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Poly[chlorido(μ_3-1,2,4-triazolato)-copper(II)]

Yu-Xiang Gao,* Li-Bin Wang and Yan-Ling Niu

Department of Chemistry, Tonghua Teachers' College, Tonghua 134002, People's Republic of China
Correspondence e-mail: yxgao_tonghua@yahoo.com.cn

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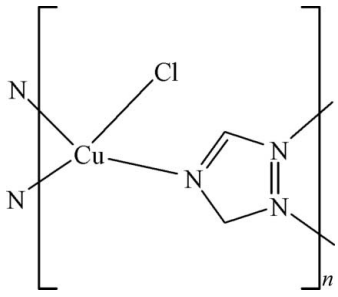
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.003 Å; R factor = 0.019; wR factor = 0.038; data-to-parameter ratio = 16.9.

The title compound, $[Cu(C_2H_2N_3)Cl]_n$, has been prepared by hydrothermal reaction of $CuCl_2$ and 1,2,4-triazole. It is isostructural with its Mn^{II}, Co^{II}, Ni^{II} and Zn^{II} analogs. The Cu^{II} atom is surrounded by three N atoms belonging to three different triazolate ligands and a Cl atom, and exhibits a slightly distorted tetrahedral coordination geometry. The triply bridging nature of the 1,2,4-triazolate ligand gives rise to a polymeric layer containing both binuclear and tetranuclear macrocyclic units. In the binuclear unit, two Cu^{II} atoms are bridged by two nearly coplanar triazolate groups through the 1,2-positions, affording a six-membered ring around an inversion center. Each binuclear unit is further connected to four parallel units through the other four N atoms of the triazolate groups. Four adjacent units, which are pairwise parallel, afford 16-membered tetranuclear macrocyclic units in which the two nearest-neighbor Cu^{II} atoms are bridged by a single triazolate ligand through the 1,4-positions.

Related literature

For the isostructural analogs, see: Gao *et al.* (2007*b*) (Mn^{II}); Wayne *et al.* (2006) (Co^{II}); Gao *et al.* (2007*a*) (Ni^{II}); Jonas *et al.* (1995) (Zn^{II}).



Experimental

Crystal data

$[Cu(C_2H_2N_3)Cl]$
M_r = 167.06
Monoclinic, $P2_1/n$
a = 6.0213 (10) Å
b = 9.960 (2) Å
c = 8.6869 (10) Å
β = 101.021 (10)°
V = 511.38 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.65 mm^{-1}
T = 293 (2) K
0.12 × 0.10 × 0.10 mm

Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.606, T_{max} = 0.654
4256 measured reflections
1096 independent reflections
917 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.038
S = 1.00
1096 reflections
65 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: BI2227).

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supplementary materials

Acta Cryst. (2007). E**63**, m2366 [**doi:10.1107/S1600536807040007**]

Poly[chlorido(μ_3-1,2,4-triazolato)copper(II)]

Y.-X. Gao, L.-B. Wang and Y.-L. Niu

Comment

The title compound, $[Cu(C_2H_2N_3)Cl]_n$, is isostructural with its Mn^{II} (Gao *et al.*, 2007*b*), Co^{II} (Wayne *et al.*, 2006), Ni^{II} (Gao *et al.*, 2007*a*) and Zn^{II} (Jonas *et al.*, 1995) analogues.

The coordination polyhedron of the Cu^{II} atom (Fig. 1) can be described as a distorted tetrahedron. The Cu^{II} atom is surrounded by three N atoms belonging to three different triazolate ligands, and a Cl atom. The Cu—N bond lengths are in the range 1.9585 (19)–2.2057 (19) Å, and the Cu—Cl bond length is 2.1955 (8) Å. The bond angles around the Cu^{II} atom are in the range 103.92 (8)–113.97 (6) °.

Polymeric layers (Fig. 2) are formed due to the triply bridging nature of the 1,2,4-triazolate ligand, which is bonded to three different Cu^{II} atoms through its three N atoms. A layer contains both binuclear and tetranuclear macrocyclic units. In the binuclear unit, two Cu^{II} atoms are bridged by two nearly coplanar triazolate groups through the 1,2-positions, affording a six-membered ring around an inversion center. The Cu···Cu separation within the binuclear unit is 3.722 (1) Å. Each binuclear unit is further connected to four parallel units through the other four N atoms of the triazolate groups. Four adjacent units, which are pairwise parallel, afford 16-membered tetranuclear macrocyclic units. In each of these, the two nearest-neighbor Cu^{II} atoms are bridged by a single triazolate ligand through the 1,4-positions. The Cu···Cu separations are 5.628 (1) and 6.026 (1) Å.

Experimental

A mixture of $CuCl_2$ (0.5 mmol), KOH (0.5 mmol), 1,2,4-triazole (0.5 mmol) and H_2O (8 ml) was sealed in a 25 ml Teflon-lined stainless steel autoclave and kept at 413 K for 2 d. On cooling to room temperature, blue crystals of the title compound were obtained in a yield of 11%. Elemental analysis calculated: C 14.37, H 1.20, N 25.15%; found: C 14.32, H 1.24, N 25.12%.

Refinement

H atoms were placed in calculated positions and allowed to ride with C—H = 0.93%A and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

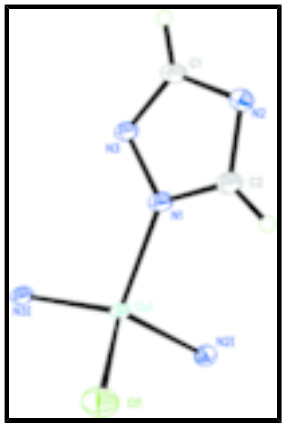

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms. The subscript I denotes the the symmetry operation $-x + 1/2, y - 1/2, -z + 3/2$).

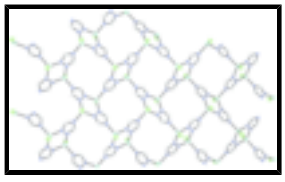

Fig. 2. View of a layer showing both the binuclear units and the tetranuclear cavities.

Poly[chlorido(μ$_3$-1,2,4-triazolato)copper(II)]

Crystal data

[Cu($C_2H_2N_3$)Cl]	F_{000} = 324
M_r = 167.06	D_x = 2.170 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1096 reflections
a = 6.0213 (10) Å	θ = 3.1–26.9º
b = 9.960 (2) Å	μ = 4.65 mm^{-1}
c = 8.6869 (10) Å	T = 293 (2) K
β = 101.021 (10)º	Block, blue
V = 511.38 (15) Å^3	0.12 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker APEX II CCD diffractometer	1096 independent reflections
Radiation source: fine-focus sealed tube	917 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 293(2) K	θ_{max} = 26.9º
φ and ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −7→7
T_{min} = 0.606, T_{max} = 0.654	k = −12→12

4256 measured reflections

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.019$

$wR(F^2) = 0.038$

$S = 1.00$

1096 reflections

65 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 0.65P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.32$ e Å^{-3}

$\Delta\rho_{min} = -0.32$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0269 (11)

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}
C1	0.2402 (4)	0.6685 (2)	1.2710 (3)	0.0277 (5)
H1	0.2495	0.6537	1.3778	0.033*
C2	0.2874 (4)	0.7543 (3)	1.0620 (3)	0.0315 (6)
H2	0.3331	0.8100	0.9880	0.038*
Cl1	0.30626 (12)	0.55329 (7)	0.67333 (8)	0.04266 (19)
Cu1	0.04412 (4)	0.58056 (3)	0.81490 (3)	0.01897 (11)
N1	0.1593 (3)	0.6475 (2)	1.0271 (2)	0.0274 (5)
N2	0.3427 (3)	0.77240 (19)	1.2138 (2)	0.0259 (4)
N3	0.1277 (3)	0.59126 (19)	1.1642 (2)	0.0247 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0344 (13)	0.0305 (13)	0.0168 (11)	−0.0032 (11)	0.0013 (9)	−0.0008 (9)
C2	0.0417 (14)	0.0305 (13)	0.0202 (11)	−0.0118 (11)	0.0010 (10)	0.0022 (10)

Cl1	0.0394 (4)	0.0548 (5)	0.0376 (4)	0.0036 (3)	0.0168 (3)	−0.0020 (3)
Cu1	0.02207 (16)	0.02000 (17)	0.01356 (15)	−0.00051 (11)	0.00020 (9)	0.00153 (10)
N1	0.0347 (11)	0.0280 (11)	0.0173 (9)	−0.0051 (9)	−0.0007 (8)	0.0027 (8)
N2	0.0292 (10)	0.0255 (10)	0.0213 (10)	−0.0034 (8)	0.0002 (8)	−0.0016 (8)
N3	0.0295 (10)	0.0266 (10)	0.0169 (9)	−0.0025 (9)	0.0015 (7)	0.0029 (8)

Geometric parameters (Å, °)

C1—N3	1.293 (3)	Cu1—N1	1.9585 (19)
C1—N2	1.348 (3)	Cu1—N2^{i}	1.9950 (19)
C1—H1	0.930	Cu1—N3^{ii}	2.0257 (19)
C2—N2	1.309 (3)	N1—N3	1.362 (3)
C2—N1	1.315 (3)	N2—Cu1^{iii}	1.9950 (19)
C2—H2	0.930	N3—Cu1^{ii}	2.0257 (19)
Cl1—Cu1	2.1955 (8)		
N3—C1—N2	114.0 (2)	N3^{ii}—Cu1—Cl1	112.32 (6)
N3—C1—H1	123.0	C2—N1—N3	107.76 (18)
N2—C1—H1	123.0	C2—N1—Cu1	125.38 (16)
N2—C2—N1	111.6 (2)	N3—N1—Cu1	126.84 (15)
N2—C2—H2	124.2	C2—N2—C1	102.67 (19)
N1—C2—H2	124.2	C2—N2—Cu1^{iii}	124.10 (17)
N1—Cu1—N2^{i}	103.92 (8)	C1—N2—Cu1^{iii}	133.17 (15)
N1—Cu1—N3^{ii}	107.36 (8)	C1—N3—N1	103.95 (18)
N2^{i}—Cu1—N3^{ii}	112.44 (8)	C1—N3—Cu1^{ii}	130.17 (16)
N1—Cu1—Cl1	113.97 (6)	N1—N3—Cu1^{ii}	125.79 (14)
N2^{i}—Cu1—Cl1	106.62 (6)		

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

Fig. 1

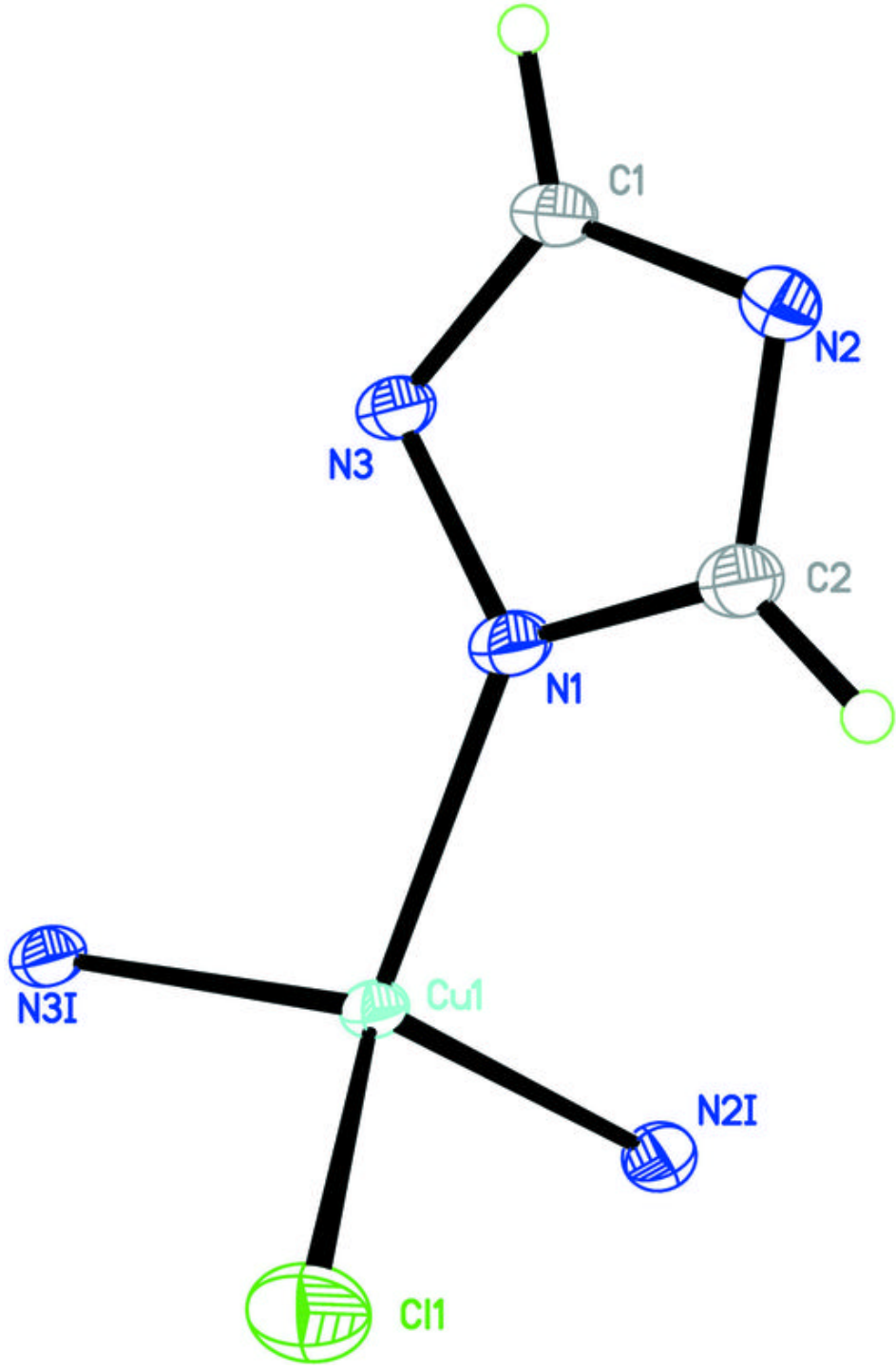

Fig. 2