733	0.1288	0.086*
H10C	0.5786	0.1633	0.3123	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0710 (3)	0.0317 (2)	0.0503 (3)	0.0104 (2)	−0.0024 (2)	−0.0063 (2)
Br2	0.0527 (3)	0.0645 (4)	0.1027 (4)	0.0055 (3)	−0.0303 (3)	0.0001 (3)
Cu1	0.0387 (4)	0.0275 (3)	0.0361 (4)	0.000	−0.0012 (3)	0.000
N1	0.041 (2)	0.0256 (17)	0.0334 (17)	0.0063 (16)	0.0008 (15)	−0.0012 (14)
O1	0.0416 (17)	0.0295 (14)	0.0475 (16)	0.0014 (13)	−0.0063 (13)	−0.0027 (13)
C1	0.042 (3)	0.031 (2)	0.030 (2)	0.002 (2)	0.0088 (18)	0.0010 (18)
C2	0.043 (2)	0.029 (2)	0.031 (2)	0.0058 (19)	0.0072 (18)	−0.0018 (18)
C3	0.044 (3)	0.039 (2)	0.039 (2)	0.013 (2)	0.0078 (19)	0.002 (2)
C4	0.035 (2)	0.046 (3)	0.045 (2)	0.006 (2)	−0.0028 (19)	0.001 (2)
C5	0.045 (3)	0.039 (2)	0.043 (2)	−0.002 (2)	−0.002 (2)	−0.002 (2)
C6	0.041 (2)	0.029 (2)	0.032 (2)	0.005 (2)	0.0022 (17)	0.0001 (18)
C7	0.049 (3)	0.029 (2)	0.032 (2)	0.001 (2)	0.0022 (19)	−0.0042 (18)
C8	0.052 (3)	0.031 (2)	0.038 (2)	0.012 (2)	−0.0001 (19)	−0.0050 (19)
C9	0.047 (4)	0.026 (3)	0.044 (3)	0.000	−0.007 (3)	0.000
C10	0.064 (3)	0.046 (3)	0.062 (3)	0.017 (3)	−0.013 (2)	0.005 (2)

Geometric parameters (Å, º)

Br1—C2	1.897 (4)	C4—C5	1.364 (6)
Br2—C4	1.893 (4)	C5—C6	1.407 (5)
Cu1—O1^{i}	1.899 (3)	C5—H5	0.9300
Cu1—O1	1.899 (3)	C6—C7	1.440 (5)
Cu1—N1^{i}	1.944 (3)	C7—H7	0.9300
Cu1—N1	1.944 (3)	C8—C9	1.531 (5)
N1—C7	1.288 (5)	C8—H8A	0.9700
N1—C8	1.475 (5)	C8—H8B	0.9700

O1—C1	1.303 (5)	C9—C10^{i}	1.522 (5)
C1—C2	1.418 (5)	C9—C10	1.522 (5)
C1—C6	1.425 (5)	C9—C8^{i}	1.531 (5)
C2—C3	1.364 (5)	C10—H10A	0.9600
C3—C4	1.387 (6)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600

O1^{i}—Cu1—O1	89.50 (16)	C5—C6—C1	121.0 (4)
O1^{i}—Cu1—N1^{i}	93.23 (12)	C5—C6—C7	116.8 (4)
O1—Cu1—N1^{i}	159.45 (11)	C1—C6—C7	122.1 (4)
O1^{i}—Cu1—N1	159.45 (11)	N1—C7—C6	125.6 (4)
O1—Cu1—N1	93.23 (12)	N1—C7—H7	117.2
N1^{i}—Cu1—N1	91.32 (18)	C6—C7—H7	117.2
C7—N1—C8	118.7 (3)	N1—C8—C9	114.3 (3)
C7—N1—Cu1	126.0 (3)	N1—C8—H8A	108.7
C8—N1—Cu1	115.0 (3)	C9—C8—H8A	108.7
C1—O1—Cu1	127.6 (2)	N1—C8—H8B	108.7
O1—C1—C2	120.1 (4)	C9—C8—H8B	108.7
O1—C1—C6	124.8 (4)	H8A—C8—H8B	107.6
C2—C1—C6	115.1 (4)	C10^{i}—C9—C10	109.2 (5)
C3—C2—C1	123.2 (4)	C10^{i}—C9—C8^{i}	107.3 (2)
C3—C2—Br1	118.7 (3)	C10—C9—C8^{i}	110.8 (2)
C1—C2—Br1	118.2 (3)	C10^{i}—C9—C8	110.8 (2)
C2—C3—C4	120.2 (4)	C10—C9—C8	107.3 (2)
C2—C3—H3	119.9	C8^{i}—C9—C8	111.3 (4)
C4—C3—H3	119.9	C9—C10—H10A	109.5
C5—C4—C3	119.9 (4)	C9—C10—H10B	109.5
C5—C4—Br2	121.1 (3)	H10A—C10—H10B	109.5
C3—C4—Br2	119.0 (3)	C9—C10—H10C	109.5
C4—C5—C6	120.6 (4)	H10A—C10—H10C	109.5
C4—C5—H5	119.7	H10B—C10—H10C	109.5
C6—C5—H5	119.7		

O1^{i}—Cu1—N1—C7	−102.7 (4)	C2—C3—C4—Br2	179.2 (3)
O1—Cu1—N1—C7	−5.5 (3)	C3—C4—C5—C6	1.0 (6)
N1^{i}—Cu1—N1—C7	154.5 (4)	Br2—C4—C5—C6	−179.9 (3)
O1^{i}—Cu1—N1—C8	70.7 (4)	C4—C5—C6—C1	0.3 (6)
O1—Cu1—N1—C8	167.9 (2)	C4—C5—C6—C7	−176.2 (4)
N1^{i}—Cu1—N1—C8	−32.2 (2)	O1—C1—C6—C5	180.0 (3)
O1^{i}—Cu1—O1—C1	167.4 (3)	C2—C1—C6—C5	−0.9 (5)
N1^{i}—Cu1—O1—C1	−94.7 (4)	O1—C1—C6—C7	−3.7 (6)
N1—Cu1—O1—C1	7.8 (3)	C2—C1—C6—C7	175.4 (3)
Cu1—O1—C1—C2	176.5 (2)	C8—N1—C7—C6	−173.3 (3)
Cu1—O1—C1—C6	−4.5 (5)	Cu1—N1—C7—C6	−0.1 (6)
O1—C1—C2—C3	179.4 (3)	C5—C6—C7—N1	−177.5 (4)
C6—C1—C2—C3	0.2 (5)	C1—C6—C7—N1	6.1 (6)
O1—C1—C2—Br1	−0.4 (5)	C7—N1—C8—C9	−115.0 (4)
C6—C1—C2—Br1	−179.5 (3)	Cu1—N1—C8—C9	71.1 (4)

C1—C2—C3—C4	1.0 (6)	N1—C8—C9—C10^{i}	83.8 (4)
Br1—C2—C3—C4	−179.2 (3)	N1—C8—C9—C10	−157.0 (4)
C2—C3—C4—C5	−1.7 (6)	N1—C8—C9—C8^{i}	−35.6 (2)

Symmetry code: (i) $-x+1, y, -z+1/2$.