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Bis{2-[(*E*)-cyclopentyliminomethyl]-6-methoxyphenolato}copper(II)

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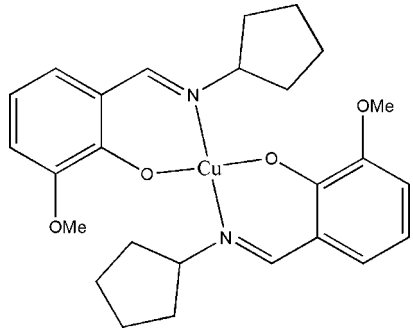
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 17.5.

The title complex, $[Cu(C_{13}H_{16}NO_2)_2]$, is a mononuclear copper(II) complex. The Cu atom is located on a crystallographic inversion centre and is coordinated by two O and two N atoms from two Schiff base ligands, forming a square-planar geometry.

Related literature

For related literature, see: Hebbachi & Benali-Cherif (2005); Liu *et al.* (2004); Usha *et al.* (2004); Wang (2007); Xu *et al.* (2005); Zhang (2004).



Experimental

Crystal data

$[Cu(C_{13}H_{16}NO_2)_2]$
M_r = 500.08
Orthorhombic, *Pbca*
a = 12.060 (2) Å
b = 10.8025 (18) Å
c = 17.863 (3) Å
V = 2327.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 293 (2) K
0.33 × 0.27 × 0.25 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.739, T_{max} = 0.793
18677 measured reflections
2662 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.03
2662 reflections
152 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: GK2077).

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supplementary materials

Acta Cryst. (2007). E**63**, m1766 [**doi:10.1107/S1600536807023860**]

Bis{2-[(*E*)-cyclopentyliminomethyl]-6-methoxyphenolato}copper(II)

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Comment

The interesting Cu(II) complexes with Schiff base ligands have been widely reported previously (Xu *et al.*, 2005; Hebbachi & Benali-Cherif, 2005; Liu *et al.*, 2004; Zhang, 2004; Wang, 2007; Usha *et al.*, 2004). We report herein the title new copper(II) complex, (I), derived from the Schiff base ligand, 2-(cyclopentyliminomethyl)-6-methoxyphenol.

(I) is a mononuclear copper(II) complex (Fig. 1).

Experimental

3-Methoxy-2-hydroxybenzaldehyde (0.2 mmol, 30.5 mg), cyclopentylamine (0.2 mmol, 17.2 mg), and $Cu(CH_3COO)_2{\cdot}H_2O$ (0.1 mmol, 20.0 mg) were dissolved in methanol. The mixture was stirred at 325 K for 30 min to give a transparent blue solution. Blue crystals were obtained by slow evaporation of the solution in air.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C–H distances in the range 0.93–0.97 Å and U_{iso}(H) set at 1.2U_{eq}(C) and 1.5U_{eq}(methyl C).

Figures

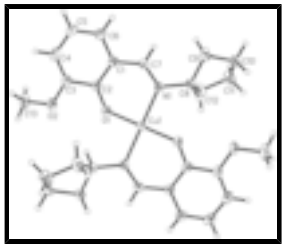

Fig. 1. The molecular structure of (I), with anisotropic displacement ellipsoids drawn at the 30% probability level.

bis{2-[(*E*)-cyclopentyliminomethyl]-6-methoxyphenolato}copper(II)

Crystal data

$[Cu(C_{13}H_{16}NO_2)_2]$	F_{000} = 1052
M_r = 500.08	D_x = 1.427 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3071 reflections
a = 12.060 (2) Å	θ = 2.3–25.4º

b = 10.8025 (18) Å	μ = 0.97 mm^{-1}
c = 17.863 (3) Å	T = 293 (2) K
V = 2327.1 (7) Å^3	Block, blue
Z = 4	0.33 × 0.27 × 0.25 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2662 independent reflections
Radiation source: fine-focus sealed tube	1921 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.048
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −15→15
T_{min} = 0.739, T_{max} = 0.793	k = −13→13
18677 measured reflections	l = −22→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.108	$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.5523P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
2662 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
152 parameters	$\Delta\rho_{min}$ = −0.52 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cu1	0.5000	1.0000	0.5000	0.03149 (14)

O1	0.48094 (13)	1.06065 (17)	0.59762 (9)	0.0476 (4)
O2	0.47911 (14)	1.21263 (17)	0.71126 (10)	0.0532 (5)
N1	0.37204 (14)	0.88125 (16)	0.51335 (9)	0.0309 (4)
C1	0.30127 (18)	0.98086 (19)	0.62636 (12)	0.0349 (5)
C2	0.39230 (17)	1.05894 (19)	0.63916 (11)	0.0339 (5)
C3	0.38780 (18)	1.13863 (19)	0.70281 (11)	0.0385 (5)
C4	0.2975 (2)	1.1376 (2)	0.74929 (13)	0.0484 (6)
H4	0.2963	1.1893	0.7909	0.058*
C5	0.2074 (2)	1.0602 (2)	0.73515 (14)	0.0524 (6)
H5	0.1461	1.0615	0.7667	0.063*
C6	0.2092 (2)	0.9832 (2)	0.67549 (14)	0.0474 (6)
H6	0.1492	0.9312	0.6666	0.057*
C7	0.30020 (17)	0.8935 (2)	0.56588 (11)	0.0353 (5)
H7	0.2404	0.8392	0.5646	0.042*
C8	0.35710 (16)	0.77989 (18)	0.45869 (11)	0.0326 (5)
H8	0.3701	0.8150	0.4089	0.039*
C9	0.24757 (18)	0.7099 (2)	0.45507 (13)	0.0416 (5)
H9A	0.2249	0.6809	0.5041	0.050*
H9B	0.1891	0.7606	0.4338	0.050*
C10	0.27792 (19)	0.6031 (2)	0.40378 (13)	0.0447 (6)
H10A	0.2262	0.5350	0.4095	0.054*
H10B	0.2782	0.6292	0.3518	0.054*
C11	0.3933 (2)	0.5656 (2)	0.42889 (18)	0.0623 (8)
H11A	0.4389	0.5443	0.3860	0.075*
H11B	0.3897	0.4947	0.4621	0.075*
C12	0.4416 (2)	0.6771 (2)	0.46972 (16)	0.0532 (7)
H12A	0.4514	0.6591	0.5225	0.064*
H12B	0.5127	0.7002	0.4485	0.064*
C13	0.4917 (2)	1.2773 (3)	0.77932 (19)	0.0682 (9)
H13A	0.4325	1.3360	0.7847	0.102*
H13B	0.5614	1.3201	0.7793	0.102*
H13C	0.4898	1.2198	0.8203	0.102*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0323 (2)	0.0320 (2)	0.0301 (2)	−0.00396 (14)	0.00267 (14)	−0.00402 (15)
O1	0.0444 (9)	0.0600 (11)	0.0385 (9)	−0.0173 (8)	0.0109 (7)	−0.0169 (8)
O2	0.0556 (10)	0.0581 (11)	0.0457 (10)	−0.0085 (8)	−0.0009 (8)	−0.0213 (9)
N1	0.0349 (10)	0.0284 (9)	0.0295 (9)	−0.0007 (7)	−0.0007 (7)	−0.0003 (7)
C1	0.0372 (12)	0.0350 (12)	0.0325 (11)	0.0033 (9)	0.0021 (9)	0.0017 (9)
C2	0.0377 (12)	0.0354 (11)	0.0286 (10)	0.0031 (9)	0.0031 (9)	0.0014 (9)
C3	0.0459 (13)	0.0366 (11)	0.0331 (11)	0.0052 (10)	−0.0029 (10)	−0.0028 (9)
C4	0.0575 (15)	0.0490 (14)	0.0387 (13)	0.0116 (12)	0.0063 (11)	−0.0088 (11)
C5	0.0502 (15)	0.0618 (16)	0.0452 (14)	0.0093 (13)	0.0164 (11)	−0.0045 (12)
C6	0.0403 (14)	0.0551 (15)	0.0469 (14)	−0.0010 (11)	0.0074 (11)	0.0003 (11)
C7	0.0326 (11)	0.0360 (12)	0.0372 (12)	−0.0038 (9)	−0.0007 (9)	0.0031 (9)
C8	0.0348 (11)	0.0288 (10)	0.0342 (11)	−0.0037 (8)	−0.0020 (9)	−0.0001 (9)

C9	0.0411 (12)	0.0405 (13)	0.0430 (13)	−0.0061 (10)	−0.0021 (10)	−0.0025 (10)
C10	0.0533 (15)	0.0346 (12)	0.0461 (13)	−0.0109 (10)	−0.0034 (11)	−0.0016 (10)
C11	0.0654 (18)	0.0343 (13)	0.087 (2)	0.0071 (12)	−0.0115 (16)	−0.0115 (13)
C12	0.0479 (15)	0.0426 (14)	0.0691 (17)	0.0101 (11)	−0.0195 (13)	−0.0094 (13)
C13	0.076 (2)	0.071 (2)	0.0575 (17)	0.0026 (15)	−0.0138 (14)	−0.0303 (16)

Geometric parameters (Å, °)

Cu1—O1	1.8770 (16)	C7—H7	0.9300
Cu1—O1^{i}	1.8770 (16)	C8—C12	1.520 (3)
Cu1—N1	2.0208 (17)	C8—C9	1.523 (3)
Cu1—N1^{i}	2.0208 (17)	C8—H8	0.9800
O1—C2	1.301 (2)	C9—C10	1.518 (3)
O2—C3	1.369 (3)	C9—H9A	0.9700
O2—C13	1.410 (4)	C9—H9B	0.9700
N1—C7	1.284 (3)	C10—C11	1.517 (3)
N1—C8	1.478 (3)	C10—H10A	0.9700
C1—C2	1.403 (3)	C10—H10B	0.9700
C1—C6	1.416 (3)	C11—C12	1.523 (3)
C1—C7	1.435 (3)	C11—H11A	0.9700
C2—C3	1.427 (3)	C11—H11B	0.9700
C3—C4	1.369 (3)	C12—H12A	0.9700
C4—C5	1.395 (4)	C12—H12B	0.9700
C4—H4	0.9300	C13—H13A	0.9600
C5—C6	1.352 (3)	C13—H13B	0.9600
C5—H5	0.9300	C13—H13C	0.9600
C6—H6	0.9300		
O1—Cu1—O1^{i}	180.00 (4)	C12—C8—C9	102.97 (17)
O1—Cu1—N1	91.06 (7)	N1—C8—H8	107.0
O1^{i}—Cu1—N1	88.94 (7)	C12—C8—H8	107.0
O1—Cu1—N1^{i}	88.94 (7)	C9—C8—H8	107.0
O1^{i}—Cu1—N1^{i}	91.06 (7)	C10—C9—C8	101.17 (17)
N1—Cu1—N1^{i}	180.0	C10—C9—H9A	111.5
C2—O1—Cu1	128.71 (14)	C8—C9—H9A	111.5
C3—O2—C13	118.1 (2)	C10—C9—H9B	111.5
C7—N1—C8	118.47 (18)	C8—C9—H9B	111.5
C7—N1—Cu1	122.43 (14)	H9A—C9—H9B	109.4
C8—N1—Cu1	119.04 (12)	C11—C10—C9	104.20 (19)
C2—C1—C6	120.1 (2)	C11—C10—H10A	110.9
C2—C1—C7	121.69 (19)	C9—C10—H10A	110.9
C6—C1—C7	118.1 (2)	C11—C10—H10B	110.9
O1—C2—C1	123.93 (19)	C9—C10—H10B	110.9
O1—C2—C3	118.5 (2)	H10A—C10—H10B	108.9
C1—C2—C3	117.56 (19)	C10—C11—C12	106.4 (2)
O2—C3—C4	125.3 (2)	C10—C11—H11A	110.5
O2—C3—C2	114.17 (19)	C12—C11—H11A	110.5
C4—C3—C2	120.6 (2)	C10—C11—H11B	110.5

C3—C4—C5	121.0 (2)	C12—C11—H11B	110.5
C3—C4—H4	119.5	H11A—C11—H11B	108.7
C5—C4—H4	119.5	C8—C12—C11	105.01 (18)
C6—C5—C4	119.9 (2)	C8—C12—H12A	110.7
C6—C5—H5	120.0	C11—C12—H12A	110.7
C4—C5—H5	120.0	C8—C12—H12B	110.7
C5—C6—C1	120.8 (2)	C11—C12—H12B	110.7
C5—C6—H6	119.6	H12A—C12—H12B	108.8
C1—C6—H6	119.6	O2—C13—H13A	109.5
N1—C7—C1	127.7 (2)	O2—C13—H13B	109.5
N1—C7—H7	116.1	H13A—C13—H13B	109.5
C1—C7—H7	116.1	O2—C13—H13C	109.5
N1—C8—C12	111.95 (17)	H13A—C13—H13C	109.5
N1—C8—C9	120.09 (17)	H13B—C13—H13C	109.5

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

Fig. 1