Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[{2-[2-(isopropylamino)-ethyliminomethyl]-4-nitrophenolato}-copper(II)]-μ-chlorido]

Li-Juan Ye[a]* and Zhonglu You[b]

[a]Department of Chemistry and Life Sciences, Xiangnan University, Chenzhou 423000, People's Republic of China, and [b]Department of Chemistry, Liaoning Teachers University, Dalian 116029, People's Republic of China
Correspondence e-mail: lijuan_ye@163.com

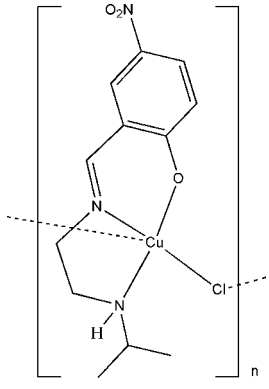
Received 4 November 2007; accepted 17 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.096; data-to-parameter ratio = 17.2.

The title compound, $[Cu(C_{12}H_{16}N_3O_3)Cl]_n$, is a chloride-bridged polymeric copper(II) complex. The Cu^{II} atom is five-coordinate in a square-pyramidal geometry, with one O and two N atoms of the Schiff base ligand and one Cl atom defining the basal plane [Cu···Cl = 2.2703 (8) Å] and a symmetry-related Cl atom occupying the apical position [2.8531 (9) Å]. The chloride-bridged polymeric chain runs along the *b* axis.

Related literature

For related literature, see: Ye & You (2007*a*,*b*).



Experimental

Crystal data

$[Cu(C_{12}H_{16}N_3O_3)Cl]$
M_r = 349.27
Monoclinic, $P2_1/n$
a = 9.762 (1) Å
b = 6.415 (1) Å
c = 22.611 (3) Å
β = 94.353 (2)°
V = 1411.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.75 mm^{-1}
T = 298 (2) K
0.33 × 0.29 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.597, T_{max} = 0.650
11191 measured reflections
3196 independent reflections
2607 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.096
S = 1.06
3196 reflections
186 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.935 (2)	Cu1—Cl1	2.2703 (8)
Cu1—N2	1.966 (3)	Cu1—Cl1^{i}	2.8531 (9)
Cu1—N3	2.048 (3)		
O3—Cu1—N2	90.74 (10)	N3—Cu1—Cl1	96.60 (9)
O3—Cu1—N3	174.91 (9)	O3—Cu1—Cl1^{i}	90.23 (7)
N2—Cu1—N3	84.29 (11)	N2—Cu1—Cl1^{i}	83.67 (8)
O3—Cu1—Cl1	88.48 (8)	N3—Cu1—Cl1^{i}	88.13 (7)
N2—Cu1—Cl1	171.01 (8)	Cl1—Cu1—Cl1^{i}	105.28 (2)

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O3^{i}	0.91 (3)	2.51 (3)	3.288 (4)	145 (3)
C8—H8B···O3^{ii}	0.97	2.47	3.345 (3)	150
C9—H9B···O2^{iii}	0.97	2.50	3.365 (4)	148

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$; (iii) $-x+1, -y+2, -z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

Financial support from the Hunan Provincial Natural Sciences Foundation of China (grant No. 03JJY3019) and the Hunan Provincial Education Ministry Foundation of China (grant No. 05C627) are acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2510).

References

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Ye, L.-J. & You, Z. (2007*a*). *Acta Cryst.* E**63**, m523–m525.
Ye, L.-J. & You, Z. (2007*b*). *Acta Cryst.* E**63**, m1837.

supplementary materials

Acta Cryst. (2007). E**63**, m3137 [**doi:10.1107/S1600536807060163**]

catena-Poly[[{2-[2-(isopropylamino)ethyliminomethyl]-4-nitrophenolato}copper(II)]-μ-chlorido]

L.-J. Ye and Z. You

Comment

Recently, we have reported a thiocyanate coordinated zinc(II) complex (Ye & You, 2007*a*) and a thiocyanate coordinated copper(II) complex (Ye & You, 2007*b*). As an extension of the work on the crystal structures of such complexes, we report herein the crystal structure of the title compound.

The title compound is a chloride-bridged polynuclear copper(II) complex (Fig. 1). The Cu^{II} atom is five-coordinated in a square-pyramidal geometry, with one O and two N atoms of the Schiff base ligand and one Cl atom defining the basal plane (Cu···Cl = 2.2703 (8) Å), and a symmetry-related Cl atom occupying the apical position (2.8531 (9) Å). Selected bond distances and angles within the coordination sphere of the metal atom are given in Table 1. The crystal structure is stabilized by N—H···O and and C—H···O hydrogen bonds (Table 2).

Experimental

5-Nitrosalicylaldehyde (0.1 mmol, 16.5 mg), *N*-isopropylethane-1,2-diamine (0.1 mmol, 10.2 mg), and copper chloride dihydrate (0.1 mmol, 17.0 mg) were dissolved in a methanol solution (10 ml). The mixture was stirred at room temperature for 30 min, giving a clear blue solution. Crystals of the title compound were formed by slow evaporation of the solvent over a week at room temperature.

Refinement

Atom H3A was located from a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å, and with the U_{iso}(H) value fixed at 0.08 $Å^2$. The remaining H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

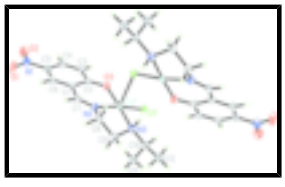


Fig. 1. Part of the polymeric structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. unlabelled atoms are related to labelled atoms by the symmetry operation (3/2 − *x*, −1/2 + *y*, 1/2 − *z*).

catena-Poly[[{2-[2-(isopropylamino)ethyliminomethyl]-4-\ nitrophenolato}copper(II)]-µ-chlorido]

Crystal data

$[Cu(C_{12}H_{16}N_3O_3)Cl]$ F_{000} = 716

M_r = 349.27	D_x = 1.643 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3124 reflections
a = 9.762 (1) Å	θ = 2.2–26.0º
b = 6.415 (1) Å	μ = 1.75 mm^{-1}
c = 22.611 (3) Å	T = 298 (2) K
β = 94.353 (2)º	Block, blue
V = 1411.9 (3) Å^3	0.33 × 0.29 × 0.27 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3196 independent reflections
Radiation source: fine-focus sealed tube	2607 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.597, T_{max} = 0.650	k = −8→8
11191 measured reflections	l = −28→29

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.096	$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 1.0385P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
3196 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
186 parameters	$\Delta\rho_{min}$ = −0.49 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 $F^2 > \sigma(F^2)$ 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	0.76386 (4)	0.83895 (5)	0.181248 (15)	0.02930 (12)
Cl1	0.87605 (8)	1.08051 (11)	0.24016 (3)	0.03700 (19)
O1	0.1740 (3)	0.9670 (5)	−0.04462 (13)	0.0726 (9)
O2	0.1089 (3)	1.2464 (5)	−0.00250 (13)	0.0774 (9)
O3	0.6076 (2)	1.0252 (3)	0.17348 (9)	0.0350 (5)
N1	0.1850 (3)	1.0962 (5)	−0.00511 (14)	0.0507 (7)
N2	0.6771 (3)	0.6547 (4)	0.11980 (11)	0.0323 (5)
N3	0.9188 (2)	0.6230 (4)	0.18510 (11)	0.0303 (5)
C1	0.4874 (3)	0.8788 (4)	0.08619 (13)	0.0315 (6)
C2	0.5112 (3)	1.0351 (4)	0.13091 (13)	0.0305 (6)
C3	0.4235 (3)	1.2127 (5)	0.12726 (15)	0.0382 (7)
H3	0.4372	1.3183	0.1553	0.046*
C4	0.3191 (3)	1.2319 (5)	0.08343 (15)	0.0415 (8)
H4	0.2629	1.3490	0.0821	0.050*
C5	0.2974 (3)	1.0762 (5)	0.04096 (14)	0.0388 (7)
C6	0.3792 (3)	0.9025 (5)	0.04230 (14)	0.0365 (7)
H6	0.3627	0.7991	0.0138	0.044*
C7	0.5695 (3)	0.6920 (4)	0.08538 (13)	0.0328 (7)
H7	0.5422	0.5905	0.0576	0.039*
C8	0.7463 (3)	0.4534 (4)	0.11834 (15)	0.0401 (8)
H8A	0.7286	0.3895	0.0796	0.048*
H8B	0.7124	0.3609	0.1479	0.048*
C9	0.8987 (3)	0.4889 (5)	0.13117 (14)	0.0370 (7)
H9A	0.9455	0.3567	0.1380	0.044*
H9B	0.9363	0.5571	0.0977	0.044*
C10	1.0653 (3)	0.6924 (5)	0.19822 (14)	0.0347 (7)
H10	1.0672	0.7827	0.2332	0.042*
C11	1.1140 (4)	0.8217 (6)	0.14826 (17)	0.0536 (9)
H11A	1.1254	0.7339	0.1146	0.080*
H11B	1.2003	0.8856	0.1608	0.080*
H11C	1.0474	0.9279	0.1376	0.080*
C12	1.1584 (4)	0.5073 (6)	0.21439 (17)	0.0523 (9)
H12A	1.1618	0.4174	0.1806	0.078*
H12B	1.1229	0.4314	0.2465	0.078*
H12C	1.2492	0.5563	0.2263	0.078*
H3A	0.893 (4)	0.546 (6)	0.2159 (12)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0326 (2)	0.02052 (18)	0.0340 (2)	0.00192 (14)	−0.00242 (14)	−0.00460 (14)
Cl1	0.0400 (4)	0.0272 (4)	0.0427 (4)	−0.0004 (3)	−0.0037 (3)	−0.0090 (3)
O1	0.071 (2)	0.074 (2)	0.0672 (19)	0.0107 (16)	−0.0334 (15)	−0.0090 (16)
O2	0.0700 (19)	0.092 (2)	0.0670 (19)	0.0411 (18)	−0.0155 (15)	0.0043 (17)
O3	0.0360 (11)	0.0289 (11)	0.0385 (12)	0.0066 (9)	−0.0067 (9)	−0.0082 (9)
N1	0.0459 (18)	0.0576 (19)	0.0476 (18)	0.0078 (15)	−0.0037 (14)	0.0140 (16)
N2	0.0373 (14)	0.0217 (12)	0.0370 (14)	0.0000 (10)	−0.0036 (11)	−0.0020 (10)
N3	0.0318 (13)	0.0247 (12)	0.0343 (14)	−0.0002 (10)	0.0011 (10)	−0.0004 (10)
C1	0.0332 (16)	0.0267 (15)	0.0341 (16)	−0.0016 (12)	−0.0004 (12)	0.0028 (12)
C2	0.0302 (15)	0.0251 (14)	0.0363 (16)	0.0003 (11)	0.0040 (12)	0.0040 (12)
C3	0.0424 (18)	0.0287 (16)	0.0432 (18)	0.0053 (13)	0.0016 (14)	−0.0010 (13)
C4	0.0407 (18)	0.0356 (17)	0.0485 (19)	0.0125 (14)	0.0055 (15)	0.0114 (15)
C5	0.0348 (17)	0.0464 (19)	0.0349 (17)	0.0031 (14)	−0.0004 (13)	0.0121 (15)
C6	0.0397 (17)	0.0340 (16)	0.0351 (17)	−0.0017 (13)	−0.0014 (13)	0.0002 (13)
C7	0.0420 (17)	0.0235 (14)	0.0319 (15)	−0.0022 (12)	−0.0030 (13)	−0.0046 (12)
C8	0.050 (2)	0.0201 (15)	0.0480 (19)	0.0028 (13)	−0.0091 (15)	−0.0089 (13)
C9	0.0436 (18)	0.0237 (15)	0.0429 (18)	0.0070 (13)	−0.0018 (14)	−0.0083 (13)
C10	0.0320 (16)	0.0322 (16)	0.0393 (17)	0.0009 (12)	−0.0020 (13)	−0.0027 (13)
C11	0.044 (2)	0.058 (2)	0.059 (2)	−0.0113 (17)	0.0042 (17)	0.0095 (19)
C12	0.042 (2)	0.049 (2)	0.064 (2)	0.0144 (16)	−0.0056 (17)	−0.0030 (18)

Geometric parameters (Å, °)

Cu1—O3	1.935 (2)	C4—C5	1.390 (5)
Cu1—N2	1.966 (3)	C4—H4	0.93
Cu1—N3	2.048 (3)	C5—C6	1.370 (4)
Cu1—Cl1	2.2703 (8)	C6—H6	0.93
Cu1—Cl1^{i}	2.8531 (9)	C7—H7	0.93
O1—N1	1.217 (4)	C8—C9	1.511 (4)
O2—N1	1.221 (4)	C8—H8A	0.97
O3—C2	1.296 (3)	C8—H8B	0.97
N1—C5	1.460 (4)	C9—H9A	0.97
N2—C7	1.281 (4)	C9—H9B	0.97
N2—C8	1.459 (4)	C10—C11	1.507 (5)
N3—C9	1.493 (4)	C10—C12	1.523 (4)
N3—C10	1.506 (4)	C10—H10	0.98
N3—H3A	0.91 (3)	C11—H11A	0.96
C1—C6	1.402 (4)	C11—H11B	0.96
C1—C2	1.431 (4)	C11—H11C	0.96
C1—C7	1.443 (4)	C12—H12A	0.96
C2—C3	1.424 (4)	C12—H12B	0.96
C3—C4	1.372 (4)	C12—H12C	0.96
C3—H3	0.93		
O3—Cu1—N2	90.74 (10)	C4—C5—N1	119.8 (3)

O3—Cu1—N3	174.91 (9)	C5—C6—C1	120.7 (3)
N2—Cu1—N3	84.29 (11)	C5—C6—H6	119.7
O3—Cu1—Cl1	88.48 (8)	C1—C6—H6	119.7
N2—Cu1—Cl1	171.01 (8)	N2—C7—C1	125.3 (3)
N3—Cu1—Cl1	96.60 (9)	N2—C7—H7	117.3
O3—Cu1—Cl1^{i}	90.23 (7)	C1—C7—H7	117.3
N2—Cu1—Cl1^{i}	83.67 (8)	N2—C8—C9	108.3 (2)
N3—Cu1—Cl1^{i}	88.13 (7)	N2—C8—H8A	110.0
Cl1—Cu1—Cl1^{i}	105.28 (2)	C9—C8—H8A	110.0
C2—O3—Cu1	128.38 (18)	N2—C8—H8B	110.0
O1—N1—O2	123.6 (3)	C9—C8—H8B	110.0
O1—N1—C5	118.9 (3)	H8A—C8—H8B	108.4
O2—N1—C5	117.5 (3)	N3—C9—C8	108.0 (2)
C7—N2—C8	120.8 (2)	N3—C9—H9A	110.1
C7—N2—Cu1	127.3 (2)	C8—C9—H9A	110.1
C8—N2—Cu1	111.87 (19)	N3—C9—H9B	110.1
C9—N3—C10	113.3 (2)	C8—C9—H9B	110.1
C9—N3—Cu1	107.72 (18)	H9A—C9—H9B	108.4
C10—N3—Cu1	119.73 (18)	N3—C10—C11	111.3 (3)
C9—N3—H3A	107 (3)	N3—C10—C12	110.9 (3)
C10—N3—H3A	109 (3)	C11—C10—C12	113.1 (3)
Cu1—N3—H3A	99 (3)	N3—C10—H10	107.0
C6—C1—C2	119.8 (3)	C11—C10—H10	107.0
C6—C1—C7	118.1 (3)	C12—C10—H10	107.0
C2—C1—C7	122.0 (3)	C10—C11—H11A	109.5
O3—C2—C3	118.8 (3)	C10—C11—H11B	109.5
O3—C2—C1	124.1 (3)	H11A—C11—H11B	109.5
C3—C2—C1	117.1 (3)	C10—C11—H11C	109.5
C4—C3—C2	121.6 (3)	H11A—C11—H11C	109.5
C4—C3—H3	119.2	H11B—C11—H11C	109.5
C2—C3—H3	119.2	C10—C12—H12A	109.5
C3—C4—C5	120.1 (3)	C10—C12—H12B	109.5
C3—C4—H4	120.0	H12A—C12—H12B	109.5
C5—C4—H4	120.0	C10—C12—H12C	109.5
C6—C5—C4	120.7 (3)	H12A—C12—H12C	109.5
C6—C5—N1	119.5 (3)	H12B—C12—H12C	109.5

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O3^{i}	0.91 (3)	2.51 (3)	3.288 (4)	145 (3)
C8—H8B···O3^{ii}	0.97	2.47	3.345 (3)	150
C9—H9B···O2^{iii}	0.97	2.50	3.365 (4)	148

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (ii) *x*, *y*−1, *z*; (iii) −*x*+1, −*y*+2, −*z*.

Fig. 1