Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloridotetrakis(imidazole)copper(II) chloride

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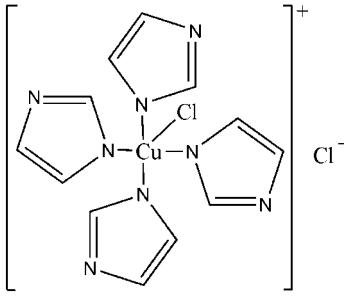
Received 29 May 2007; accepted 10 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.025; wR factor = 0.072; data-to-parameter ratio = 13.8.

The title compound, $[CuCl(C_3H_3N_2)_4]Cl$, exhibits a square-pyramidal coordination of Cu^{II} by four N atoms of four imidazole ligands and one chlorine atom located at the apex of the pyramid.

Related literature

For related literature, see Li *et al.* (2004).



Experimental

Crystal data

$[CuCl(C_3H_3N_2)_4]Cl$
M_r = 402.74
Monoclinic, $P2_1/n$
a = 8.8662 (3) Å
b = 13.3199 (4) Å
c = 13.9190 (4) Å
β = 90.0420 (10)°
V = 1643.79 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.66 mm^{-1}
T = 293 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker AXS CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.788, T_{max} = 0.851
18750 measured reflections
2885 independent reflections
2735 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.072
S = 1.00
2885 reflections
209 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N5	1.996 (7)	Cu1—N7	2.018 (7)
Cu1—N3	2.000 (7)	Cu1—Cl1	2.621 (2)
Cu1—N1	2.016 (6)		
N5—Cu1—N3	174.9 (3)	N1—Cu1—N7	157.5 (3)
N5—Cu1—N1	90.1 (3)	N5—Cu1—Cl1	92.2 (2)
N3—Cu1—N1	89.7 (3)	N3—Cu1—Cl1	92.8 (2)
N5—Cu1—N7	88.9 (3)	N1—Cu1—Cl1	98.2 (2)
N3—Cu1—N7	89.3 (3)	N7—Cu1—Cl1	104.3 (2)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Science Project of Taishan University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2113).

References

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  doi:10.1107/S1600536807044108

supplementary materials

Acta Cryst. (2007). E**63**, m2536 [**doi:10.1107/S1600536807044108**]

Chloridotetrakis(imidazole)copper(II) chloride

T. B. Li, Y. L. Hu, J. K. Li and G. F. He

Experimental

The aimed compound was prepared by adding imidazole (27.2 mg, 0.4 mmol) to a solution of $CuCl_2 2H_2O$ (17.2 mg, 0.1 mmol) in CH_3OH and stirred vigorously for about 4 h, then the blue precipitate were filtered off and dried in vacuum. Single crystals suitable for X-ray structural analysis were obtained from DMF solution by slow evaporation. The crystal packing (Fig. 2) involves C—H···Cl hydrogen bonds formed between CH of the imidazole group and the coordinated chlorine (C8—H8···Cl1^{i} with C8···Cl1^{i} of 3.806 (2) Å; H8···Cl1^{i}of 2.878 (2) Å; C8—H8—Cl1^{i} = 175.3 (2) °; symmetry code i = 1/2 − *x*, 1/2 + *y*, 1/2 − *z*) generating a chain along the axis b.

Figures

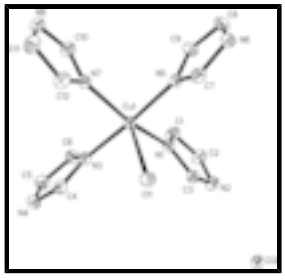


Fig. 1. Molecular structure of the title compound with ellipsoids drawn at the 30% probability level.
Fig. 2. Crystal packing diagram in the *bc* plane.

Chloridotetrakis(imidazole)copper(II) chloride

Crystal data

$[CuCl(C_3H_3N_2)_4]Cl$	F_{000} = 812
M_r = 402.74	D_x = 1.627 Mg m^{-3}
Monoclinic, *P*2(1)/*n*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8636 reflections
a = 8.8662 (3) Å	θ = 2.7–27.4º
b = 13.3199 (4) Å	μ = 1.66 mm^{-1}
c = 13.9190 (4) Å	*T* = 293 (2) K
β = 90.0420 (10)º	Block, blue
V = 1643.79 (9) Å^3	0.15 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker AXS CCD area-detector diffractometer	2885 independent reflections

Radiation source: fine-focus sealed tube	2735 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 293(2)$ K	$\theta_{max} = 25.0°$
phi and ω scans	$\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 8$
$T_{min} = 0.788$, $T_{max} = 0.851$	$k = -15 \rightarrow 15$
18750 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.025$	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.4934P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.56$ e Å^{-3}
2885 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}
209 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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	0.68669 (11)	0.21337 (6)	0.37745 (7)	0.0240 (4)
Cl1	0.4436 (2)	0.10148 (15)	0.37916 (18)	0.0334 (5)
Cl2	0.0547 (2)	0.40803 (17)	0.37502 (18)	0.0368 (5)
N1	0.5854 (8)	0.3488 (5)	0.3741 (5)	0.0277 (14)
N2	0.4028 (8)	0.4602 (5)	0.3706 (6)	0.0353 (17)
N3	0.6950 (9)	0.2209 (5)	0.5209 (5)	0.0286 (16)
N4	0.6740 (10)	0.1813 (6)	0.6730 (5)	0.0383 (19)
N5	0.6957 (9)	0.2123 (5)	0.2342 (5)	0.0273 (16)

N6	0.6674 (10)	0.1741 (6)	0.0824 (5)	0.0354 (18)
N7	0.8583 (8)	0.1139 (5)	0.3799 (6)	0.0276 (15)
N8	1.0860 (8)	0.0512 (6)	0.3744 (7)	0.0389 (17)
C1	0.6476 (10)	0.4434 (6)	0.3757 (7)	0.036 (2)
H1	0.7503	0.4576	0.3777	0.043*
C2	0.5353 (10)	0.5125 (7)	0.3739 (8)	0.040 (2)
H2	0.5463	0.5819	0.3747	0.047*
C3	0.4385 (10)	0.3618 (6)	0.3713 (7)	0.0313 (18)
H3	0.3684	0.3099	0.3701	0.038*
C4	0.6407 (11)	0.1555 (7)	0.5825 (7)	0.034 (2)
H4	0.5862	0.0985	0.5654	0.040*
C5	0.7553 (13)	0.2692 (8)	0.6689 (7)	0.042 (2)
H5	0.7941	0.3050	0.7206	0.050*
C6	0.7675 (12)	0.2930 (7)	0.5751 (7)	0.036 (2)
H6	0.8169	0.3491	0.5508	0.043*
C7	0.6289 (11)	0.1510 (7)	0.1729 (7)	0.033 (2)
H7	0.5643	0.0991	0.1901	0.039*
C8	0.7656 (13)	0.2535 (8)	0.0856 (7)	0.039 (2)
H8	0.8116	0.2852	0.0338	0.047*
C9	0.7816 (12)	0.2764 (6)	0.1798 (7)	0.034 (2)
H9	0.8417	0.3277	0.2040	0.041*
C10	1.0017 (10)	0.1352 (7)	0.3754 (8)	0.036 (2)
H10	1.0406	0.1999	0.3732	0.043*
C11	0.9878 (11)	−0.0278 (7)	0.3794 (9)	0.043 (2)
H11	1.0129	−0.0956	0.3802	0.052*
C12	0.8481 (10)	0.0114 (6)	0.3829 (7)	0.036 (2)
H12	0.7590	−0.0253	0.3868	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0257 (6)	0.0258 (5)	0.0206 (5)	0.0039 (4)	0.0002 (5)	0.0001 (4)
Cl1	0.0294 (11)	0.0342 (11)	0.0366 (12)	−0.0065 (8)	−0.0001 (11)	0.0031 (10)
Cl2	0.0312 (11)	0.0486 (12)	0.0305 (11)	0.0088 (9)	0.0003 (11)	0.0022 (11)
N1	0.030 (4)	0.028 (3)	0.025 (3)	0.003 (3)	0.001 (4)	0.000 (3)
N2	0.032 (4)	0.033 (4)	0.041 (4)	0.006 (3)	0.000 (4)	−0.001 (4)
N3	0.029 (4)	0.032 (4)	0.024 (4)	0.004 (3)	0.000 (3)	0.000 (3)
N4	0.036 (5)	0.055 (5)	0.024 (4)	0.003 (4)	0.001 (4)	0.006 (4)
N5	0.028 (4)	0.029 (4)	0.025 (4)	0.005 (3)	−0.001 (3)	−0.002 (3)
N6	0.033 (4)	0.047 (5)	0.026 (4)	0.004 (4)	0.000 (3)	−0.006 (3)
N7	0.027 (4)	0.030 (3)	0.026 (3)	0.002 (3)	0.000 (3)	0.000 (3)
N8	0.028 (4)	0.048 (4)	0.041 (4)	0.008 (3)	0.000 (4)	0.003 (4)
C1	0.029 (4)	0.031 (4)	0.047 (5)	−0.002 (3)	−0.001 (5)	0.000 (5)
C2	0.037 (5)	0.025 (4)	0.057 (6)	−0.001 (4)	−0.002 (5)	0.000 (5)
C3	0.030 (5)	0.032 (4)	0.032 (5)	−0.001 (4)	−0.001 (4)	0.000 (4)
C4	0.031 (5)	0.036 (5)	0.033 (5)	0.001 (4)	−0.001 (4)	0.005 (4)
C5	0.040 (6)	0.058 (6)	0.028 (5)	−0.002 (5)	−0.004 (5)	−0.007 (4)
C6	0.038 (6)	0.037 (5)	0.033 (5)	−0.005 (4)	−0.002 (4)	0.001 (4)

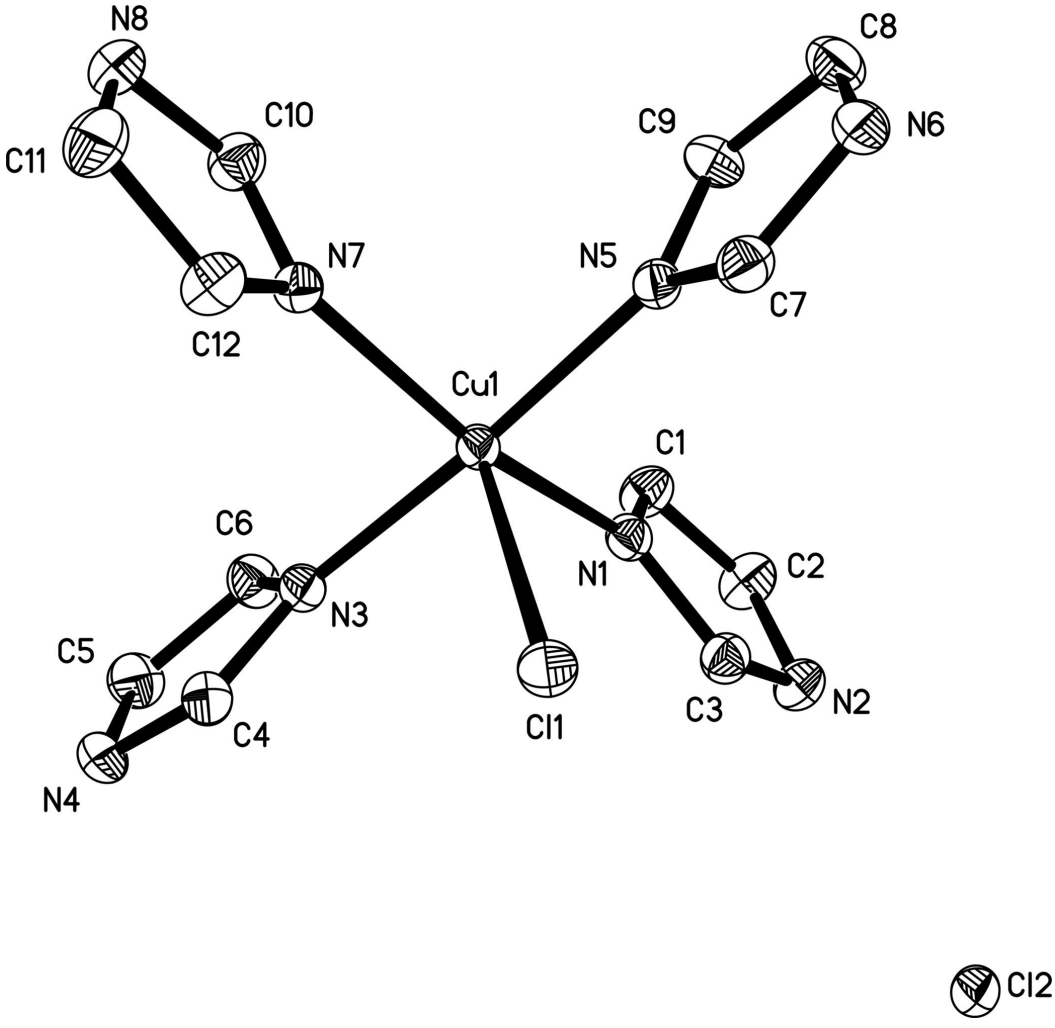
C7	0.030 (5)	0.035 (5)	0.033 (5)	0.002 (4)	−0.001 (4)	−0.004 (4)
C8	0.048 (6)	0.042 (5)	0.028 (4)	0.004 (5)	0.007 (4)	0.006 (4)
C9	0.039 (6)	0.033 (5)	0.030 (5)	−0.005 (4)	0.006 (4)	0.001 (4)
C10	0.035 (5)	0.032 (4)	0.041 (5)	0.001 (4)	0.001 (5)	0.002 (4)
C11	0.045 (6)	0.033 (5)	0.052 (6)	0.010 (4)	0.000 (5)	−0.001 (5)
C12	0.031 (5)	0.030 (4)	0.048 (5)	0.000 (3)	0.001 (5)	−0.001 (4)

Geometric parameters (Å, °)

Cu1—N5	1.996 (7)	N8—C10	1.346 (12)
Cu1—N3	2.000 (7)	N8—C11	1.367 (13)
Cu1—N1	2.016 (6)	C1—C2	1.356 (13)
Cu1—N7	2.018 (7)	C1—H1	0.9300
Cu1—Cl1	2.621 (2)	C2—H2	0.9300
N1—C3	1.314 (12)	C3—H3	0.9300
N1—C1	1.375 (11)	C4—H4	0.9300
N2—C3	1.348 (11)	C5—C6	1.348 (14)
N2—C2	1.367 (12)	C5—H5	0.9300
N3—C4	1.314 (12)	C6—H6	0.9300
N3—C6	1.380 (12)	C7—H7	0.9300
N4—C4	1.338 (12)	C8—C9	1.353 (13)
N4—C5	1.376 (14)	C8—H8	0.9300
N5—C7	1.320 (12)	C9—H9	0.9300
N5—C9	1.372 (12)	C10—H10	0.9300
N6—C7	1.341 (12)	C11—C12	1.345 (13)
N6—C8	1.370 (15)	C11—H11	0.9300
N7—C10	1.304 (11)	C12—H12	0.9300
N7—C12	1.369 (11)		
N5—Cu1—N3	174.9 (3)	N2—C2—H2	126.7
N5—Cu1—N1	90.1 (3)	N1—C3—N2	111.1 (8)
N3—Cu1—N1	89.7 (3)	N1—C3—H3	124.4
N5—Cu1—N7	88.9 (3)	N2—C3—H3	124.4
N3—Cu1—N7	89.3 (3)	N3—C4—N4	111.3 (8)
N1—Cu1—N7	157.5 (3)	N3—C4—H4	124.4
N5—Cu1—Cl1	92.2 (2)	N4—C4—H4	124.4
N3—Cu1—Cl1	92.8 (2)	C6—C5—N4	106.4 (9)
N1—Cu1—Cl1	98.2 (2)	C6—C5—H5	126.8
N7—Cu1—Cl1	104.3 (2)	N4—C5—H5	126.8
C3—N1—C1	106.1 (7)	C5—C6—N3	109.1 (9)
C3—N1—Cu1	124.0 (6)	C5—C6—H6	125.4
C1—N1—Cu1	129.8 (6)	N3—C6—H6	125.4
C3—N2—C2	107.1 (7)	N5—C7—N6	110.5 (8)
C4—N3—C6	106.0 (8)	N5—C7—H7	124.7
C4—N3—Cu1	127.2 (6)	N6—C7—H7	124.7
C6—N3—Cu1	126.7 (6)	C9—C8—N6	105.7 (8)
C4—N4—C5	107.2 (8)	C9—C8—H8	127.1
C7—N5—C9	106.1 (8)	N6—C8—H8	127.1
C7—N5—Cu1	129.2 (6)	C8—C9—N5	109.7 (8)
C9—N5—Cu1	124.7 (6)	C8—C9—H9	125.2

C7—N6—C8	108.0 (7)	N5—C9—H9	125.2
C10—N7—C12	106.4 (8)	N7—C10—N8	111.2 (8)
C10—N7—Cu1	126.3 (6)	N7—C10—H10	124.4
C12—N7—Cu1	127.3 (6)	N8—C10—H10	124.4
C10—N8—C11	106.6 (7)	C12—C11—N8	106.8 (8)
C2—C1—N1	109.1 (8)	C12—C11—H11	126.6
C2—C1—H1	125.5	N8—C11—H11	126.6
N1—C1—H1	125.5	C11—C12—N7	109.0 (8)
C1—C2—N2	106.6 (7)	C11—C12—H12	125.5
C1—C2—H2	126.7	N7—C12—H12	125.5
N5—Cu1—N1—C3	90.8 (8)	N1—Cu1—N7—C12	179.6 (8)
N3—Cu1—N1—C3	−94.3 (8)	Cl1—Cu1—N7—C12	−0.7 (8)
N7—Cu1—N1—C3	178.2 (8)	C3—N1—C1—C2	0.0 (12)
Cl1—Cu1—N1—C3	−1.5 (8)	Cu1—N1—C1—C2	−178.9 (7)
N5—Cu1—N1—C1	−90.4 (8)	N1—C1—C2—N2	−0.4 (12)
N3—Cu1—N1—C1	84.5 (8)	C3—N2—C2—C1	0.5 (12)
N7—Cu1—N1—C1	−3.0 (13)	C1—N1—C3—N2	0.3 (12)
Cl1—Cu1—N1—C1	177.3 (8)	Cu1—N1—C3—N2	179.4 (6)
N5—Cu1—N3—C4	−148 (3)	C2—N2—C3—N1	−0.5 (12)
N1—Cu1—N3—C4	124.3 (8)	C6—N3—C4—N4	0.0 (11)
N7—Cu1—N3—C4	−78.2 (8)	Cu1—N3—C4—N4	176.4 (7)
Cl1—Cu1—N3—C4	26.1 (8)	C5—N4—C4—N3	−0.1 (12)
N5—Cu1—N3—C6	27 (3)	C4—N4—C5—C6	0.1 (12)
N1—Cu1—N3—C6	−60.1 (8)	N4—C5—C6—N3	−0.1 (12)
N7—Cu1—N3—C6	97.4 (8)	C4—N3—C6—C5	0.1 (12)
Cl1—Cu1—N3—C6	−158.3 (8)	Cu1—N3—C6—C5	−176.3 (7)
N3—Cu1—N5—C7	157 (3)	C9—N5—C7—N6	−0.7 (10)
N1—Cu1—N5—C7	−115.8 (8)	Cu1—N5—C7—N6	−178.4 (6)
N7—Cu1—N5—C7	86.6 (8)	C8—N6—C7—N5	0.9 (11)
Cl1—Cu1—N5—C7	−17.6 (8)	C7—N6—C8—C9	−0.6 (12)
N3—Cu1—N5—C9	−20 (3)	N6—C8—C9—N5	0.2 (12)
N1—Cu1—N5—C9	66.9 (7)	C7—N5—C9—C8	0.3 (11)
N7—Cu1—N5—C9	−90.7 (7)	Cu1—N5—C9—C8	178.1 (7)
Cl1—Cu1—N5—C9	165.1 (7)	C12—N7—C10—N8	0.6 (12)
N5—Cu1—N7—C10	84.6 (9)	Cu1—N7—C10—N8	−177.2 (6)
N3—Cu1—N7—C10	−90.6 (9)	C11—N8—C10—N7	−0.5 (13)
N1—Cu1—N7—C10	−3.0 (15)	C10—N8—C11—C12	0.2 (13)
Cl1—Cu1—N7—C10	176.7 (9)	N8—C11—C12—N7	0.2 (13)
N5—Cu1—N7—C12	−92.7 (8)	C10—N7—C12—C11	−0.5 (12)
N3—Cu1—N7—C12	92.1 (8)	Cu1—N7—C12—C11	177.3 (8)

Fig. 1


N8
C10
C11
N7
C12
C8
C9
N6
N5
C7
Cu1
C1
C6
N1
C2
N3
C5
C3
N2
C4
Cl1
N4
Cl2