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Di-μ-chlorido-bis[2,2′-(propane-1,3-diyl)-bis(2*H*-benzotriazole)-$\kappa^2N^1,N^{1'}$]-copper(I)]

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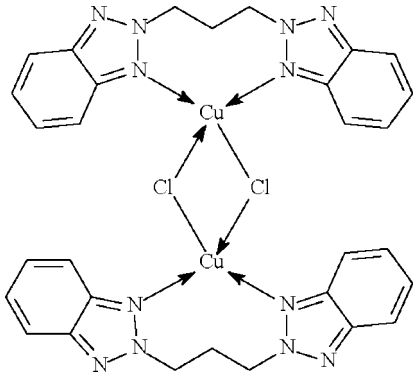
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.104; data-to-parameter ratio = 17.3.

Cupric chloride undergoes reduction in its reaction with 2,2′-(propane-1,3-diyl)bis(2*H*-benzotriazole) to form the centrosymmetic title compound, $[Cu_2Cl_2(C_{15}H_{14}N_6)_2]$. The organic ligand chelates the Cu^I atom and two adducts are linked through two chloride bridges into a dinuclear molecule. The metal atom shows tetrahedral coordination.

Related literature

For the isomeric chain structure, see Borsting & Steel (2004). For the synthesis of the ligand, see: Xie *et al.* (2000).



Experimental

Crystal data

$[Cu_2Cl_2(C_{15}H_{14}N_6)_2]$
M_r = 754.62
Monoclinic, $P2_1/n$
a = 9.886 (3) Å
b = 10.055 (3) Å
c = 15.876 (4) Å
β = 106.401 (4)°
V = 1514.0 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 295 (2) K
0.23 × 0.20 × 0.19 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2006)
T_{min} = 0.592, T_{max} = 0.748
17855 measured reflections
3592 independent reflections
3425 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.104
S = 1.06
3592 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.034 (2)	Cu1—Cl1	2.3028 (7)
Cu1—N4	2.076 (2)	Cu1—Cl1^{i}	2.5131 (8)
N1—Cu1—N4	112.58 (7)	N4—Cu1—Cl1	111.68 (5)
N1—Cu1—Cl1	121.38 (5)	N4—Cu1—Cl1^{i}	100.66 (5)
N1—Cu1—Cl1^{i}	106.40 (5)	Cl1—Cu1—Cl1^{i}	101.04 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrystalClear* (Rigaku/MSC, 2006); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2279).

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supplementary materials

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Di-μ-chlorido-bis[2,2'-(propane-1,3-diyl)bis(2*H*-benzotriazole)-$\kappa^2N^1,N^{1'}$]copper(I)]

X.-L. Zhou, L.-P. Wang, X.-R. Meng and S. W. Ng

Comment

The 2,2'-(propane-1,3-diyl)bis(2*H*-benzotriazole) heterocycle binds to two copper(I) atoms in the 1:1 adduct with copper(I) chloride to furnish a linear chain structure. The copper atom shows tetrahedral coordination (Table 1) as is covalently bonded to one chlorine atom and datively bonded to the adjacent one (Borsting & Steel, 2004). The present compound is a 1:1 adduct but the compound exists as a monomeric dinculear molecule as the heterocycle functions instead as a bidentate chelate (Fig. 1). However, bond dimensions involving the copper atom are not significantly difference, so that the different architectures reflect the flexible nature of the ligand, which possess three methylene linkages separating the fused-rings.

Experimental

A methanol solution (5 ml) of 2,2'-(propane-1,3-diyl)bis(2*H*-benzotriazole) (Xie *et al.*, 2000) (55.6 mg, 0.2 mmol) was added to methanol solution (5 ml) of copper(II) dichloride dihydrate (17.1 mg, 0.1 mmol). The clear solution was set aside for a week for the growth of crystals. The yellow copper(I) chloride adduct is air stable.

Refinement

The carbon-bound H atoms were placed in calculated positions [C—H = 0.93 to 0.97 Å], and were included in the refinement in the riding model approximation with U_{iso}(H) = 1.2U_{eq}(C).

Figures

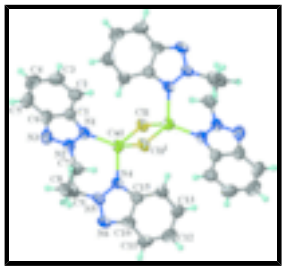


Fig. 1. Thermal ellipsoid plot of $(C_{15}H_{14}N_6)_2Cl_2Cu_2$; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. Symmetry code *i*: $1-x$, $1-y$, $1-z$.

Di-μ-chlorido-bis[2,2'-(propane-1,3-diyl)bis(2*H*-benzotriazole)-\ $\kappa^2N^1,N^{1'}$]copper(I)]

Crystal data

$[Cu_2Cl_2(C_{15}H_{14}N_6)_2]$	F_{000} = 768
M_r = 754.62	D_x = 1.655 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2yn	Cell parameters from 3803 reflections
a = 9.886 (3) Å	θ = 2.1–27.9º
b = 10.055 (3) Å	μ = 1.63 mm^{-1}
c = 15.876 (4) Å	T = 295 (2) K
β = 106.401 (4)º	Prism, yellow
V = 1514.0 (7) Å^3	0.23 × 0.20 × 0.19 mm
Z = 2	

Data collection

Rigaku Saturn diffractometer	3592 independent reflections
Radiation source: fine-focus sealed tube	3425 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 295(2) K	θ_{max} = 27.9º
ω scans	θ_{min} = 2.8º
Absorption correction: Multi-scan (CrystalClear; Rigaku/MSC, 2006)	h = −13→12
T_{min} = 0.592, T_{max} = 0.748	k = −12→13
17855 measured reflections	l = −20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H-atom parameters constrained
$wR(F^2)$ = 0.104	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.7057P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
3592 reflections	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
208 parameters	$\Delta\rho_{min}$ = −0.81 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.37039 (3)	0.44465 (3)	0.431367 (18)	0.04155 (11)
Cl1	0.53996 (5)	0.58239 (5)	0.40490 (3)	0.03700 (13)
N1	0.16588 (17)	0.50352 (17)	0.40525 (10)	0.0339 (3)
N2	0.06485 (18)	0.42252 (17)	0.41610 (11)	0.0364 (4)
N3	−0.06712 (19)	0.4634 (2)	0.38526 (13)	0.0444 (4)
N4	0.38999 (18)	0.25130 (16)	0.39053 (11)	0.0352 (3)
N5	0.29088 (18)	0.16622 (17)	0.34729 (10)	0.0366 (3)
N6	0.3327 (2)	0.04471 (17)	0.33617 (13)	0.0431 (4)
C1	0.0923 (2)	0.6102 (2)	0.36354 (12)	0.0348 (4)
C2	0.1380 (2)	0.7295 (2)	0.33471 (13)	0.0412 (4)

H2	0.2333	0.7481	0.3440	0.049*
C3	0.0357 (3)	0.8171 (2)	0.29235 (15)	0.0504 (5)
H3	0.0623	0.8968	0.2719	0.060*
C4	−0.1112 (3)	0.7899 (3)	0.27846 (16)	0.0568 (6)
H4	−0.1773	0.8517	0.2484	0.068*
C5	−0.1564 (3)	0.6767 (3)	0.30800 (16)	0.0537 (6)
H5	−0.2518	0.6605	0.3002	0.064*
C6	−0.0523 (2)	0.5844 (2)	0.35115 (14)	0.0401 (4)
C7	0.0958 (2)	0.2884 (2)	0.45160 (13)	0.0398 (4)
H7A	0.0414	0.2703	0.4925	0.048*
H7B	0.1951	0.2816	0.4832	0.048*
C8	0.0595 (2)	0.1869 (2)	0.37756 (14)	0.0425 (4)
H8A	−0.0402	0.1937	0.3471	0.051*
H8B	0.0767	0.0984	0.4026	0.051*
C9	0.1437 (2)	0.2046 (2)	0.31134 (13)	0.0398 (4)
H9A	0.1014	0.1511	0.2598	0.048*
H9B	0.1391	0.2970	0.2931	0.048*
C10	0.4737 (2)	0.04905 (19)	0.37568 (14)	0.0390 (4)
C11	0.5774 (3)	−0.0498 (2)	0.38292 (17)	0.0509 (6)
H11	0.5546	−0.1354	0.3613	0.061*
C12	0.7128 (3)	−0.0132 (3)	0.42332 (16)	0.0509 (5)
H12	0.7843	−0.0754	0.4286	0.061*
C13	0.7485 (2)	0.1159 (2)	0.45750 (16)	0.0474 (5)
H13	0.8425	0.1354	0.4850	0.057*
C14	0.6498 (2)	0.2130 (2)	0.45152 (15)	0.0429 (4)
H14	0.6740	0.2978	0.4742	0.052*
C15	0.5096 (2)	0.17771 (19)	0.40924 (12)	0.0348 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03493 (17)	0.03753 (17)	0.04959 (18)	−0.00308 (9)	0.00770 (12)	−0.00336 (10)
Cl1	0.0374 (2)	0.0393 (2)	0.0299 (2)	−0.01079 (18)	0.00249 (17)	0.00473 (17)
N1	0.0309 (8)	0.0358 (8)	0.0344 (8)	−0.0022 (6)	0.0080 (6)	−0.0020 (6)
N2	0.0313 (8)	0.0411 (9)	0.0367 (8)	−0.0042 (7)	0.0093 (6)	−0.0022 (7)
N3	0.0321 (9)	0.0526 (11)	0.0486 (10)	−0.0010 (8)	0.0115 (8)	−0.0040 (8)
N4	0.0374 (8)	0.0316 (8)	0.0344 (8)	−0.0036 (6)	0.0064 (6)	−0.0065 (6)
N5	0.0399 (9)	0.0339 (8)	0.0335 (7)	−0.0058 (7)	0.0063 (6)	−0.0061 (6)
N6	0.0503 (11)	0.0310 (8)	0.0444 (9)	−0.0062 (7)	0.0073 (8)	−0.0058 (7)
C1	0.0350 (9)	0.0379 (10)	0.0295 (8)	0.0014 (8)	0.0060 (7)	−0.0053 (7)
C2	0.0478 (11)	0.0374 (10)	0.0380 (10)	0.0001 (9)	0.0115 (8)	−0.0031 (8)
C3	0.0694 (16)	0.0388 (11)	0.0416 (11)	0.0080 (10)	0.0134 (10)	−0.0009 (9)
C4	0.0585 (14)	0.0567 (14)	0.0488 (12)	0.0221 (12)	0.0049 (11)	−0.0015 (11)
C5	0.0389 (11)	0.0632 (15)	0.0533 (13)	0.0137 (11)	0.0038 (10)	−0.0044 (11)
C6	0.0341 (10)	0.0472 (11)	0.0374 (10)	0.0032 (8)	0.0077 (8)	−0.0065 (8)
C7	0.0425 (11)	0.0401 (10)	0.0370 (9)	−0.0067 (8)	0.0114 (8)	0.0033 (8)
C8	0.0383 (10)	0.0421 (11)	0.0445 (10)	−0.0086 (9)	0.0076 (8)	−0.0023 (9)
C9	0.0382 (10)	0.0445 (11)	0.0317 (9)	−0.0064 (8)	0.0019 (7)	−0.0062 (8)

C10	0.0486 (12)	0.0297 (9)	0.0366 (9)	−0.0023 (8)	0.0088 (8)	−0.0011 (7)
C11	0.0640 (15)	0.0319 (10)	0.0518 (13)	0.0067 (10)	0.0082 (11)	−0.0037 (9)
C12	0.0564 (14)	0.0431 (12)	0.0510 (12)	0.0149 (11)	0.0112 (11)	0.0020 (10)
C13	0.0411 (11)	0.0490 (13)	0.0496 (12)	0.0023 (10)	0.0086 (9)	−0.0012 (10)
C14	0.0416 (11)	0.0369 (10)	0.0471 (11)	−0.0024 (8)	0.0073 (9)	−0.0069 (8)
C15	0.0403 (10)	0.0323 (9)	0.0314 (8)	−0.0011 (8)	0.0093 (7)	−0.0026 (7)

Geometric parameters (Å, °)

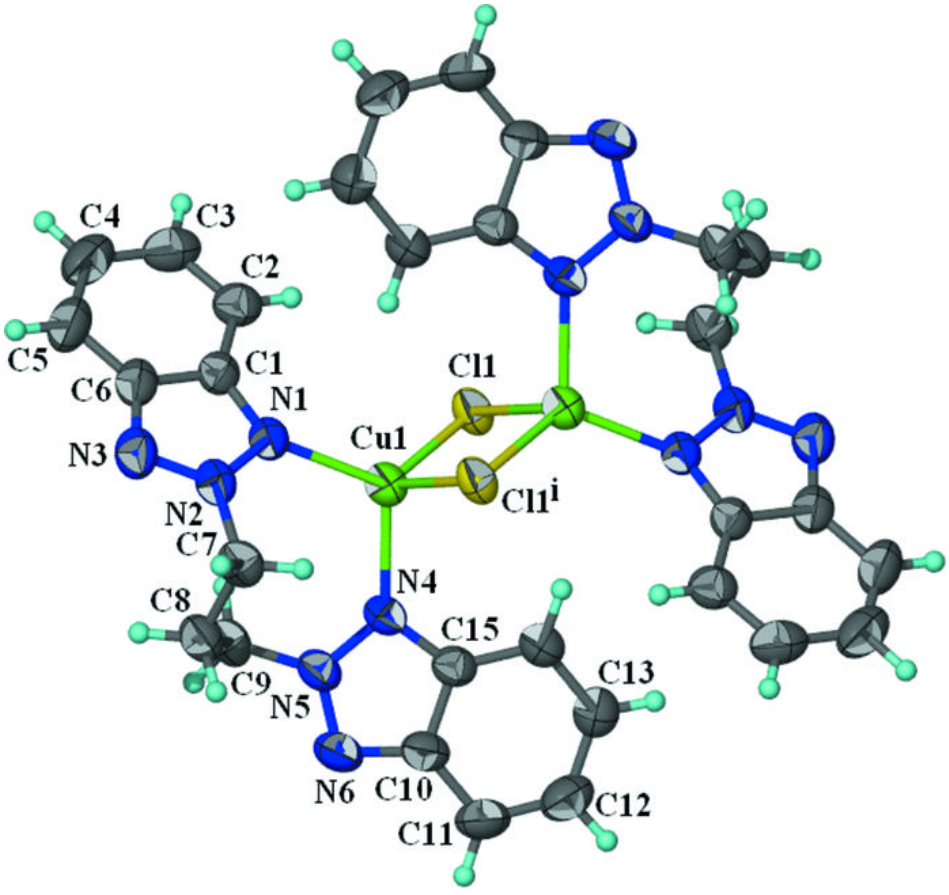
Cu1—N1	2.034 (2)	C4—H4	0.9300
Cu1—N4	2.076 (2)	C5—C6	1.411 (3)
Cu1—Cl1	2.3028 (7)	C5—H5	0.9300
Cu1—Cl1^{i}	2.5131 (8)	C7—C8	1.521 (3)
Cl1—Cu1^{i}	2.5131 (8)	C7—H7A	0.9700
N1—N2	1.337 (2)	C7—H7B	0.9700
N1—C1	1.359 (3)	C8—C9	1.524 (3)
N2—N3	1.323 (3)	C8—H8A	0.9700
N2—C7	1.460 (3)	C8—H8B	0.9700
N3—C6	1.356 (3)	C9—H9A	0.9700
N4—N5	1.335 (2)	C9—H9B	0.9700
N4—C15	1.355 (3)	C10—C15	1.406 (3)
N5—N6	1.318 (2)	C10—C11	1.409 (3)
N5—C9	1.457 (3)	C11—C12	1.361 (4)
N6—C10	1.358 (3)	C11—H11	0.9300
C1—C2	1.404 (3)	C12—C13	1.413 (4)
C1—C6	1.411 (3)	C12—H12	0.9300
C2—C3	1.366 (3)	C13—C14	1.365 (3)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.433 (4)	C14—C15	1.405 (3)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.354 (4)		
N1—Cu1—N4	112.58 (7)	C1—C6—C5	121.2 (2)
N1—Cu1—Cl1	121.38 (5)	N2—C7—C8	110.08 (17)
N1—Cu1—Cl1^{i}	106.40 (5)	N2—C7—H7A	109.6
N4—Cu1—Cl1	111.68 (5)	C8—C7—H7A	109.6
N4—Cu1—Cl1^{i}	100.66 (5)	N2—C7—H7B	109.6
Cl1—Cu1—Cl1^{i}	101.04 (2)	C8—C7—H7B	109.6
Cu1—Cl1—Cu1^{i}	78.957 (19)	H7A—C7—H7B	108.2
N2—N1—C1	103.12 (16)	C7—C8—C9	113.52 (17)
N2—N1—Cu1	122.15 (13)	C7—C8—H8A	108.9
C1—N1—Cu1	133.93 (14)	C9—C8—H8A	108.9
N3—N2—N1	117.21 (17)	C7—C8—H8B	108.9
N3—N2—C7	120.49 (17)	C9—C8—H8B	108.9
N1—N2—C7	121.96 (17)	H8A—C8—H8B	107.7
N2—N3—C6	102.74 (17)	N5—C9—C8	112.22 (17)
N5—N4—C15	103.35 (16)	N5—C9—H9A	109.2
N5—N4—Cu1	129.87 (13)	C8—C9—H9A	109.2
C15—N4—Cu1	126.57 (13)	N5—C9—H9B	109.2

N6—N5—N4	116.77 (17)	C8—C9—H9B	109.2
N6—N5—C9	120.65 (17)	H9A—C9—H9B	107.9
N4—N5—C9	122.56 (17)	N6—C10—C15	108.71 (18)
N5—N6—C10	103.20 (16)	N6—C10—C11	130.0 (2)
N1—C1—C2	131.01 (19)	C15—C10—C11	121.2 (2)
N1—C1—C6	107.76 (18)	C12—C11—C10	116.3 (2)
C2—C1—C6	121.2 (2)	C12—C11—H11	121.9
C3—C2—C1	116.7 (2)	C10—C11—H11	121.9
C3—C2—H2	121.6	C11—C12—C13	122.4 (2)
C1—C2—H2	121.6	C11—C12—H12	118.8
C2—C3—C4	122.0 (2)	C13—C12—H12	118.8
C2—C3—H3	119.0	C14—C13—C12	122.3 (2)
C4—C3—H3	119.0	C14—C13—H13	118.8
C5—C4—C3	121.8 (2)	C12—C13—H13	118.8
C5—C4—H4	119.1	C13—C14—C15	116.2 (2)
C3—C4—H4	119.1	C13—C14—H14	121.9
C4—C5—C6	117.0 (2)	C15—C14—H14	121.9
C4—C5—H5	121.5	N4—C15—C14	130.47 (19)
C6—C5—H5	121.5	N4—C15—C10	107.97 (18)
N3—C6—C1	109.17 (19)	C14—C15—C10	121.54 (19)
N3—C6—C5	129.6 (2)		
N1—Cu1—Cl1—Cu1^{i}	117.13 (6)	C2—C3—C4—C5	1.1 (4)
N4—Cu1—Cl1—Cu1^{i}	−106.28 (5)	C3—C4—C5—C6	−1.7 (4)
Cl1^{i}—Cu1—Cl1—Cu1^{i}	0.0	N2—N3—C6—C1	0.2 (2)
N4—Cu1—N1—N2	40.36 (16)	N2—N3—C6—C5	179.3 (2)
Cl1—Cu1—N1—N2	176.60 (12)	N1—C1—C6—N3	0.3 (2)
Cl1^{i}—Cu1—N1—N2	−68.98 (14)	C2—C1—C6—N3	−179.66 (18)
N4—Cu1—N1—C1	−127.53 (17)	N1—C1—C6—C5	−178.99 (19)
Cl1—Cu1—N1—C1	8.7 (2)	C2—C1—C6—C5	1.1 (3)
Cl1^{i}—Cu1—N1—C1	123.13 (17)	C4—C5—C6—N3	−178.5 (2)
C1—N1—N2—N3	0.7 (2)	C4—C5—C6—C1	0.6 (3)
Cu1—N1—N2—N3	−170.33 (14)	N3—N2—C7—C8	72.4 (2)
C1—N1—N2—C7	174.18 (17)	N1—N2—C7—C8	−100.8 (2)
Cu1—N1—N2—C7	3.1 (2)	N2—C7—C8—C9	61.2 (2)
N1—N2—N3—C6	−0.6 (2)	N6—N5—C9—C8	93.2 (2)
C7—N2—N3—C6	−174.12 (18)	N4—N5—C9—C8	−88.6 (2)
N1—Cu1—N4—N5	3.63 (19)	C7—C8—C9—N5	71.6 (2)
Cl1—Cu1—N4—N5	−136.92 (15)	N5—N6—C10—C15	−0.1 (2)
Cl1^{i}—Cu1—N4—N5	116.54 (16)	N5—N6—C10—C11	−177.7 (2)
N1—Cu1—N4—C15	−170.15 (15)	N6—C10—C11—C12	176.9 (2)
Cl1—Cu1—N4—C15	49.30 (17)	C15—C10—C11—C12	−0.5 (3)
Cl1^{i}—Cu1—N4—C15	−57.23 (16)	C10—C11—C12—C13	0.9 (4)
C15—N4—N5—N6	0.4 (2)	C11—C12—C13—C14	−0.7 (4)
Cu1—N4—N5—N6	−174.49 (14)	C12—C13—C14—C15	0.0 (4)
C15—N4—N5—C9	−177.89 (17)	N5—N4—C15—C14	177.8 (2)
Cu1—N4—N5—C9	7.2 (3)	Cu1—N4—C15—C14	−7.1 (3)
N4—N5—N6—C10	−0.2 (2)	N5—N4—C15—C10	−0.4 (2)

C9—N5—N6—C10	178.15 (17)	Cu1—N4—C15—C10	174.66 (13)
N2—N1—C1—C2	179.3 (2)	C13—C14—C15—N4	−177.6 (2)
Cu1—N1—C1—C2	−11.2 (3)	C13—C14—C15—C10	0.4 (3)
N2—N1—C1—C6	−0.6 (2)	N6—C10—C15—N4	0.4 (2)
Cu1—N1—C1—C6	168.93 (14)	C11—C10—C15—N4	178.2 (2)
N1—C1—C2—C3	178.5 (2)	N6—C10—C15—C14	−178.04 (19)
C6—C1—C2—C3	−1.7 (3)	C11—C10—C15—C14	−0.2 (3)
C1—C2—C3—C4	0.6 (3)		

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

Fig. 1


C4
C3
C2
C5
C1
C6
N1
Cl1
Cu1
N3
N2
Cl1i
C7
N4
C8
C15
C13
C9
N5
N6
C10
C12
C11