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[Bis(3-aminopropyl-κN)(2-furylmethyl)-amine-κN]dichloridocopper(II)

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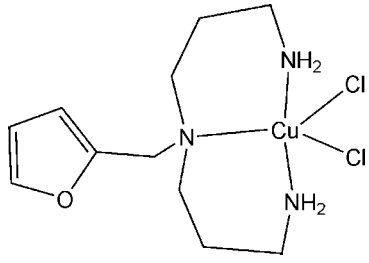
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.027; wR factor = 0.076; data-to-parameter ratio = 15.1.

In the title complex, $[CuCl_2(C_{11}H_{21}N_3O)]$, the five-coordinate Cu atom has a distorted square-pyramidal configuration. The crystal packing is stabilized by intermolecular N—H···Cl hydrogen-bonding interactions. The furan ring is disordered over two position, with site occupancy factors of *ca.* 0.6 and 0.4.

Related literature

For related literature, see: Jee *et al.* (2003); Kang *et al.* (1995); Kurisaki *et al.* (2005); Zhang *et al.* (2006); Zhu *et al.* (1996).



Experimental

Crystal data

$[CuCl_2(C_{11}H_{21}N_3O)]$
M_r = 345.75
Triclinic, $P\overline{1}$
a = 6.7493 (4) Å
b = 9.7335 (5) Å
c = 11.9658 (6) Å
α = 94.358 (1)°
β = 104.696 (1)°
γ = 104.181 (1)°
V = 729.16 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.584, T_{max} = 0.756
7493 measured reflections
3156 independent reflections
2934 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.076
S = 1.07
3156 reflections
209 parameters
17 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O1	0.97	2.46	3.098 (6)	124
C7—H7B···Cl2^{i}	0.97	2.77	3.732 (2)	170
N3—H3D···Cl2^{i}	0.90	2.65	3.5345 (18)	168
N3—H3C···Cl2^{ii}	0.90	2.64	3.4086 (17)	144
N2—H2D···Cl1^{iii}	0.90	2.40	3.2865 (19)	170

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y, -z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HG2341).

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supplementary materials

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[Bis(3-aminopropyl-*κN*)(2-furylmethyl)amine-*κN*]dichloridocopper(II)

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Comment

Polyamines with pendant arm have received much attention because of their strong coordination ability with transition metal ions and interesting biochemical properties (Kurisaki *et al.*, 2005; Kang *et al.*, 1995; Jee *et al.*, 2003; Zhu *et al.*, 1996). Up to the present, many linear and cyclic polyamine complexes with branched chain have been made in order to search for their potential uses. In order to search for new complexes of polyamine with pendant arms, we report the synthesis and crystal structure of the title complex, dichloro[*N*,*N*'-bis(3-aminopropyl-κ*N*,κ*N*') −2-furanmethylamine-κ*N*]copper(II), (I).

In the structure of (I), the copper atom is coordinated with three N atoms and two chloride anions (Fig. 1). The equatorial positions are occupied by three nitrogen atoms and one chloride in which the Cu—N and Cu—Cl bond lengths fall in the range 1.9930 (16)–2.3810 (5) Å. The deviation of the Cu atom from the N_3Cl basal plane is 0.3536 (2) Å. One Cl atom occupies the axial position with the elongated Cu—Cl distance of 2.5163 (6) Å. Intermolecular N—H···Cl hydrogen bonds play an important role in stabilizing the crystal packing.

Experimental

All the solvents and chemicals were of analytical grade and used without further purification. Furanmethylamine and acrylonitrile were purified by distillation. *N*,*N*'-bis(3-aminopropyl) −2-furanmethylamine was prepared by a similar method to that described in the literature (Zhang *et al.*, 2006). The title complex was synthesized by the following procedure: a methanol solution (10 ml) of $CuCl_2$ (0.134 g, 1 mmol) was added to a methanol solution (10 ml) of [*N*,*N*'-bis(3-aminopropyl) −2-furanmethylamine (0.22 g, 1 mmol). The mixture was stirred at ambient temperature for about one day and then filtered. A methanol solution (5 ml) of $NaClO_4$(0.142 g, 1 mmol) was added to the filtrate and the stirring was continued for 2 h. Blue crystals suitable for the X-ray diffraction were obtained by slow diffusion of diethyl ether into the mother solution over one month.

Refinement

Furan was disordered and major to minor of occupancy was 0.61 (1): 0.39 (1). H atoms bonded to C atoms of CH_2 and furan were placed in calculated positions, with C—H distances 0.97Å (for CH_2) and 0.93Å (for furan), and included in the refinement in the riding-model approximation with U_{iso}(H) = 1.2 U_{eq}(C). Other H atoms bonded to N atoms were located in a difference map and refined with distance restraints of N—H = 0.90 Å, and with U_{iso}(H) = 1.2 U_{eq}(N).

Figures

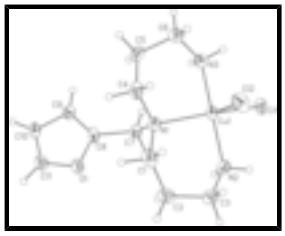

Fig. 1. A view of the title complex cation, showing the labeling of the non-H atoms and 30% probability ellipsoids.

[Bis(3-aminopropyl-κ*N*)(2-furylmethyl)amine-κ*N*]dichloridocopper(II)

Crystal data

$[CuCl_2(C_{11}H_{21}N_3O)]$	$Z = 2$
$M_r = 345.75$	$F_{000} = 358$
Triclinic, $P\overline{1}$	$D_x = 1.575$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.7493$ (4) Å	Cell parameters from 4753 reflections
$b = 9.7335$ (5) Å	$\theta = 2.2$–28.3º
$c = 11.9658$ (6) Å	$\mu = 1.86$ mm^{-1}
$\alpha = 94.358$ (1)º	$T = 298$ (2) K
$\beta = 104.696$ (1)º	Block, blue
$\gamma = 104.181$ (1)º	0.30 × 0.20 × 0.16 mm
$V = 729.16$ (7) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3156 independent reflections
Radiation source: fine-focus sealed tube	2934 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 298$(2) K	$\theta_{max} = 27.0$º
phi and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -8 \rightarrow 8$
$T_{min} = 0.584$, $T_{max} = 0.756$	$k = -12 \rightarrow 12$
7493 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.027$	H-atom parameters constrained
$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.1388P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
3156 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
209 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
17 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
Cu1	0.31362 (3)	0.24158 (2)	0.095524 (17)	0.03385 (9)	
C1	0.4985 (3)	0.1845 (3)	0.33945 (18)	0.0492 (5)	
H1A	0.5099	0.1986	0.4222	0.059*	
H1B	0.6378	0.2288	0.3305	0.059*	
C2	0.4441 (4)	0.0255 (3)	0.2990 (2)	0.0576 (6)	
H2A	0.2972	−0.0180	0.2965	0.069*	
H2B	0.5335	−0.0164	0.3553	0.069*	
C3	0.4735 (4)	−0.0094 (3)	0.1794 (2)	0.0562 (5)	
H3A	0.6173	0.0391	0.1793	0.067*	
H3B	0.4526	−0.1117	0.1616	0.067*	
C4	0.4435 (3)	0.4152 (2)	0.33239 (17)	0.0473 (5)	
H4A	0.5840	0.4458	0.3208	0.057*	
H4B	0.4625	0.4211	0.4159	0.057*	
C5	0.3204 (4)	0.5202 (2)	0.2869 (2)	0.0543 (6)	
H5A	0.1728	0.4818	0.2854	0.065*	
H5B	0.3771	0.6094	0.3407	0.065*	
C6	0.3291 (4)	0.5515 (2)	0.1663 (2)	0.0518 (5)	
H6A	0.2587	0.6255	0.1456	0.062*	
H6B	0.4764	0.5866	0.1661	0.062*	
C7	0.1299 (3)	0.2061 (2)	0.29461 (16)	0.0369 (4)	
H7A	0.0799	0.1042	0.2661	0.044*	
H7B	0.0333	0.2517	0.2468	0.044*	
C8	0.119 (3)	0.2299 (16)	0.4226 (12)	0.040 (3)	0.608 (12)
C11	0.1618 (14)	0.1877 (10)	0.6011 (8)	0.0581 (17)	0.608 (12)
H11	0.1950	0.1457	0.6682	0.070*	0.608 (12)

C10	0.0701 (12)	0.2934 (8)	0.5932 (6)	0.0441 (13)	0.608 (12)
H10	0.0318	0.3398	0.6518	0.053*	0.608 (12)
O1	0.2010 (11)	0.1482 (5)	0.5006 (5)	0.0572 (15)	0.608 (12)
C9	0.0425 (18)	0.3213 (12)	0.4752 (8)	0.0432 (17)	0.608 (12)
H9	−0.0174	0.3903	0.4419	0.052*	0.608 (12)
C8'	0.115 (5)	0.222 (2)	0.4068 (19)	0.038 (4)	0.392 (12)
C10'	0.103 (2)	0.2105 (17)	0.5948 (12)	0.068 (4)	0.392 (12)
H10'	0.1185	0.1813	0.6680	0.082*	0.392 (12)
C11'	0.053 (2)	0.3265 (15)	0.5613 (12)	0.060 (3)	0.392 (12)
H11'	0.0185	0.3920	0.6083	0.072*	0.392 (12)
C9'	0.1286 (19)	0.1389 (8)	0.4902 (12)	0.059 (3)	0.392 (12)
H9'	0.1510	0.0486	0.4826	0.071*	0.392 (12)
O1'	0.059 (2)	0.3387 (14)	0.4501 (11)	0.055 (3)	0.392 (12)
Cl1	0.12864 (9)	0.17685 (6)	−0.10687 (4)	0.05026 (14)	
Cl2	0.70195 (8)	0.33846 (7)	0.10934 (5)	0.05553 (15)	
N1	0.3464 (2)	0.26238 (17)	0.27872 (13)	0.0351 (3)	
N2	0.3189 (3)	0.03707 (18)	0.08969 (15)	0.0450 (4)	
H2D	0.1882	−0.0145	0.0892	0.054*	
H2C	0.3373	0.0105	0.0202	0.054*	
N3	0.2241 (3)	0.42131 (17)	0.07939 (14)	0.0407 (4)	
H3C	0.2356	0.4457	0.0098	0.049*	
H3D	0.0846	0.3991	0.0750	0.049*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03157 (13)	0.03896 (14)	0.03096 (13)	0.00929 (9)	0.00983 (9)	0.00263 (9)
C1	0.0379 (10)	0.0731 (14)	0.0370 (10)	0.0214 (10)	0.0055 (8)	0.0078 (9)
C2	0.0583 (14)	0.0710 (15)	0.0585 (13)	0.0382 (12)	0.0180 (11)	0.0277 (11)
C3	0.0566 (13)	0.0565 (13)	0.0687 (14)	0.0320 (11)	0.0236 (11)	0.0143 (11)
C4	0.0433 (11)	0.0508 (11)	0.0347 (9)	−0.0030 (9)	0.0074 (8)	−0.0070 (8)
C5	0.0671 (15)	0.0392 (10)	0.0519 (12)	0.0039 (10)	0.0235 (11)	−0.0096 (9)
C6	0.0603 (13)	0.0369 (10)	0.0560 (13)	0.0068 (9)	0.0200 (11)	0.0029 (9)
C7	0.0328 (9)	0.0401 (9)	0.0356 (9)	0.0082 (7)	0.0092 (7)	−0.0001 (7)
C8	0.038 (4)	0.056 (5)	0.027 (3)	0.008 (3)	0.016 (3)	0.004 (3)
C11	0.074 (4)	0.082 (3)	0.042 (2)	0.044 (3)	0.031 (3)	0.022 (2)
C10	0.047 (2)	0.056 (3)	0.034 (3)	0.016 (2)	0.018 (2)	0.003 (2)
O1	0.078 (4)	0.081 (2)	0.0387 (19)	0.052 (2)	0.029 (2)	0.0234 (17)
C9	0.045 (3)	0.049 (3)	0.043 (4)	0.019 (2)	0.020 (3)	0.010 (2)
C8'	0.033 (5)	0.042 (5)	0.039 (7)	0.015 (4)	0.006 (5)	0.006 (4)
C10'	0.078 (7)	0.098 (8)	0.040 (4)	0.027 (6)	0.034 (5)	0.008 (5)
C11'	0.055 (5)	0.078 (6)	0.045 (6)	0.006 (4)	0.027 (4)	−0.001 (4)
C9'	0.060 (6)	0.071 (5)	0.057 (5)	0.025 (4)	0.026 (4)	0.021 (4)
O1'	0.057 (3)	0.063 (5)	0.050 (5)	0.011 (3)	0.032 (3)	−0.003 (3)
Cl1	0.0550 (3)	0.0574 (3)	0.0319 (2)	0.0085 (2)	0.0095 (2)	−0.0003 (2)
Cl2	0.0330 (2)	0.0742 (4)	0.0657 (3)	0.0146 (2)	0.0198 (2)	0.0286 (3)
N1	0.0299 (7)	0.0420 (8)	0.0309 (7)	0.0085 (6)	0.0068 (6)	0.0007 (6)
N2	0.0489 (10)	0.0448 (9)	0.0465 (9)	0.0172 (8)	0.0196 (8)	0.0024 (7)

N3	0.0400 (9)	0.0413 (8)	0.0410 (8)	0.0116 (7)	0.0117 (7)	0.0055 (7)

Geometric parameters (Å, °)

Cu1—N3	1.9930 (16)	C7—C8'	1.372 (19)
Cu1—N2	1.9959 (17)	C7—N1	1.495 (2)
Cu1—N1	2.1353 (15)	C7—C8	1.555 (12)
Cu1—Cl1	2.3810 (5)	C7—H7A	0.9700
Cu1—Cl2	2.5163 (6)	C7—H7B	0.9700
C1—N1	1.497 (3)	C8—C9	1.326 (9)
C1—C2	1.511 (3)	C8—O1	1.370 (11)
C1—H1A	0.9700	C11—C10	1.322 (6)
C1—H1B	0.9700	C11—O1	1.343 (8)
C2—C3	1.518 (3)	C11—H11	0.9300
C2—H2A	0.9700	C10—C9	1.433 (7)
C2—H2B	0.9700	C10—H10	0.9300
C3—N2	1.477 (3)	C9—H9	0.9300
C3—H3A	0.9700	C8'—C9'	1.331 (9)
C3—H3B	0.9700	C8'—O1'	1.385 (15)
C4—N1	1.490 (2)	C10'—C11'	1.317 (8)
C4—C5	1.517 (3)	C10'—C9'	1.455 (9)
C4—H4A	0.9700	C10'—H10'	0.9300
C4—H4B	0.9700	C11'—O1'	1.353 (11)
C5—C6	1.509 (3)	C11'—H11'	0.9300
C5—H5A	0.9700	C9'—H9'	0.9300
C5—H5B	0.9700	N2—H2D	0.9000
C6—N3	1.475 (3)	N2—H2C	0.9000
C6—H6A	0.9700	N3—H3C	0.9000
C6—H6B	0.9700	N3—H3D	0.9000
N3—Cu1—N2	164.28 (7)	C8—C7—H7A	108.5
N3—Cu1—N1	92.82 (6)	C8'—C7—H7B	108.8
N2—Cu1—N1	91.68 (7)	N1—C7—H7B	108.5
N3—Cu1—Cl1	84.66 (5)	C8—C7—H7B	108.5
N2—Cu1—Cl1	85.11 (5)	H7A—C7—H7B	107.5
N1—Cu1—Cl1	155.99 (4)	C9—C8—O1	109.9 (9)
N3—Cu1—Cl2	99.22 (5)	C9—C8—C7	130.9 (9)
N2—Cu1—Cl2	95.14 (5)	O1—C8—C7	119.1 (9)
N1—Cu1—Cl2	97.20 (4)	C10—C11—O1	111.9 (8)
Cl1—Cu1—Cl2	106.78 (2)	C10—C11—H11	124.1
N1—C1—C2	116.70 (17)	O1—C11—H11	124.1
N1—C1—H1A	108.1	C11—C10—C9	105.4 (8)
C2—C1—H1A	108.1	C11—C10—H10	127.3
N1—C1—H1B	108.1	C9—C10—H10	127.3
C2—C1—H1B	108.1	C11—O1—C8	105.9 (7)
H1A—C1—H1B	107.3	C8—C9—C10	106.7 (8)
C1—C2—C3	113.1 (2)	C8—C9—H9	126.6
C1—C2—H2A	109.0	C10—C9—H9	126.6
C3—C2—H2A	109.0	C9'—C8'—C7	133.0 (16)
C1—C2—H2B	109.0	C9'—C8'—O1'	106.0 (14)

C3—C2—H2B	109.0	C7—C8'—O1'	120.8 (10)
H2A—C2—H2B	107.8	C11'—C10'—C9'	103.5 (11)
N2—C3—C2	109.90 (18)	C11'—C10'—H10'	128.2
N2—C3—H3A	109.7	C9'—C10'—H10'	128.2
C2—C3—H3A	109.7	C10'—C11'—O1'	111.8 (13)
N2—C3—H3B	109.7	C10'—C11'—H11'	124.1
C2—C3—H3B	109.7	O1'—C11'—H11'	124.1
H3A—C3—H3B	108.2	C8'—C9'—C10'	109.9 (13)
N1—C4—C5	116.33 (17)	C8'—C9'—H9'	125.1
N1—C4—H4A	108.2	C10'—C9'—H9'	125.1
C5—C4—H4A	108.2	C11'—O1'—C8'	108.4 (12)
N1—C4—H4B	108.2	C4—N1—C7	111.55 (15)
C5—C4—H4B	108.2	C4—N1—C1	104.91 (15)
H4A—C4—H4B	107.4	C7—N1—C1	111.46 (15)
C6—C5—C4	113.80 (19)	C4—N1—Cu1	109.90 (12)
C6—C5—H5A	108.8	C7—N1—Cu1	107.77 (10)
C4—C5—H5A	108.8	C1—N1—Cu1	111.28 (12)
C6—C5—H5B	108.8	C3—N2—Cu1	121.57 (15)
C4—C5—H5B	108.8	C3—N2—H2D	106.9
H5A—C5—H5B	107.7	Cu1—N2—H2D	106.9
N3—C6—C5	110.68 (17)	C3—N2—H2C	106.9
N3—C6—H6A	109.5	Cu1—N2—H2C	106.9
C5—C6—H6A	109.5	H2D—N2—H2C	106.7
N3—C6—H6B	109.5	C6—N3—Cu1	121.74 (14)
C5—C6—H6B	109.5	C6—N3—H3C	106.9
H6A—C6—H6B	108.1	Cu1—N3—H3C	106.9
C8'—C7—N1	116.5 (13)	C6—N3—H3D	106.9
N1—C7—C8	114.9 (8)	Cu1—N3—H3D	106.9
C8'—C7—H7A	106.6	H3C—N3—H3D	106.7
N1—C7—H7A	108.5		
N1—C1—C2—C3	71.7 (3)	C8—C7—N1—C1	64.8 (5)
C1—C2—C3—N2	−65.9 (3)	C8'—C7—N1—Cu1	−174.3 (7)
N1—C4—C5—C6	−73.3 (2)	C8—C7—N1—Cu1	−172.9 (5)
C4—C5—C6—N3	64.4 (3)	C2—C1—N1—C4	−177.78 (18)
N1—C7—C8—C9	105.3 (19)	C2—C1—N1—C7	61.4 (2)
N1—C7—C8—O1	−73.6 (15)	C2—C1—N1—Cu1	−59.0 (2)
O1—C11—C10—C9	1.8 (10)	N3—Cu1—N1—C4	−39.90 (13)
C10—C11—O1—C8	−3.1 (13)	N2—Cu1—N1—C4	155.16 (13)
C9—C8—O1—C11	3.3 (17)	Cl1—Cu1—N1—C4	−123.10 (13)
C7—C8—O1—C11	−177.6 (12)	Cl2—Cu1—N1—C4	59.76 (13)
O1—C8—C9—C10	−2.2 (18)	N3—Cu1—N1—C7	81.85 (12)
C7—C8—C9—C10	178.8 (16)	N2—Cu1—N1—C7	−83.09 (12)
C11—C10—C9—C8	0.3 (14)	Cl1—Cu1—N1—C7	−1.35 (19)
N1—C7—C8'—C9'	−92 (3)	Cl2—Cu1—N1—C7	−178.49 (11)
N1—C7—C8'—O1'	95 (2)	N3—Cu1—N1—C1	−155.67 (13)
C9'—C10'—C11'—O1'	−4.0 (17)	N2—Cu1—N1—C1	39.40 (14)
C7—C8'—C9'—C10'	179 (3)	Cl1—Cu1—N1—C1	121.14 (14)
O1'—C8'—C9'—C10'	−6(3)	Cl2—Cu1—N1—C1	−56.00 (13)
C11'—C10'—C9'—C8'	6(2)	C2—C3—N2—Cu1	59.8 (2)

C10'—C11'—O1'—C8'	0(2)	N3—Cu1—N2—C3	−150.6 (2)
C9'—C8'—O1'—C11'	4(3)	N1—Cu1—N2—C3	−44.01 (16)
C7—C8'—O1'—C11'	179 (2)	Cl1—Cu1—N2—C3	159.83 (16)
C5—C4—N1—C7	−58.9 (2)	Cl2—Cu1—N2—C3	53.38 (16)
C5—C4—N1—C1	−179.74 (17)	C5—C6—N3—Cu1	−56.2 (2)
C5—C4—N1—Cu1	60.5 (2)	N2—Cu1—N3—C6	148.3 (2)
C8'—C7—N1—C4	−53.6 (8)	N1—Cu1—N3—C6	41.86 (16)
C8—C7—N1—C4	−52.1 (5)	Cl1—Cu1—N3—C6	−162.08 (15)
C8'—C7—N1—C1	63.3 (8)	Cl2—Cu1—N3—C6	−55.91 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1A···O1	0.97	2.46	3.098 (6)	124
C7—H7B···Cl2^{i}	0.97	2.77	3.732 (2)	170
N3—H3D···Cl2^{i}	0.90	2.65	3.5345 (18)	168
N3—H3C···Cl2^{ii}	0.90	2.64	3.4086 (17)	144
N2—H2D···Cl1^{iii}	0.90	2.40	3.2865 (19)	170

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

Fig. 1