Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

({[2-(1*H*-Benzimidazol-2-yl)ethyl]iminomethyl}phenolato)chloridocopper(II)

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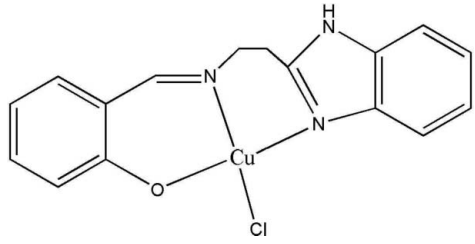
Received 3 May 2007; accepted 17 May 2007

Key indicators: single-crystal X-ray study; T = 571 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.096; data-to-parameter ratio = 13.1.

In the title compound, $[Cu(C_{16}H_{14}N_3O)Cl]$, the Cu^{II} ion exhibits a distorted tetrahedral geometry. The coordination environment of the Cu^{II} ion is composed of one benzimidazole N atom, one imino N atom, one phenolato O atom and one Cl^- anion. Intermolecular N—H···O hydrogen bonds play key roles in stabilizing the crystal packing.

Related literature

For related literature, see: Atwood *et al.* (1998); Bush *et al.* (1994); Masters *et al.* (1985); Maurya *et al.* (2006); Syme *et al.* (2004).



Experimental

Crystal data

$[Cu(C_{16}H_{14}N_3O)Cl]$
M_r = 363.29
Triclinic, $P\overline{1}$
a = 8.009 (3) Å
b = 9.303 (3) Å
c = 10.192 (3) Å
α = 87.815 (4)°
β = 87.548 (4)°
γ = 82.267 (4)°
V = 751.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.64 mm^{-1}
T = 571 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.736, T_{max} = 0.854
3708 measured reflections
2599 independent reflections
2293 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.096
S = 1.12
2599 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H16···O1^{i}	0.86	1.90	2.753 (4)	170

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

We thank the National Natural Science Foundation of China for financial support (No. 30470408) and Jian-Ping Guo for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2057).

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 doi:10.1107/S1600536807024397

supplementary materials

Acta Cryst. (2007). E**63**, m1729 [**doi:10.1107/S1600536807024397**]

({[2-(1*H*-Benzimidazol-2-yl)ethyl]iminomethyl}phenolato)chloridocopper(II)

X.-Y. Ma, X.-D. Dong, Y.-P. Li and Z.-G. Zhang

Comment

The aggregation of the amyloid-beta peptide to form senile plaques is a key event in Alzheimer's disease (Masters *et al.*, 1985). Complexation of copper and zinc with the amyloid-beta peptide induces aggregation of the peptide (Atwood *et al.*, 1998; Bush *et al.*, 1994; Syme *et al.*, 2004). Detailed knowledge of the metal- Amyloid-beta coordination environment could aid in the development of compounds with more effective and specific metal chelating properties as eventual treatments in Alzheimer's disease. As our efforts to develop model complexes as mimics of the metal site, we report a novel copper complex in this paper.

A displacement ellipsoid drawing of (I) is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. Cu(II) ion exhibits a distorted tetrahedral geometry. The coordination sphere of Cu(II) ion is composed of one benzoimidazole N atom, one imino N atom, one phenolato O atom and one Cl anion. As shown in Fig. 2, intermolecular N—H···O hydrogen bonds play key roles in stabilizing the crystal packing. The detailed hydrogen bond information is listed in Table 2.

Experimental

All chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification.

At room temperature, a methanol solution of $CuCl_2·2H_2O$ (0.5 mmol, 5 ml) and a methanol solution of *N*-salicylidine-2-aminoethylbenzimidazole (0.5 mmol, 10 ml, Maurya *et al.*, 2006) were mixed together. The mixture was stirred for about six hours and then filtered. The filtrate was allowed to evaporate at room temperature, affording the green crystal (I).

Refinement

H atoms attached to C atoms were placed in geometrically idealized positions, with Csp^3—H=0.970 Å and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C), and with Csp^2 = 0.930 Å, constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). The H atom on N atom was located in a difference Fourier map and its position and isotropic displacement parameters were refined, with N—H distance was fixed at 0.86 Å.

Figures

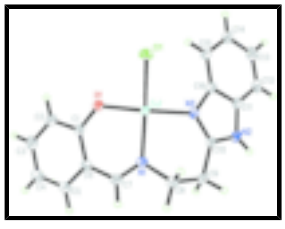

Fig. 1. The structure of the title compound in 30% probability ellipsoids.

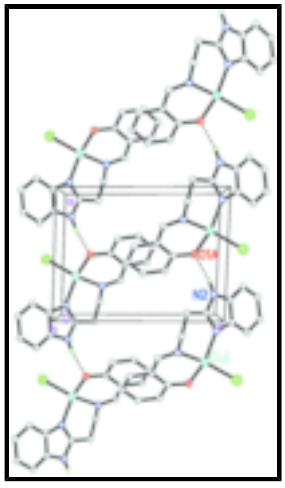

Fig. 2. A packing diagram, viewed down the *b* axis. Hydrogen bonds are indicated by dashed lines. [Symmetry code: (A) $x-1, y, z$]

({[2-(1*H*-Benzimidazol-2-yl)ethyl]iminomethyl}phenolato)chloridocopper(II)

Crystal data

$[Cu(C_{16}H_{14}ON_3)Cl]$	$Z = 2$
$M_r = 363.29$	$F_{000} = 370$
Triclinic, $P\overline{1}$	$D_x = 1.606$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.009$ (3) Å	Cell parameters from 1643 reflections
$b = 9.303$ (3) Å	$\theta = 2.2$–26.6º
$c = 10.192$ (3) Å	$\mu = 1.64$ mm^{-1}
$\alpha = 87.815$ (4)º	$T = 571$ (2) K
$\beta = 87.548$ (4)º	Block, green
$\gamma = 82.267$ (4)º	0.20 × 0.20 × 0.10 mm
$V = 751.3$ (4) Å^3	

Data collection

Bruker SMART CCD diffractometer	2599 independent reflections
Radiation source: fine-focus sealed tube	2293 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 571(2)$ K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 9$
$T_{min} = 0.736$, $T_{max} = 0.854$	$k = -9 \rightarrow 11$
3708 measured reflections	$l = -11 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 0.4537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
2599 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.39$ 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 $F^2 > 2$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	0.32075 (6)	0.15770 (6)	0.09550 (4)	0.03379 (17)
Cl1	0.45923 (12)	0.15497 (12)	−0.09963 (9)	0.0441 (3)
O1	0.4966 (3)	0.2340 (3)	0.1815 (2)	0.0364 (7)
N1	0.2375 (4)	0.0735 (3)	0.2598 (3)	0.0310 (7)
N2	−0.1942 (4)	0.2427 (4)	0.0546 (3)	0.0371 (8)
H16	−0.2948	0.2365	0.0852	0.045*
N3	0.0840 (4)	0.2006 (3)	0.0333 (3)	0.0319 (7)
C1	0.5099 (4)	0.2481 (4)	0.3089 (4)	0.0323 (9)
C2	0.6238 (5)	0.3345 (5)	0.3519 (4)	0.0398 (10)
H2	0.6862	0.3832	0.2901	0.048*
C3	0.6470 (5)	0.3500 (5)	0.4830 (4)	0.0464 (11)
H3	0.7257	0.4076	0.5081	0.056*
C4	0.5554 (5)	0.2816 (5)	0.5775 (4)	0.0486 (11)
H4	0.5720	0.2921	0.6662	0.058*
C5	0.4401 (5)	0.1984 (4)	0.5393 (4)	0.0412 (10)
H5	0.3776	0.1526	0.6032	0.049*
C6	0.4126 (4)	0.1795 (4)	0.4062 (4)	0.0310 (9)
C7	0.2891 (5)	0.0901 (4)	0.3741 (4)	0.0339 (9)
H7	0.2419	0.0391	0.4433	0.041*
C8	0.1105 (5)	−0.0237 (4)	0.2442 (4)	0.0385 (10)
H8A	0.0996	−0.0822	0.3242	0.046*
H8B	0.1461	−0.0886	0.1731	0.046*

C9	−0.0580 (5)	0.0634 (5)	0.2148 (4)	0.0385 (10)
H9A	−0.1376	−0.0032	0.1986	0.046*
H9B	−0.0996	0.1173	0.2919	0.046*
C10	−0.0531 (4)	0.1680 (4)	0.0993 (4)	0.0326 (9)
C11	−0.1515 (4)	0.3313 (4)	−0.0485 (4)	0.0335 (9)
C12	−0.2493 (5)	0.4289 (4)	−0.1289 (4)	0.0414 (10)
H12	−0.3660	0.4461	−0.1172	0.050*
C13	−0.1657 (5)	0.4988 (5)	−0.2260 (4)	0.0459 (11)
H13	−0.2267	0.5662	−0.2814	0.055*
C14	0.0094 (5)	0.4713 (5)	−0.2444 (4)	0.0462 (11)
H14	0.0618	0.5184	−0.3135	0.055*
C15	0.1063 (5)	0.3762 (5)	−0.1626 (4)	0.0412 (10)
H15	0.2231	0.3608	−0.1735	0.049*
C16	0.0237 (4)	0.3041 (4)	−0.0634 (4)	0.0324 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0250 (3)	0.0526 (3)	0.0254 (3)	−0.0124 (2)	0.00124 (19)	0.0014 (2)
Cl1	0.0364 (6)	0.0643 (7)	0.0292 (6)	−0.0022 (5)	0.0072 (4)	0.0041 (5)
O1	0.0271 (14)	0.0581 (19)	0.0260 (15)	−0.0135 (13)	0.0011 (11)	−0.0011 (13)
N1	0.0277 (17)	0.0395 (19)	0.0265 (18)	−0.0078 (14)	0.0012 (14)	0.0013 (14)
N2	0.0208 (16)	0.054 (2)	0.037 (2)	−0.0087 (15)	0.0039 (14)	−0.0036 (17)
N3	0.0222 (16)	0.044 (2)	0.0303 (18)	−0.0092 (14)	−0.0028 (14)	0.0037 (15)
C1	0.0231 (19)	0.041 (2)	0.031 (2)	0.0026 (17)	−0.0003 (16)	−0.0013 (18)
C2	0.037 (2)	0.050 (3)	0.034 (2)	−0.0128 (19)	0.0034 (19)	−0.0034 (19)
C3	0.044 (3)	0.056 (3)	0.042 (3)	−0.014 (2)	−0.009 (2)	−0.009 (2)
C4	0.058 (3)	0.064 (3)	0.025 (2)	−0.012 (2)	−0.006 (2)	−0.004 (2)
C5	0.047 (3)	0.046 (3)	0.029 (2)	−0.008 (2)	−0.002 (2)	0.0062 (19)
C6	0.030 (2)	0.035 (2)	0.028 (2)	−0.0023 (17)	−0.0016 (17)	0.0015 (17)
C7	0.032 (2)	0.037 (2)	0.031 (2)	−0.0021 (17)	0.0067 (17)	0.0044 (17)
C8	0.040 (2)	0.042 (2)	0.036 (2)	−0.0136 (19)	0.0014 (19)	0.0020 (19)
C9	0.029 (2)	0.054 (3)	0.035 (2)	−0.0156 (19)	0.0030 (18)	0.0022 (19)
C10	0.026 (2)	0.049 (3)	0.024 (2)	−0.0129 (18)	0.0025 (16)	−0.0055 (17)
C11	0.027 (2)	0.040 (2)	0.035 (2)	−0.0071 (17)	−0.0018 (17)	−0.0057 (18)
C12	0.030 (2)	0.045 (3)	0.049 (3)	−0.0022 (19)	−0.008 (2)	−0.007 (2)
C13	0.046 (3)	0.042 (3)	0.049 (3)	−0.004 (2)	−0.014 (2)	0.004 (2)
C14	0.041 (2)	0.050 (3)	0.050 (3)	−0.015 (2)	−0.007 (2)	0.013 (2)
C15	0.028 (2)	0.053 (3)	0.045 (3)	−0.0143 (19)	−0.0027 (19)	0.008 (2)
C16	0.027 (2)	0.038 (2)	0.034 (2)	−0.0082 (17)	−0.0031 (17)	−0.0045 (18)

Geometric parameters (Å, °)

Cu1—O1	1.918 (3)	C5—C6	1.404 (5)
Cu1—N1	1.951 (3)	C5—H5	0.9300
Cu1—N3	2.009 (3)	C6—C7	1.431 (5)
Cu1—Cl1	2.2347 (12)	C7—H7	0.9300
O1—C1	1.321 (4)	C8—C9	1.514 (5)
N1—C7	1.274 (5)	C8—H8A	0.9700

N1—C8	1.466 (5)	C8—H8B	0.9700
N2—C10	1.333 (5)	C9—C10	1.501 (5)
N2—C11	1.371 (5)	C9—H9A	0.9700
N2—H16	0.8600	C9—H9B	0.9700
N3—C10	1.327 (4)	C11—C12	1.384 (5)
N3—C16	1.406 (5)	C11—C16	1.395 (5)
C1—C2	1.389 (5)	C12—C13	1.365 (6)
C1—C6	1.420 (5)	C12—H12	0.9300
C2—C3	1.372 (6)	C13—C14	1.397 (6)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.375 (6)	C14—C15	1.376 (5)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.360 (6)	C15—C16	1.385 (5)
C4—H4	0.9300	C15—H15	0.9300
O1—Cu1—N1	92.21 (12)	N1—C7—H7	116.9
O1—Cu1—N3	145.14 (13)	C6—C7—H7	116.9
N1—Cu1—N3	90.28 (12)	N1—C8—C9	110.3 (3)
O1—Cu1—Cl1	93.09 (8)	N1—C8—H8A	109.6
N1—Cu1—Cl1	155.59 (10)	C9—C8—H8A	109.6
N3—Cu1—Cl1	98.78 (9)	N1—C8—H8B	109.6
C1—O1—Cu1	127.4 (2)	C9—C8—H8B	109.6
C7—N1—C8	119.2 (3)	H8A—C8—H8B	108.1
C7—N1—Cu1	126.2 (3)	C10—C9—C8	114.3 (3)
C8—N1—Cu1	114.5 (2)	C10—C9—H9A	108.7
C10—N2—C11	108.3 (3)	C8—C9—H9A	108.7
C10—N2—H16	125.8	C10—C9—H9B	108.7
C11—N2—H16	125.8	C8—C9—H9B	108.7
C10—N3—C16	104.9 (3)	H9A—C9—H9B	107.6
C10—N3—Cu1	125.4 (2)	N3—C10—N2	112.6 (3)
C16—N3—Cu1	127.2 (2)	N3—C10—C9	126.3 (3)
O1—C1—C2	119.2 (3)	N2—C10—C9	121.1 (3)
O1—C1—C6	123.4 (4)	N2—C11—C12	131.5 (3)
C2—C1—C6	117.4 (4)	N2—C11—C16	105.6 (3)
C3—C2—C1	121.9 (4)	C12—C11—C16	122.9 (4)
C3—C2—H2	119.0	C13—C12—C11	116.6 (4)
C1—C2—H2	119.0	C13—C12—H12	121.7
C2—C3—C4	120.9 (4)	C11—C12—H12	121.7
C2—C3—H3	119.6	C12—C13—C14	121.6 (4)
C4—C3—H3	119.6	C12—C13—H13	119.2
C5—C4—C3	118.9 (4)	C14—C13—H13	119.2
C5—C4—H4	120.5	C15—C14—C13	121.6 (4)
C3—C4—H4	120.5	C15—C14—H14	119.2
C4—C5—C6	122.0 (4)	C13—C14—H14	119.2
C4—C5—H5	119.0	C14—C15—C16	117.7 (4)
C6—C5—H5	119.0	C14—C15—H15	121.2
C5—C6—C1	118.8 (4)	C16—C15—H15	121.2
C5—C6—C7	118.6 (3)	C15—C16—C11	119.7 (4)
C1—C6—C7	122.6 (3)	C15—C16—N3	131.7 (3)
N1—C7—C6	126.3 (3)	C11—C16—N3	108.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H16···O1^{i}	0.86	1.90	2.753 (4)	170

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

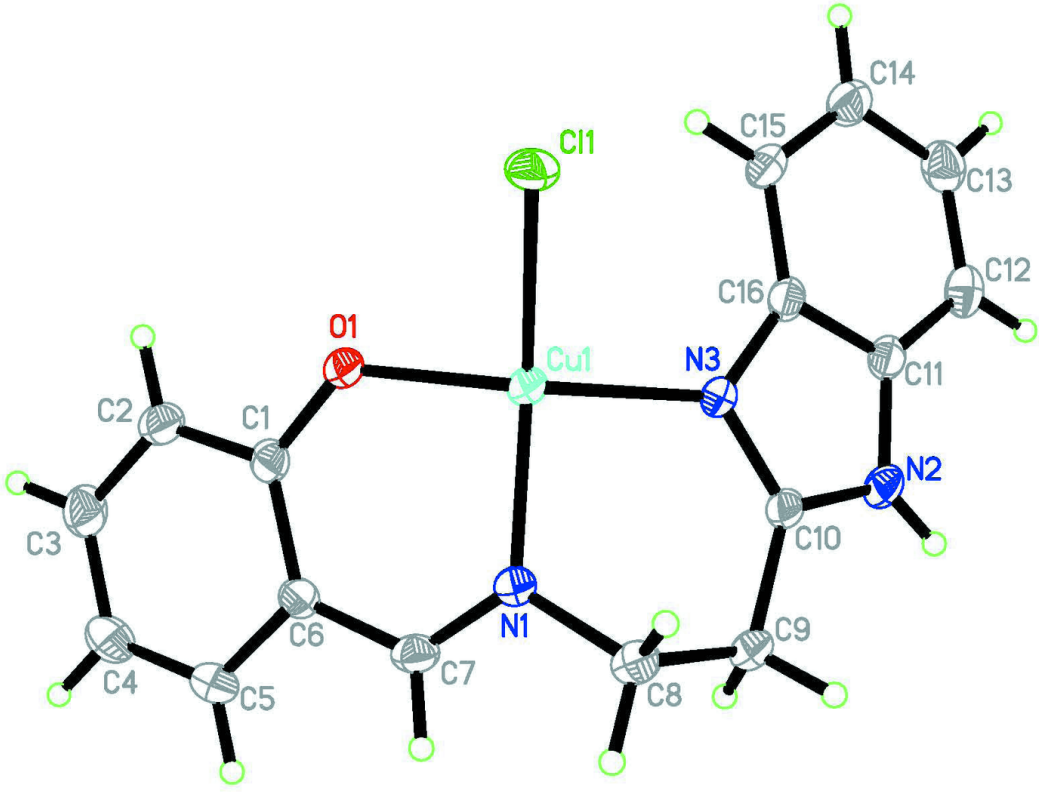
C14
C15
Cl1
C13
C12
C16
O1
Cu1
N3
C11
C2
C1
N2
C3
C10
N1
C6
C9
C7
C4
C5
C8

Fig. 2