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Dichlorido{2-[(3,4-dimethylphenyl)-iminomethyl]pyridine-κ^2N,N'}copper(II)

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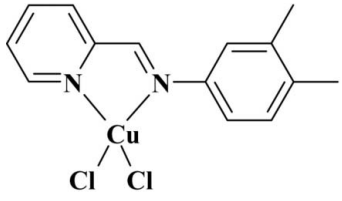
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.126; data-to-parameter ratio = 18.3.

In the title complex, $[CuCl_2(C_{14}H_{14}N_2)]$, the Cu^{II} atom exhibits a very distorted tetrahedral coordination geometry involving two chloride ions and two N-atom donors from the Schiff base ligand. The range for the six bond angles about the Cu^{2+} cation is 81.49 (11)–145.95 (9)°. The chelate ring including the Cu^{II} atom is approximately planar, with a maximum deviation of 0.039 (4) Å for one of the C atoms; this plane forms a dihedral angle of 46.69 (9)° with the $CuCl_2$ plane.

Related literature

For related structures, see: Mahmoudi *et al.* (2009); Wang & Zhong (2009). For background information on diimine complexes, see: Khalaj *et al.* (2010); Salehzadeh *et al.* (2011).



Experimental

Crystal data

$[CuCl_2(C_{14}H_{14}N_2)]$
M_r = 344.71
Triclinic, $P\overline{1}$
a = 8.1171 (4) Å
b = 9.5784 (4) Å
c = 10.0609 (5) Å
α = 67.236 (2)°
β = 88.513 (2)°
γ = 81.336 (2)°
V = 712.61 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 150 K
0.18 × 0.16 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.725, T_{max} = 0.830
6451 measured reflections
3189 independent reflections
2256 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.126
S = 1.07
3189 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.988 (3)	Cu1—Cl2	2.2035 (10)
Cu1—N2	2.025 (3)	Cu1—Cl1	2.2204 (10)

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2154).

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supplementary materials

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Dichlorido{2-[(3,4-dimethylphenyl)iminomethyl]pyridine-κ^2N,N'}copper(II)

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Comment

Diimine ligands derived from 2-aminopyridine and aniline derivatives are useful bidentate terminal ligands and some complexes with them as ligand have already been published (Mahmoudi *et al.*, 2009; Salehzadeh *et al.*, 2011). We report herein the crystal structure of the title complex [$CuCl_2(C_{14}H_{14}N_2)$] which was prepared by the reaction of $CuCl_2$ with the bidentate ligand *N*-(3,4-dimethylphenyl)-pyridine-2-ylmethyleneamine.

The molecular structure of the title complex is shown in Fig. 1. The Cu^{II} ion is in a very distorted tetrahedral environment formed by a bis-chelating ligand and two Cl anions. The dihedral angle between the chelate plane Cu1–N1–C5–C6–N2 and the Cl1–Cu1–Cl2 plane is 46.69(9° and the range for the six bond angles about Cu1 is 81.49 (11)° (N1-Cu1-N2)–145.95 (9)° (N2-Cu1-Cl1). These values show an appreciable distortion towards square planar geometry. A comparison of the dihedral angles between the planes of the pyridine, chelate and the benzene rings indicate that the ligand is distorted from planarity, with a twist of 26.00 (17)° between the chelate (N1—C5—C6—N2) and the benzene (C7–C12) planes. The Cu—Cl and Cu—N bond dimensions compare well with the values found in other tetrahedral diimine complexes of copper(II) chloride (Mahmoudi *et al.*, 2009; Wang & Zhong, 2009).

Experimental

The title complex was prepared by the reaction of $CuCl_2$ (13.4 mg, 0.1 mmol) and *N*-(3,4-dimethylphenyl)-(pyridine-2-ylmethylene)amine (21.0 mg, 0.1 mmol) in 10 ml acetonitrile at room temperature. The green single crystals were obtained after the solution had been allowed to stand at room temperature for two days.

Refinement

Hydrogen atoms were placed in calculated positions with C—H = 0.95–0.98Å and included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C_{aromatic})$ or $1.5U_{eq}(C_{methyl})$.

Figures

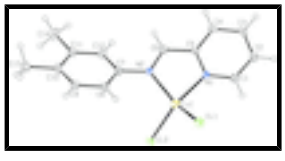

Fig. 1. A view of the structure of the title complex, with displacement ellipsoids drawn at the 50% probability level.

Dichlorido{2-[(3,4-dimethylphenyl)iminomethyl]pyridine- κ^2N,N'}copper(II)

Crystal data

$[CuCl_2(C_{14}H_{14}N_2)]$	$Z = 2$
$M_r = 344.71$	$F(000) = 350$
Triclinic, $P\overline{1}$	$D_x = 1.607$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.1171$ (4) Å	Cell parameters from 6451 reflections
$b = 9.5784$ (4) Å	$\theta = 3.2$–$27.4°$
$c = 10.0609$ (5) Å	$\mu = 1.89$ mm^{-1}
$\alpha = 67.236$ (2)°	$T = 150$ K
$\beta = 88.513$ (2)°	Block, green
$\gamma = 81.336$ (2)°	0.18 × 0.16 × 0.10 mm
$V = 712.61$ (6) Å^3	

Data collection

Nonius KappaCCD diffractometer	3189 independent reflections
Radiation source: fine-focus sealed tube	2256 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.039$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 27.4°$, $\theta_{min} = 3.2°$
φ scans and ω scans with κ offsets	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$k = -11 \rightarrow 12$
$T_{min} = 0.725$, $T_{max} = 0.830$	$l = -12 \rightarrow 13$
6451 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.126$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.324P]$ where $P = (F_o^2 + 2F_c^2)/3$
3189 reflections	$(\Delta/\sigma)_{max} < 0.001$
174 parameters	$\Delta\rho_{max} = 0.83$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.62$ e Å^{-3}

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	0.78165 (5)	0.20424 (5)	0.33299 (5)	0.02388 (17)
Cl1	1.03716 (11)	0.14201 (11)	0.26876 (12)	0.0344 (3)
Cl2	0.82609 (12)	0.35601 (10)	0.44190 (11)	0.0285 (2)
N1	0.7024 (4)	0.0099 (3)	0.3557 (3)	0.0214 (7)
N2	0.5411 (4)	0.2901 (3)	0.2659 (3)	0.0210 (7)
C1	0.7928 (5)	−0.1295 (4)	0.3991 (4)	0.0246 (8)
H1A	0.9088	−0.1414	0.4200	0.030*
C2	0.7211 (5)	−0.2577 (4)	0.4146 (4)	0.0268 (9)
H2A	0.7879	−0.3557	0.4440	0.032*
C3	0.5523 (5)	−0.2417 (4)	0.3868 (4)	0.0276 (9)
H3A	0.5013	−0.3282	0.3973	0.033*
C4	0.4583 (5)	−0.0967 (4)	0.3432 (4)	0.0242 (8)
H4A	0.3416	−0.0824	0.3242	0.029*
C5	0.5375 (4)	0.0264 (4)	0.3280 (4)	0.0199 (7)
C6	0.4535 (5)	0.1850 (4)	0.2758 (4)	0.0226 (8)
H6A	0.3379	0.2099	0.2500	0.027*
C7	0.4663 (5)	0.4479 (4)	0.2081 (4)	0.0221 (8)
C8	0.5689 (5)	0.5567 (4)	0.1391 (4)	0.0239 (8)
H8A	0.6856	0.5271	0.1362	0.029*
C9	0.4977 (5)	0.7090 (4)	0.0747 (4)	0.0267 (8)
H9A	0.5672	0.7830	0.0249	0.032*
C10	0.3303 (5)	0.7572 (4)	0.0800 (4)	0.0281 (9)
C11	0.2260 (5)	0.6473 (4)	0.1520 (4)	0.0250 (8)
C12	0.2963 (5)	0.4939 (4)	0.2149 (4)	0.0265 (8)
H12A	0.2271	0.4191	0.2634	0.032*
C13	0.2548 (5)	0.9237 (4)	0.0073 (4)	0.0321 (9)
H13A	0.3406	0.9834	−0.0456	0.048*
H13B	0.2103	0.9620	0.0803	0.048*
H13C	0.1645	0.9337	−0.0601	0.048*
C14	0.0420 (5)	0.6938 (4)	0.1616 (5)	0.0363 (10)
H14A	−0.0082	0.6034	0.2197	0.054*
H14B	−0.0102	0.7396	0.0644	0.054*
H14C	0.0245	0.7687	0.2068	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0176 (3)	0.0229 (3)	0.0336 (3)	−0.00222 (18)	0.0004 (2)	−0.0139 (2)
Cl1	0.0182 (5)	0.0407 (6)	0.0514 (7)	−0.0050 (4)	0.0058 (4)	−0.0255 (5)
Cl2	0.0269 (5)	0.0226 (4)	0.0390 (6)	−0.0013 (4)	−0.0050 (4)	−0.0156 (4)
N1	0.0205 (16)	0.0209 (15)	0.0232 (17)	−0.0002 (12)	−0.0008 (13)	−0.0100 (13)
N2	0.0222 (16)	0.0190 (15)	0.0228 (16)	−0.0036 (12)	0.0033 (13)	−0.0092 (13)
C1	0.023 (2)	0.0270 (19)	0.023 (2)	0.0004 (15)	0.0001 (16)	−0.0107 (17)
C2	0.033 (2)	0.0204 (18)	0.028 (2)	−0.0005 (16)	0.0044 (18)	−0.0118 (17)
C3	0.038 (2)	0.0225 (19)	0.027 (2)	−0.0094 (17)	0.0055 (18)	−0.0130 (17)
C4	0.024 (2)	0.030 (2)	0.023 (2)	−0.0081 (16)	0.0011 (16)	−0.0129 (17)
C5	0.0194 (18)	0.0211 (17)	0.0207 (19)	−0.0042 (14)	0.0025 (15)	−0.0095 (15)
C6	0.0180 (18)	0.0235 (18)	0.027 (2)	−0.0008 (14)	0.0016 (16)	−0.0114 (17)
C7	0.026 (2)	0.0196 (17)	0.0217 (19)	−0.0018 (15)	0.0007 (16)	−0.0092 (15)
C8	0.0213 (19)	0.0262 (19)	0.026 (2)	−0.0054 (15)	0.0013 (16)	−0.0110 (17)
C9	0.031 (2)	0.0251 (19)	0.023 (2)	−0.0063 (16)	−0.0010 (17)	−0.0079 (17)
C10	0.040 (2)	0.0171 (17)	0.023 (2)	0.0025 (16)	0.0032 (18)	−0.0054 (16)
C11	0.024 (2)	0.027 (2)	0.024 (2)	−0.0012 (16)	0.0016 (16)	−0.0096 (17)
C12	0.025 (2)	0.0255 (19)	0.027 (2)	−0.0038 (16)	0.0050 (17)	−0.0090 (17)
C13	0.043 (3)	0.0233 (19)	0.029 (2)	−0.0015 (17)	−0.0030 (19)	−0.0103 (18)
C14	0.030 (2)	0.029 (2)	0.039 (3)	0.0047 (17)	0.0020 (19)	−0.0039 (19)

Geometric parameters (Å, °)

Cu1—N1	1.988 (3)	C7—C8	1.391 (5)
Cu1—N2	2.025 (3)	C7—C12	1.392 (5)
Cu1—Cl2	2.2035 (10)	C8—C9	1.384 (5)
Cu1—Cl1	2.2204 (10)	C8—H8A	0.9500
N1—C1	1.335 (4)	C9—C10	1.374 (5)
N1—C5	1.348 (5)	C9—H9A	0.9500
N2—C6	1.290 (4)	C10—C11	1.413 (5)
N2—C7	1.433 (4)	C10—C13	1.510 (5)
C1—C2	1.391 (5)	C11—C12	1.390 (5)
C1—H1A	0.9500	C11—C14	1.505 (5)
C2—C3	1.379 (5)	C12—H12A	0.9500
C2—H2A	0.9500	C13—H13A	0.9800
C3—C4	1.390 (5)	C13—H13B	0.9800
C3—H3A	0.9500	C13—H13C	0.9800
C4—C5	1.383 (5)	C14—H14A	0.9800
C4—H4A	0.9500	C14—H14B	0.9800
C5—C6	1.462 (5)	C14—H14C	0.9800
C6—H6A	0.9500		
N1—Cu1—N2	81.49 (11)	C8—C7—C12	119.9 (3)
N1—Cu1—Cl2	145.38 (9)	C8—C7—N2	117.6 (3)
N2—Cu1—Cl2	99.33 (8)	C12—C7—N2	122.5 (3)
N1—Cu1—Cl1	95.98 (9)	C9—C8—C7	118.7 (3)

N2—Cu1—Cl1	145.95 (9)	C9—C8—H8A	120.7
Cl2—Cu1—Cl1	101.41 (4)	C7—C8—H8A	120.7
C1—N1—C5	119.2 (3)	C10—C9—C8	122.5 (3)
C1—N1—Cu1	127.1 (3)	C10—C9—H9A	118.8
C5—N1—Cu1	113.6 (2)	C8—C9—H9A	118.8
C6—N2—C7	120.0 (3)	C9—C10—C11	119.0 (3)
C6—N2—Cu1	112.6 (2)	C9—C10—C13	121.6 (3)
C7—N2—Cu1	127.4 (2)	C11—C10—C13	119.4 (3)
N1—C1—C2	121.5 (3)	C12—C11—C10	118.8 (3)
N1—C1—H1A	119.2	C12—C11—C14	120.0 (3)
C2—C1—H1A	119.2	C10—C11—C14	121.2 (3)
C3—C2—C1	119.6 (3)	C11—C12—C7	121.1 (3)
C3—C2—H2A	120.2	C11—C12—H12A	119.4
C1—C2—H2A	120.2	C7—C12—H12A	119.4
C2—C3—C4	118.8 (3)	C10—C13—H13A	109.5
C2—C3—H3A	120.6	C10—C13—H13B	109.5
C4—C3—H3A	120.6	H13A—C13—H13B	109.5
C5—C4—C3	118.8 (3)	C10—C13—H13C	109.5
C5—C4—H4A	120.6	H13A—C13—H13C	109.5
C3—C4—H4A	120.6	H13B—C13—H13C	109.5
N1—C5—C4	122.1 (3)	C11—C14—H14A	109.5
N1—C5—C6	114.1 (3)	C11—C14—H14B	109.5
C4—C5—C6	123.7 (3)	H14A—C14—H14B	109.5
N2—C6—C5	118.0 (3)	C11—C14—H14C	109.5
N2—C6—H6A	121.0	H14A—C14—H14C	109.5
C5—C6—H6A	121.0	H14B—C14—H14C	109.5

Fig. 1