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Chlorido{4-chloro-2-[(2-morpholinoethyl)iminomethyl]phenolato-κ^3N,N',O}copper(II)

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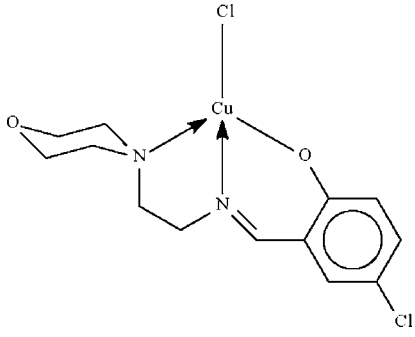
Key indicators: single-crystal X-ray study; T = 140 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.113; data-to-parameter ratio = 17.4.

The Cu^{II} atom in the title compound, $[Cu(C_{13}H_{16}ClN_2O_2)Cl]$, exists in a distorted square-planar coordination environment as the deprotonated Schiff base chelates to the Cu^{II} atom through three atom sites. In the crystal structure, adjacent molecules are linked by a Cu···Cl [3.011 (1) Å] bridge, generating a linear chain running along the b axis of the orthorhombic unit cell.

Related literature

A similar deprotonated Schiff base is bidentate in bis{5-methoxy-2-[(2-morpholinoethyl)iminomethyl]phenolato}-nickel; see: Mohd Lair *et al.* (2009).



Experimental

Crystal data

$[Cu(C_{13}H_{16}ClN_2O_2)Cl]$
M_r = 366.72
Orthorhombic, *Pbcn*
a = 23.0936 (6) Å
b = 8.4890 (2) Å
c = 14.0582 (3) Å
V = 2756.0 (1) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.97 mm^{-1}
T = 140 K
0.40 × 0.10 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.506, T_{max} = 0.962
17248 measured reflections
3156 independent reflections
2416 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.113
S = 1.09
3156 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.907 (2)	Cu1—N2	2.105 (3)
Cu1—N1	1.947 (3)	Cu1—Cl1	2.2620 (9)

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2547).

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supporting information

Acta Cryst. (2009). E**65**, m870 [doi:10.1107/S1600536809025215]

Chlorido{4-chloro-2-[(2-morpholinoethyl)iminomethyl]phenolato-κ^3N,N',O}copper(II)

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S1. Experimental

The Schiff base was synthesized by condensing N-2-(aminoethyl)morpholine (0.80 g, 6.1 mmol) and 5-chlorosalicyl-aldehyde (0.96 g, 6.1 mmol) in ethanol; the reactants were heated for 2 hours. Copper(II) chloride (1.00 g, 6.1 mmol) was added and the heating continued for another 5 hour. The solvent was removed and the product recrystallized from methanol.

S2. Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.95–0.99 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2 times $U_{eq}(C)$.

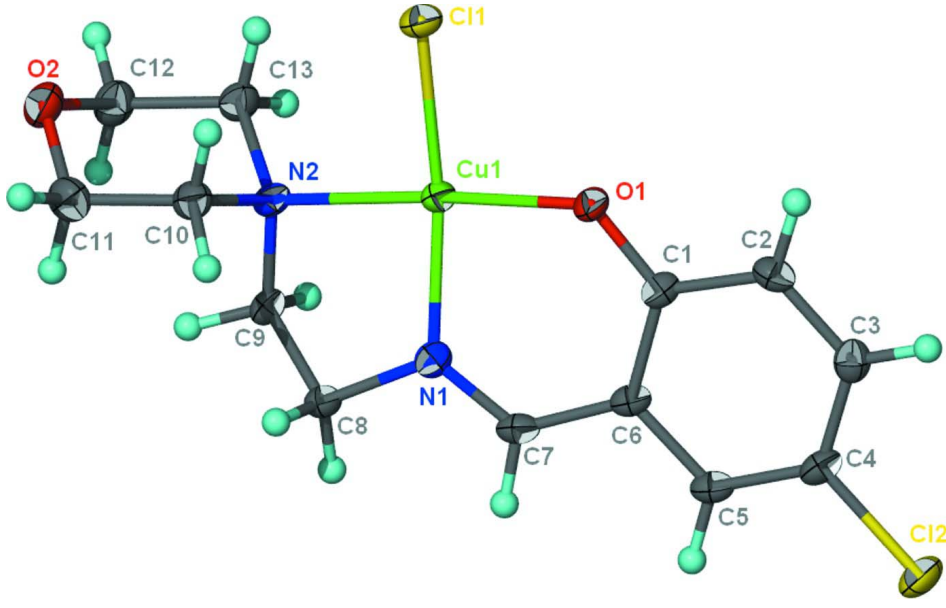

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the $CuCl(C_{13}H_{16}ClN_2O_2)$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Chlorido{4-chloro-2-[(2-morpholinoethyl)iminomethyl]phenolato-κ^3N,N',O}copper(II)

Crystal data

$[Cu(C_{13}H_{16}ClN_2O_2)Cl]$
$M_r = 366.72$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 23.0936$ (6) Å
$b = 8.4890$ (2) Å
$c = 14.0582$ (3) Å
$V = 2756.0$ (1) Å^3
$Z = 8$
$F(000) = 1496$
$D_x = 1.768$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4043 reflections
$\theta = 2.6$–$28.1°$
$\mu = 1.97$ mm^{-1}
$T = 140$ K
Plate, green
0.40 × 0.10 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.506$, $T_{max} = 0.962$
17248 measured reflections
3156 independent reflections
2416 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -29 \rightarrow 30$
$k = -10 \rightarrow 10$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.113$
$S = 1.09$
3156 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 6.7938P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.229938 (18)	0.65838 (5)	0.49762 (3)	0.01385 (13)
Cl1	0.24525 (4)	0.85643 (10)	0.39295 (6)	0.0181 (2)
Cl2	0.43295 (4)	0.32750 (12)	0.83746 (7)	0.0253 (2)
O1	0.30890 (10)	0.6693 (3)	0.53670 (17)	0.0159 (5)
O2	0.03792 (12)	0.7569 (3)	0.36877 (18)	0.0225 (6)
N1	0.20874 (13)	0.5357 (3)	0.60938 (19)	0.0141 (6)
N2	0.14182 (13)	0.6347 (3)	0.46204 (19)	0.0131 (6)
C1	0.33436 (15)	0.5909 (4)	0.6049 (2)	0.0131 (7)
C2	0.39494 (16)	0.6087 (4)	0.6170 (2)	0.0158 (7)
H2	0.4156	0.6769	0.5756	0.019*
C3	0.42459 (16)	0.5294 (4)	0.6873 (2)	0.0157 (7)
H3	0.4652	0.5438	0.6942	0.019*
C4	0.39495 (16)	0.4279 (4)	0.7485 (2)	0.0169 (7)
C5	0.33647 (16)	0.4082 (4)	0.7404 (2)	0.0158 (7)

H5	0.3168	0.3396	0.7829	0.019*
C6	0.30502 (15)	0.4889 (4)	0.6696 (2)	0.0139 (7)
C7	0.24355 (16)	0.4685 (4)	0.6681 (2)	0.0149 (7)
H7	0.2271	0.3998	0.7141	0.018*
C8	0.14665 (15)	0.5035 (4)	0.6176 (2)	0.0147 (7)
H8A	0.1272	0.5891	0.6531	0.018*
H8B	0.1401	0.4030	0.6517	0.018*
C9	0.12305 (15)	0.4933 (4)	0.5171 (2)	0.0147 (7)
H9A	0.1376	0.3966	0.4859	0.018*
H9B	0.0802	0.4882	0.5189	0.018*
C10	0.11098 (16)	0.7815 (4)	0.4921 (2)	0.0168 (7)
H10A	0.1293	0.8732	0.4607	0.020*
H10B	0.1155	0.7949	0.5617	0.020*
C11	0.04724 (17)	0.7799 (5)	0.4681 (3)	0.0209 (8)
H11A	0.0280	0.6943	0.5040	0.025*
H11B	0.0296	0.8810	0.4879	0.025*
C12	0.06457 (16)	0.6146 (5)	0.3373 (3)	0.0202 (8)
H12A	0.0585	0.6029	0.2679	0.024*
H12B	0.0459	0.5239	0.3693	0.024*
C13	0.12914 (16)	0.6129 (5)	0.3585 (2)	0.0173 (7)
H13A	0.1457	0.5114	0.3371	0.021*
H13B	0.1482	0.6981	0.3220	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0132 (2)	0.0170 (2)	0.0113 (2)	−0.00069 (18)	−0.00083 (15)	0.00270 (17)
Cl1	0.0202 (4)	0.0186 (4)	0.0154 (4)	−0.0010 (4)	−0.0009 (3)	0.0058 (3)
Cl2	0.0222 (5)	0.0295 (5)	0.0243 (5)	−0.0005 (4)	−0.0077 (4)	0.0126 (4)
O1	0.0146 (13)	0.0158 (13)	0.0174 (11)	0.0000 (10)	−0.0020 (10)	0.0069 (10)
O2	0.0209 (14)	0.0274 (15)	0.0193 (13)	0.0077 (12)	−0.0033 (11)	0.0008 (11)
N1	0.0152 (15)	0.0145 (15)	0.0126 (13)	−0.0010 (12)	−0.0018 (11)	−0.0015 (11)
N2	0.0163 (15)	0.0126 (14)	0.0103 (12)	0.0011 (12)	−0.0014 (11)	−0.0013 (11)
C1	0.0171 (18)	0.0117 (17)	0.0106 (15)	0.0007 (14)	−0.0021 (13)	−0.0006 (12)
C2	0.0173 (19)	0.0149 (17)	0.0151 (16)	−0.0030 (15)	0.0029 (13)	−0.0001 (13)
C3	0.0154 (18)	0.0144 (18)	0.0173 (16)	−0.0016 (14)	−0.0018 (13)	−0.0031 (13)
C4	0.0221 (19)	0.0159 (18)	0.0126 (15)	0.0024 (15)	−0.0035 (14)	0.0028 (13)
C5	0.0225 (19)	0.0127 (18)	0.0121 (15)	0.0002 (15)	0.0005 (13)	0.0006 (13)
C6	0.0191 (18)	0.0119 (16)	0.0106 (15)	0.0005 (14)	0.0001 (13)	−0.0007 (12)
C7	0.0205 (19)	0.0142 (17)	0.0100 (14)	0.0009 (14)	0.0029 (13)	−0.0002 (13)
C8	0.0140 (17)	0.0166 (17)	0.0133 (15)	−0.0007 (14)	−0.0002 (13)	0.0032 (13)
C9	0.0146 (17)	0.0161 (17)	0.0135 (16)	0.0003 (14)	−0.0030 (12)	0.0022 (13)
C10	0.0194 (18)	0.0146 (17)	0.0164 (16)	0.0035 (15)	0.0008 (14)	−0.0009 (14)
C11	0.022 (2)	0.0218 (19)	0.0191 (17)	0.0042 (17)	0.0028 (15)	−0.0031 (15)
C12	0.020 (2)	0.0238 (19)	0.0171 (17)	0.0009 (16)	−0.0031 (14)	−0.0020 (15)
C13	0.0191 (19)	0.0198 (18)	0.0130 (15)	0.0019 (15)	−0.0011 (13)	−0.0012 (14)

Geometric parameters (Å, º)

Cu1—O1	1.907 (2)	C4—C5	1.366 (5)
Cu1—N1	1.947 (3)	C5—C6	1.410 (5)
Cu1—N2	2.105 (3)	C5—H5	0.9500
Cu1—Cl1	2.2620 (9)	C6—C7	1.430 (5)
Cu1—Cl1^{i}	3.0107 (10)	C7—H7	0.9500
Cl2—C4	1.750 (3)	C8—C9	1.516 (4)
O1—C1	1.307 (4)	C8—H8A	0.9900
O2—C11	1.427 (4)	C8—H8B	0.9900
O2—C12	1.426 (5)	C9—H9A	0.9900
N1—C7	1.285 (4)	C9—H9B	0.9900
N1—C8	1.464 (4)	C10—C11	1.510 (5)
N2—C9	1.492 (4)	C10—H10A	0.9900
N2—C13	1.496 (4)	C10—H10B	0.9900
N2—C10	1.497 (4)	C11—H11A	0.9900
C1—C2	1.417 (5)	C11—H11B	0.9900
C1—C6	1.427 (5)	C12—C13	1.521 (5)
C2—C3	1.378 (5)	C12—H12A	0.9900
C2—H2	0.9500	C12—H12B	0.9900
C3—C4	1.396 (5)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
O1—Cu1—N1	91.95 (11)	N1—C7—C6	125.2 (3)
O1—Cu1—N2	176.00 (11)	N1—C7—H7	117.4
N1—Cu1—N2	84.12 (12)	C6—C7—H7	117.4
O1—Cu1—Cl1	90.10 (7)	N1—C8—C9	106.8 (3)
N1—Cu1—Cl1	164.06 (9)	N1—C8—H8A	110.4
N2—Cu1—Cl1	93.88 (8)	C9—C8—H8A	110.4
O1—Cu1—Cl1^{i}	90.02 (8)	N1—C8—H8B	110.4
N1—Cu1—Cl1^{i}	89.25 (9)	C9—C8—H8B	110.4
N2—Cu1—Cl1^{i}	89.22 (8)	H8A—C8—H8B	108.6
Cl1—Cu1—Cl1^{i}	106.56 (3)	N2—C9—C8	109.5 (3)
C1—O1—Cu1	128.1 (2)	N2—C9—H9A	109.8
C11—O2—C12	110.8 (3)	C8—C9—H9A	109.8
C7—N1—C8	118.6 (3)	N2—C9—H9B	109.8
C7—N1—Cu1	126.7 (3)	C8—C9—H9B	109.8
C8—N1—Cu1	114.2 (2)	H9A—C9—H9B	108.2
C9—N2—C13	110.4 (3)	N2—C10—C11	113.1 (3)
C9—N2—C10	112.6 (3)	N2—C10—H10A	109.0
C13—N2—C10	106.5 (3)	C11—C10—H10A	109.0
C9—N2—Cu1	103.6 (2)	N2—C10—H10B	109.0
C13—N2—Cu1	115.6 (2)	C11—C10—H10B	109.0
C10—N2—Cu1	108.2 (2)	H10A—C10—H10B	107.8
O1—C1—C2	118.5 (3)	O2—C11—C10	111.5 (3)
O1—C1—C6	124.3 (3)	O2—C11—H11A	109.3
C2—C1—C6	117.2 (3)	C10—C11—H11A	109.3
C3—C2—C1	121.6 (3)	O2—C11—H11B	109.3

C3—C2—H2	119.2	C10—C11—H11B	109.3
C1—C2—H2	119.2	H11A—C11—H11B	108.0
C2—C3—C4	120.0 (3)	O2—C12—C13	111.7 (3)
C2—C3—H3	120.0	O2—C12—H12A	109.3
C4—C3—H3	120.0	C13—C12—H12A	109.3
C5—C4—C3	120.6 (3)	O2—C12—H12B	109.3
C5—C4—Cl2	119.7 (3)	C13—C12—H12B	109.3
C3—C4—Cl2	119.7 (3)	H12A—C12—H12B	107.9
C4—C5—C6	120.5 (3)	N2—C13—C12	112.4 (3)
C4—C5—H5	119.7	N2—C13—H13A	109.1
C6—C5—H5	119.7	C12—C13—H13A	109.1
C5—C6—C7	117.6 (3)	N2—C13—H13B	109.1
C5—C6—C1	120.0 (3)	C12—C13—H13B	109.1
C7—C6—C1	122.4 (3)	H13A—C13—H13B	107.8

N1—Cu1—O1—C1	11.0 (3)	Cl2—C4—C5—C6	179.6 (3)
Cl1—Cu1—O1—C1	175.2 (3)	C4—C5—C6—C7	−177.2 (3)
Cl1^{i}—Cu1—O1—C1	−78.2 (3)	C4—C5—C6—C1	0.6 (5)
O1—Cu1—N1—C7	−12.6 (3)	O1—C1—C6—C5	179.4 (3)
N2—Cu1—N1—C7	166.6 (3)	C2—C1—C6—C5	−1.3 (5)
Cl1—Cu1—N1—C7	−109.8 (4)	O1—C1—C6—C7	−2.9 (5)
Cl1^{i}—Cu1—N1—C7	77.4 (3)	C2—C1—C6—C7	176.3 (3)
O1—Cu1—N1—C8	175.5 (2)	C8—N1—C7—C6	−179.5 (3)
N2—Cu1—N1—C8	−5.2 (2)	Cu1—N1—C7—C6	9.0 (5)
Cl1—Cu1—N1—C8	78.3 (4)	C5—C6—C7—N1	178.7 (3)
Cl1^{i}—Cu1—N1—C8	−94.5 (2)	C1—C6—C7—N1	1.0 (5)
N1—Cu1—N2—C9	−21.8 (2)	C7—N1—C8—C9	−141.6 (3)
Cl1—Cu1—N2—C9	174.03 (19)	Cu1—N1—C8—C9	30.9 (3)
Cl1^{i}—Cu1—N2—C9	67.48 (19)	C13—N2—C9—C8	169.0 (3)
N1—Cu1—N2—C13	−142.8 (3)	C10—N2—C9—C8	−72.1 (3)
Cl1—Cu1—N2—C13	53.1 (2)	Cu1—N2—C9—C8	44.6 (3)
Cl1^{i}—Cu1—N2—C13	−53.4 (2)	N1—C8—C9—N2	−50.7 (4)
N1—Cu1—N2—C10	97.9 (2)	C9—N2—C10—C11	−67.4 (4)
Cl1—Cu1—N2—C10	−66.2 (2)	C13—N2—C10—C11	53.8 (4)
Cl1^{i}—Cu1—N2—C10	−172.8 (2)	Cu1—N2—C10—C11	178.7 (2)
Cu1—O1—C1—C2	175.2 (2)	C12—O2—C11—C10	57.0 (4)
Cu1—O1—C1—C6	−5.6 (5)	N2—C10—C11—O2	−57.2 (4)
O1—C1—C2—C3	−179.9 (3)	C11—O2—C12—C13	−57.2 (4)
C6—C1—C2—C3	0.8 (5)	C9—N2—C13—C12	69.1 (4)
C1—C2—C3—C4	0.4 (5)	C10—N2—C13—C12	−53.5 (4)
C2—C3—C4—C5	−1.2 (5)	Cu1—N2—C13—C12	−173.8 (2)
C2—C3—C4—Cl2	179.9 (3)	O2—C12—C13—N2	57.4 (4)
C3—C4—C5—C6	0.7 (5)		

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