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Dichlorido(1,10-phenanthroline)-copper(II)

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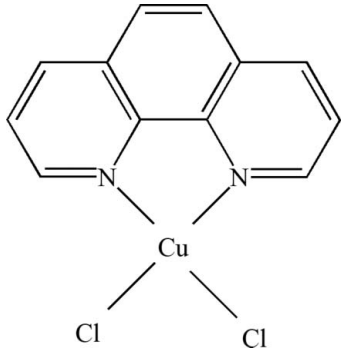
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 13.7.

In the title compound, $[CuCl_2(C_{12}H_8N_2)]$, the Cu^{II} atom adopts a distorted tetrahedral coordination formed by two N atoms from one 1,10-phenanthroline ligand and two Cl atoms. In the crystal structure, molecules form intermolecular C—H···Cl contacts and π–π stacking interactions [centroid-to-centroid distances = 3.803 and 3.671 Å]. The shortest intermolecular Cu···Cl contacts are 4.306 (3) Å.

Related literature

For the related dimeric and polymeric structures, $[(C_{12}H_8N_2)CuCl_2]_2$ and $[(C_{12}H_8N_2)Cu_2Cl_2]_n$, see: Viossat *et al.* (1998); Wang *et al.* (2002).



Experimental

Crystal data

$[CuCl_2(C_{12}H_8N_2)]$
M_r = 314.65
Monoclinic, $P2_1/c$
a = 8.000 (5) Å
b = 15.669 (8) Å
c = 11.348 (5) Å
β = 122.53 (3)°
V = 1199.3 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.24 mm^{-1}
T = 293 (2) K
0.26 × 0.07 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
7416 measured reflections
2220 independent reflections
1510 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 0.99
2220 reflections
162 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl2^{i}	0.93	2.88	3.572 (3)	132
C3—H3···Cl2^{ii}	0.93	2.80	3.669 (3)	157
C7—H7···Cl2^{iii}	0.93	2.79	3.513 (3)	135

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2255).

References

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Wang, S., Li, Y., Wang, E., Luan, G., Hu, C., Hu, N. & Jia, H. (2002). *J. Solid State Chem.* **167**, 402–406.

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supplementary materials

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Dichlorido(1,10-phenanthroline)copper(II)

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Comment

As shown in Fig. 1, the title compound is a monomeric complex in which the Cu^{II} atom is four-coordinated in a distorted tetrahedral geometry by two N atoms from one 1,10-phenanthroline ligand and two Cl atoms. In the crystal structure, molecules form intermolecular C—H···Cl contacts and π-π stacking interactions (Fig. 2). The dihedral angle and centroid-to-centroid distance between rings [C4–C8, C12] and [C1–C5, N1]^{i} (symmetry code: (i) $1-x, 1-y, 1-z$) are 1.4° and 3.803 Å, respectively. Between rings [C4–C8, C12] and [C8–C12, N2]^{ii} (symmetry code: (ii) $2-x, 1-y, 1-z$), the corresponding measurements are 3.0° and 3.671 Å.

Experimental

A mixture of 1,10-phenanthroline (0.161 g, 0.001 mol) and $CuCl_2$ (0.135 g, 0.001 mol) was added to methanol (20 ml), and the mixture was heated at 365 K for 5 h under reflux with stirring. The resulting solution was then filtered and single crystals suitable for X-ray diffraction analysis formed after a week by slow evaporation of the solvent.

Refinement

All H atoms were located at calculated positions and refined as riding on their parent C atoms with the C—H = 0.93 Å and $U_{iso}(H) = 1.2\ U_{eq}(C)$.

Figures

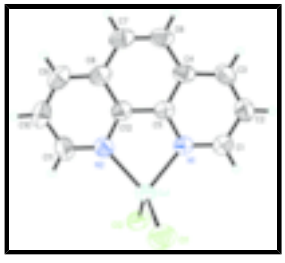

Fig. 1. The molecular structure, showing displacement ellipsoids at 50% probability for non-H atoms.

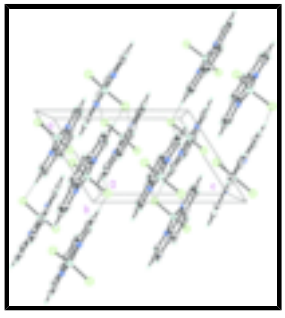

Fig. 2. Packing diagram viewed along the *b* axis.

Dichlorido(1,10-phenanthroline)copper(II)

Crystal data

$[CuCl_2(C_{12}H_8N_2)]$	F_{000} = 628
M_r = 314.65	D_x = 1.743 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3375 reflections
a = 8.000 (5) Å	θ = 1.0–28.3º
b = 15.669 (8) Å	μ = 2.24 mm^{-1}
c = 11.348 (5) Å	T = 293 (2) K
β = 122.53 (3)º	Block, blue
V = 1199.3 (12) Å^3	0.26 × 0.07 × 0.06 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	1510 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.042
Monochromator: graphite	θ_{max} = 25.5º
T = 293(2) K	θ_{min} = 2.5º
phi and ω scans	h = −9→9
Absorption correction: none	k = −18→18
7416 measured reflections	l = −13→13
2220 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.091	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.001
2220 reflections	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
162 parameters	$\Delta\rho_{min}$ = −0.32 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.73800 (6)	0.22097 (2)	0.95569 (4)	0.04570 (17)
Cl1	0.57194 (15)	0.31386 (6)	0.99943 (11)	0.0681 (3)
Cl2	0.92896 (14)	0.27755 (5)	0.89018 (11)	0.0621 (3)
N1	0.5460 (4)	0.12799 (16)	0.8272 (3)	0.0438 (7)
N2	0.8850 (4)	0.11559 (17)	1.0788 (3)	0.0456 (7)
C1	0.3787 (5)	0.1347 (2)	0.7024 (4)	0.0508 (9)
H1	0.3393	0.1885	0.6621	0.055 (10)*
C2	0.2612 (5)	0.0655 (2)	0.6306 (4)	0.0591 (10)
H2	0.1457	0.0728	0.5432	0.074 (12)*
C3	0.3154 (5)	−0.0135 (2)	0.6880 (4)	0.0550 (10)
H3	0.2374	−0.0606	0.6402	0.060 (10)*
C4	0.4892 (5)	−0.0243 (2)	0.8191 (4)	0.0452 (8)
C5	0.6006 (5)	0.04917 (19)	0.8855 (3)	0.0398 (7)
C6	0.5560 (5)	−0.1041 (2)	0.8883 (4)	0.0539 (9)
H6	0.4798	−0.1528	0.8468	0.066 (11)*
C7	0.7274 (5)	−0.1107 (2)	1.0122 (4)	0.0564 (10)
H7	0.7685	−0.1639	1.0547	0.069 (12)*
C8	0.8498 (5)	−0.0375 (2)	1.0818 (4)	0.0481 (8)
C9	1.0331 (5)	−0.0415 (3)	1.2071 (4)	0.0587 (10)
H9	1.0841	−0.0936	1.2513	0.057 (10)*
C10	1.1382 (6)	0.0321 (3)	1.2647 (4)	0.0596 (10)
H10	1.2618	0.0301	1.3477	0.065 (11)*
C11	1.0576 (5)	0.1093 (2)	1.1984 (3)	0.0542 (9)
H11	1.1290	0.1590	1.2401	0.047 (9)*
C12	0.7828 (5)	0.0422 (2)	1.0188 (3)	0.0420 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0442 (3)	0.0321 (2)	0.0536 (3)	−0.00146 (18)	0.0216 (2)	−0.00104 (19)
Cl1	0.0739 (7)	0.0533 (6)	0.0802 (7)	0.0106 (5)	0.0436 (6)	−0.0022 (5)
Cl2	0.0557 (6)	0.0442 (5)	0.0879 (7)	0.0035 (4)	0.0397 (5)	0.0093 (5)
N1	0.0454 (16)	0.0361 (15)	0.0458 (16)	−0.0035 (13)	0.0219 (14)	0.0025 (13)
N2	0.0447 (16)	0.0437 (16)	0.0436 (16)	0.0004 (13)	0.0206 (14)	−0.0038 (13)
C1	0.050 (2)	0.045 (2)	0.053 (2)	0.0025 (17)	0.0241 (18)	0.0037 (17)
C2	0.050 (2)	0.061 (3)	0.051 (2)	−0.0022 (19)	0.0165 (19)	−0.0053 (19)
C3	0.046 (2)	0.048 (2)	0.062 (3)	−0.0079 (17)	0.023 (2)	−0.0093 (19)

C4	0.046 (2)	0.0351 (18)	0.063 (2)	−0.0001 (15)	0.0349 (18)	−0.0065 (16)
C5	0.0423 (18)	0.0372 (18)	0.0472 (19)	0.0015 (15)	0.0289 (16)	0.0014 (15)
C6	0.054 (2)	0.0359 (19)	0.077 (3)	0.0008 (17)	0.039 (2)	−0.0028 (18)
C7	0.062 (3)	0.039 (2)	0.079 (3)	0.0106 (18)	0.045 (2)	0.0073 (19)
C8	0.053 (2)	0.044 (2)	0.057 (2)	0.0087 (17)	0.0355 (18)	0.0054 (17)
C9	0.057 (2)	0.061 (3)	0.060 (2)	0.019 (2)	0.033 (2)	0.018 (2)
C10	0.051 (2)	0.077 (3)	0.044 (2)	0.019 (2)	0.0209 (19)	0.010 (2)
C11	0.045 (2)	0.063 (2)	0.046 (2)	−0.0009 (19)	0.0181 (18)	−0.0077 (19)
C12	0.0442 (19)	0.0400 (19)	0.0479 (19)	0.0046 (15)	0.0289 (16)	0.0022 (16)

Geometric parameters (Å, °)

Cu1—N1	2.049 (3)	C4—C5	1.402 (4)
Cu1—N2	2.072 (3)	C4—C6	1.419 (5)
Cu1—Cl1	2.1998 (13)	C5—C12	1.433 (5)
Cu1—Cl2	2.2122 (14)	C6—C7	1.340 (5)
N1—C1	1.330 (4)	C6—H6	0.930
N1—C5	1.357 (4)	C7—C8	1.437 (5)
N2—C11	1.320 (4)	C7—H7	0.930
N2—C12	1.362 (4)	C8—C9	1.391 (5)
C1—C2	1.379 (5)	C8—C12	1.396 (5)
C1—H1	0.930	C9—C10	1.368 (6)
C2—C3	1.357 (5)	C9—H9	0.930
C2—H2	0.930	C10—C11	1.387 (5)
C3—C4	1.397 (5)	C10—H10	0.930
C3—H3	0.930	C11—H11	0.930
N1—Cu1—N2	81.35 (11)	N1—C5—C4	122.7 (3)
N1—Cu1—Cl1	108.56 (9)	N1—C5—C12	117.5 (3)
N2—Cu1—Cl1	124.60 (8)	C4—C5—C12	119.8 (3)
N1—Cu1—Cl2	115.78 (9)	C7—C6—C4	121.1 (3)
N2—Cu1—Cl2	107.56 (9)	C7—C6—H6	119.4
Cl1—Cu1—Cl2	114.87 (5)	C4—C6—H6	119.5
C1—N1—C5	117.8 (3)	C6—C7—C8	121.7 (3)
C1—N1—Cu1	129.9 (2)	C6—C7—H7	119.4
C5—N1—Cu1	112.3 (2)	C8—C7—H7	118.9
C11—N2—C12	117.8 (3)	C9—C8—C12	117.8 (3)
C11—N2—Cu1	130.8 (2)	C9—C8—C7	123.9 (3)
C12—N2—Cu1	111.4 (2)	C12—C8—C7	118.2 (3)
N1—C1—C2	122.9 (3)	C10—C9—C8	119.4 (4)
N1—C1—H1	118.4	C10—C9—H9	120.2
C2—C1—H1	118.7	C8—C9—H9	120.4
C3—C2—C1	119.6 (4)	C9—C10—C11	119.3 (4)
C3—C2—H2	120.2	C9—C10—H10	120.1
C1—C2—H2	120.3	C11—C10—H10	120.6
C2—C3—C4	120.0 (3)	N2—C11—C10	123.1 (4)
C2—C3—H3	120.2	N2—C11—H11	118.5
C4—C3—H3	119.8	C10—C11—H11	118.3
C3—C4—C5	117.0 (3)	N2—C12—C8	122.6 (3)
C3—C4—C6	124.0 (3)	N2—C12—C5	117.4 (3)

C5—C4—C6	119.0 (3)	C8—C12—C5	120.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl2^{i}	0.93	2.88	3.572 (3)	132
C3—H3···Cl2^{ii}	0.93	2.80	3.669 (3)	157
C7—H7···Cl2^{iii}	0.93	2.79	3.513 (3)	135

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

Fig. 1

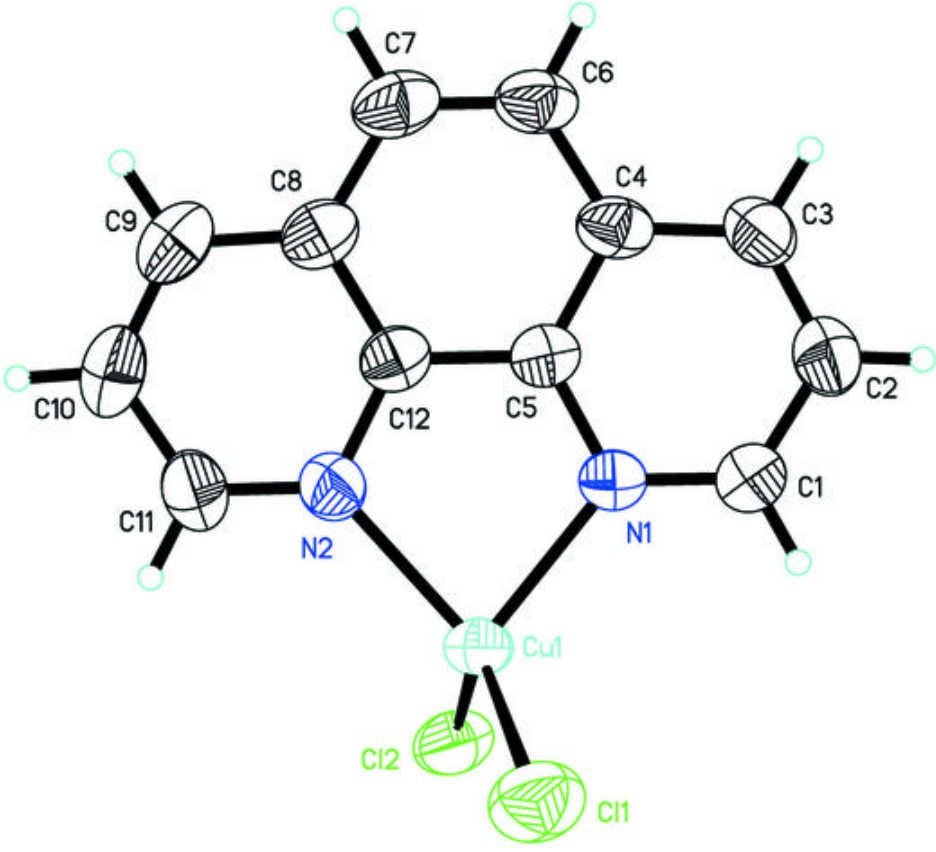

Fig. 2