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Di-μ-chlorido-bis{aqua[5-ethyl-2-(5-isopropyl-5-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-2-yl)nicotinato]copper(II)}

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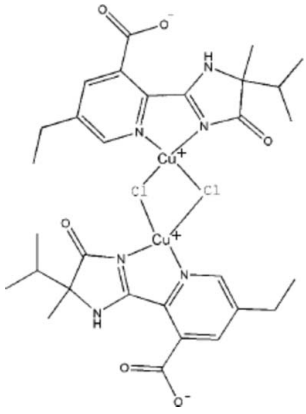
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.049; wR factor = 0.088; data-to-parameter ratio = 14.5.

In the title centrosymmetric complex, $[Cu_2(C_{15}H_{18}N_3O_3)_2(H_2O)_2Cl_2]$, the bridging Cu_2Cl_2 ring, which is exactly planar by virtue of a crystallographic inversion center, has two different Cu—Cl distances. The dihedral angle between the pyridine and imidazole ring planes is 2.49 (4)°. In the crystal structure, intermolecular O—H···O hydrogen bonds link dimer molecules into a one-dimensional chain in the c-axis direction. The atoms of the isopropyl and ethyl groups are disordered over two sites with approximate occupancies of 0.75:0.25 and 0.5:0.5, respectively.

Related literature

For background information, see: Solomon *et al.* (1996); Hay *et al.* (1995); Johnson *et al.* (1984). For related structures, see: Puschmann, Batsanov *et al.* (2001); Puschmann, Howard *et al.* (2001).



Experimental

Crystal data

$[Cu_2(C_{15}H_{18}N_3O_3)_2(H_2O)_2Cl_2]$
M_r = 810.68
Monoclinic, $P2_1/c$
a = 12.960 (2) Å
b = 13.2235 (19) Å
c = 10.4526 (16) Å
β = 97.012 (3)°
V = 1778.0 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 291 (2) K
0.34 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.647, T_{max} = 0.695
9418 measured reflections
3487 independent reflections
2260 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.088
S = 1.01
3487 reflections
241 parameters
177 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.930 (3)	Cu1—Cl1	2.2301 (11)
Cu1—O4	1.944 (2)	Cu1—Cl1^{i}	2.7249 (11)
Cu1—N1	2.041 (3)		
N2—Cu1—O4	89.01 (11)	N2—Cu1—Cl1^{i}	93.48 (9)
N2—Cu1—N1	79.86 (12)	O4—Cu1—Cl1^{i}	99.06 (9)
O4—Cu1—N1	166.85 (11)	N1—Cu1—Cl1^{i}	88.66 (8)
N2—Cu1—Cl1	172.96 (9)	Cl1—Cu1—Cl1^{i}	93.06 (3)
O4—Cu1—Cl1	92.56 (9)	Cu1—Cl1—Cu1^{i}	86.94 (3)
N1—Cu1—Cl1	97.67 (9)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4B···O1^{ii}	0.84	1.70	2.537 (4)	174
O4—H4A···O3	0.83	1.97	2.759 (4)	159
N3—H3A···O2	0.86	1.72	2.493 (4)	148

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Berndt (2005); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

The authors thank Dr Hai-Bin Song of Nankai University and Dr Jian-Ge Wang of Luoyang Normal University for their help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2432).

References

Brandenburg, K. & Berndt, M. (2005). *DIAMOND*. Release 3.0c. Crystal Impact GbR, Bonn, Germany.

Bruker (1998). *SHELXTL* (Version 5.10), *SAINT* (Version 5.10) and *SMART* (Version 5.0). Bruker AXS Inc., Madison, Wisoconsin, USA.

Hay, P. G., Thibeault, J. C. & Hoffmann, R. (1995). *J. Am. Chem. Soc.* **97**, 4884–4899.

Johnson, R. A., Von Dreele, R. B. & Brown, T. M. (1984). *Inorg. Chem.* **23**, 4302–4309.

Puschmann, H., Batsanov, A. S., Howard, J. A. K., Soto, B., Bonne, R. & Au-Alvarez, O. (2001). *Acta Cryst.* E**57**, m524–m526.

Puschmann, H., Howard, J. A. K., Soto, B., Bonne, R. & Au-Alvarez, O. (2001). *Acta Cryst.* E**57**, m551–m552.

Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97.* University of Göttingen, Germany.

Solomon, E. I., Sundaram, U. M. & Machokin, T. E. (1996). *Chem. Rev.* **96**, 2563–2605.

supplementary materials

Acta Cryst. (2007). E**63**, m1972-m1973 [**doi:10.1107/S1600536807029819**]

Di-μ-chlorido-bis{aqua[5-ethyl-2-(5-isopropyl-5-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-2-yl)nicotinato]copper(II)}

Y. Zhao, K. Qian, Y.-G. Tu, J.-K. Li and W. Liu

Comment

The synthesis and characterization of binuclear copper(II) complexes has made an impact on bio-inorganic chemistry (Solomon *et al.*, 1996). The exchange mechanism of bridged copper(II) complexes has been published (Johnson *et al.*, 1984). An excellent treatise on the orbital interaction in metal dimer complexes was also published (Hoffman *et al.*, 1975).

The molecular structure is shown in Fig. 1. The bridging Cu_2Cl_2 unit is exactly planar. The Cu1—Cl1 and Cu1—$Cl1^i$ [symmetry code: (i) $1-x, 1-y, 1-z$] distances are not equal [2.2301 (11) and 2.7249 (11) Å]. The distance between Cu and $Cu1^i$ is less than the value in di-u-chloro- bis{chloro[1,2-diphenyl-2-(phenylamino)ethanoximato]copper(II)} (Puschmann, Batsanov *et al.*, 2001) [3.4275 (4) *versus* 3.5172 (4) Å] and is longer than that in di-[μ]-chloro-bis{chloro[1,2-diphenyl-2-(4-chlorophenylamino) ethanoximato]copper(II)} [3.3514 (3) Å] [Puschmann, Howard *et al.*, 2001]. In the asymmetric unit, the dihedral angle between the plane of the pyridine ring and the imidazole group plane is 2.49 (4) °. In the crystal structure, there is a O4—H4B···$O1^{ii}$ [symmetry code: (ii) $x, y, z+1$] hydrogen bond (H4B···O1 = 1.70 Å), which links molecules into chains in the *c* axis direction.

Experimental

A heavy-walled Pyrex tube containing a mixture of $CuCl_2{\cdot}2H_2O$ (0.02 g), 5-Ethyl-2-(5-isopropyl-5-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-2-yl)- nicotinic acid (0.03 g), 0.65 mol/l NaOH solution (0.3 ml) and H_2O (2 ml) was frozen in liquid N_2, sealed under vacuum and placed in an oven at 423 K. Blue single crystals suitable for X-ray analysis were then obtained after heating for one month.

Refinement

The water H atoms were located in a difference Fourier map and included in the 'as found' positions with with U_{iso}(H)= 1.5U_{eq}(O); All other H atoms were included in calculated positions and refined as riding (C—H= 0.93–0.98 Å; N—H = 0.86 Å), with U_{iso}(H)= 1.5 U_{eq}(C) for methyl and 1.2 U_{eq}(C,*N*) for all other H atoms. Atoms C9 and C10 of the ethyl group are disordered over two sites with refined occupancies of 0.503 (7) and 0.497 (7) for the major and minor components, respectively. Atoms C13, C14 and C15 of the isopropyl group are disordered, with the ratio between the major and minor components refining to 75 (3):25 (3).

Figures

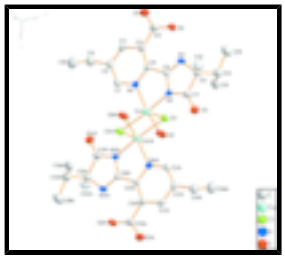


Fig. 1. : The molecular structure, showing 30% probability displacement ellipsoids. Hydrogen atoms and the minor components of disorder have been omitted [Symmetry code: (A) 1 − *x*, 1 − *y*, 1 − *z*].

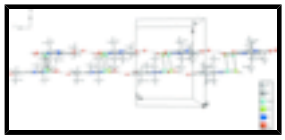


Fig. 2. : The crystal packing, viewed approximately along the *a* axis, showing the hydrogen bonded chain formed along the *c* axis. Hydrogen bonds are shown as dashed lines.

Di-μ-chloro-bis{aqua[5-ethyl-2-(5-isopropyl-5-methyl-4-oxo-4,5-dihydro- 1*H*-imidazol-2-yl)nicotinato]copper(II)}

Crystal data

$[Cu_2(C_{15}H_{18}N_3O_3)_2(H_2O)_2Cl_2]$	F_{000} = 836
M_r = 810.68	D_x = 1.514 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2342 reflections
a = 12.960 (2) Å	θ = 2.3–22.5º
b = 13.2235 (19) Å	μ = 1.40 mm^{-1}
c = 10.4526 (16) Å	T = 291 (2) K
β = 97.012 (3)º	Block, blue
V = 1778.0 (5) Å^3	0.34 × 0.30 × 0.28 mm
Z = 2	

Data collection

Bruker SMART CCD diffractometer	3487 independent reflections
Radiation source: fine-focus sealed tube	2260 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→15
T_{min} = 0.647, T_{max} = 0.695	k = −13→16
9418 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.088$	$w = 1/[\sigma^2(F_o^2) + (0.0218P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
3487 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
241 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
177 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)
C9	0.2667 (15)	0.6115 (10)	0.0561 (13)	0.070 (2)	0.503 (7)
H9A	0.2619	0.6002	−0.0361	0.084*	0.503 (7)
H9B	0.2342	0.5553	0.0954	0.084*	0.503 (7)
C10	0.2156 (7)	0.7105 (7)	0.0849 (12)	0.093 (2)	0.503 (7)
H10A	0.2163	0.7178	0.1764	0.139*	0.503 (7)
H10B	0.1450	0.7108	0.0442	0.139*	0.503 (7)
H10C	0.2529	0.7656	0.0522	0.139*	0.503 (7)
C9'	0.2633 (15)	0.6291 (11)	0.0901 (12)	0.070 (2)	0.497 (7)
H9'1	0.2357	0.5614	0.0754	0.084*	0.497 (7)
H9'2	0.2370	0.6557	0.1664	0.084*	0.497 (7)
C10'	0.2247 (8)	0.6943 (8)	−0.0233 (12)	0.093 (2)	0.497 (7)
H10D	0.2377	0.7640	−0.0016	0.139*	0.497 (7)
H10E	0.1514	0.6840	−0.0453	0.139*	0.497 (7)
H10F	0.2603	0.6765	−0.0954	0.139*	0.497 (7)
C13	0.9367 (14)	0.5454 (8)	0.3180 (14)	0.0696 (14)	0.75 (3)
H13	0.9938	0.5488	0.3886	0.084*	0.75 (3)
C14	0.8774 (9)	0.4486 (4)	0.3335 (11)	0.0709 (19)	0.75 (3)
H14A	0.8248	0.4404	0.2612	0.106*	0.75 (3)
H14B	0.8453	0.4517	0.4114	0.106*	0.75 (3)
H14C	0.9244	0.3923	0.3376	0.106*	0.75 (3)
C15	0.9844 (10)	0.5461 (10)	0.1909 (8)	0.091 (3)	0.75 (3)

H15A	1.0368	0.4946	0.1931	0.136*	0.75 (3)
H15B	1.0152	0.6110	0.1792	0.136*	0.75 (3)
H15C	0.9311	0.5332	0.1206	0.136*	0.75 (3)
C13'	0.944 (4)	0.564 (2)	0.316 (4)	0.0696 (14)	0.25 (3)
H13'	0.9881	0.5655	0.3984	0.084*	0.25 (3)
C14'	0.905 (3)	0.4542 (8)	0.305 (3)	0.0709 (19)	0.25 (3)
H14D	0.8854	0.4326	0.3862	0.106*	0.25 (3)
H14E	0.9587	0.4113	0.2805	0.106*	0.25 (3)
H14F	0.8451	0.4502	0.2403	0.106*	0.25 (3)
C15'	1.019 (2)	0.585 (3)	0.216 (3)	0.091 (3)	0.25 (3)
H15D	0.9803	0.5870	0.1312	0.136*	0.25 (3)
H15E	1.0699	0.5325	0.2195	0.136*	0.25 (3)
H15F	1.0522	0.6490	0.2345	0.136*	0.25 (3)
Cu1	0.57594 (3)	0.60289 (3)	0.47672 (4)	0.04189 (16)	
Cl1	0.42446 (7)	0.60139 (7)	0.55756 (9)	0.0512 (3)	
N1	0.5182 (2)	0.6183 (2)	0.2872 (3)	0.0371 (7)	
N2	0.7035 (2)	0.6214 (2)	0.4018 (3)	0.0390 (7)	
N3	0.7798 (2)	0.6384 (2)	0.2244 (3)	0.0524 (9)	
H3A	0.7853	0.6439	0.1435	0.063*	
O1	0.5822 (2)	0.6509 (2)	−0.1448 (3)	0.0809 (10)	
O2	0.7255 (2)	0.6343 (2)	−0.0127 (2)	0.0674 (9)	
O3	0.8461 (2)	0.6231 (2)	0.5567 (2)	0.0669 (9)	
O4	0.6551 (2)	0.6095 (2)	0.6469 (2)	0.0786 (9)	
H4A	0.7179	0.6116	0.6397	0.118*	
H4B	0.6323	0.6276	0.7148	0.118*	
C1	0.4177 (3)	0.6166 (3)	0.2445 (4)	0.0473 (10)	
H1	0.3702	0.6106	0.3039	0.057*	
C2	0.3808 (3)	0.6234 (3)	0.1149 (4)	0.0527 (11)	
C3	0.4533 (3)	0.6309 (3)	0.0314 (4)	0.0501 (11)	
H3	0.4303	0.6356	−0.0562	0.060*	
C4	0.5595 (3)	0.6318 (2)	0.0701 (3)	0.0386 (9)	
C5	0.5886 (3)	0.6261 (2)	0.2032 (3)	0.0325 (9)	
C6	0.6938 (3)	0.6284 (2)	0.2732 (3)	0.0366 (9)	
C7	0.8071 (3)	0.6269 (3)	0.4445 (4)	0.0492 (10)	
C8	0.8673 (3)	0.6389 (3)	0.3283 (4)	0.0537 (11)	
C11	0.6306 (4)	0.6391 (3)	−0.0363 (4)	0.0498 (11)	
C12	0.9234 (3)	0.7421 (3)	0.3368 (4)	0.0748 (14)	
H12A	0.9545	0.7535	0.2593	0.112*	
H12B	0.9764	0.7422	0.4095	0.112*	
H12C	0.8741	0.7948	0.3470	0.112*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C9	0.053 (3)	0.089 (4)	0.066 (5)	−0.001 (3)	0.000 (4)	0.000 (4)
C10	0.073 (4)	0.099 (4)	0.103 (5)	0.001 (3)	−0.006 (4)	0.008 (4)
C9'	0.053 (3)	0.089 (4)	0.066 (5)	−0.001 (3)	0.000 (4)	0.000 (4)
C10'	0.073 (4)	0.099 (4)	0.103 (5)	0.001 (3)	−0.006 (4)	0.008 (4)

C13	0.057 (3)	0.089 (4)	0.063 (3)	0.012 (3)	0.010 (2)	0.008 (3)
C14	0.063 (5)	0.077 (3)	0.075 (4)	0.017 (3)	0.018 (3)	0.000 (3)
C15	0.072 (4)	0.114 (5)	0.091 (4)	0.004 (4)	0.033 (3)	−0.009 (4)
C13'	0.057 (3)	0.089 (4)	0.063 (3)	0.012 (3)	0.010 (2)	0.008 (3)
C14'	0.063 (5)	0.077 (3)	0.075 (4)	0.017 (3)	0.018 (3)	0.000 (3)
C15'	0.072 (4)	0.114 (5)	0.091 (4)	0.004 (4)	0.033 (3)	−0.009 (4)
Cu1	0.0406 (3)	0.0545 (3)	0.0317 (3)	−0.0056 (3)	0.0091 (2)	−0.0009 (2)
Cl1	0.0510 (6)	0.0529 (6)	0.0537 (7)	0.0025 (5)	0.0230 (5)	0.0001 (5)
N1	0.0360 (18)	0.0410 (19)	0.0342 (18)	−0.0005 (15)	0.0035 (14)	0.0028 (13)
N2	0.0292 (17)	0.058 (2)	0.0291 (17)	−0.0044 (15)	0.0026 (13)	0.0047 (14)
N3	0.0369 (19)	0.091 (3)	0.0300 (19)	−0.0031 (18)	0.0070 (15)	0.0113 (16)
O1	0.076 (2)	0.137 (3)	0.0288 (17)	0.016 (2)	0.0030 (15)	0.0025 (17)
O2	0.0510 (18)	0.116 (3)	0.0367 (17)	0.0012 (18)	0.0123 (14)	0.0056 (15)
O3	0.0456 (18)	0.118 (2)	0.0346 (17)	−0.0046 (17)	−0.0075 (14)	0.0030 (15)
O4	0.0585 (19)	0.148 (3)	0.0307 (16)	−0.0201 (19)	0.0088 (13)	−0.0151 (17)
C1	0.035 (2)	0.059 (3)	0.048 (3)	0.002 (2)	0.0064 (19)	0.007 (2)
C2	0.035 (2)	0.062 (3)	0.059 (3)	0.001 (2)	−0.006 (2)	0.010 (2)
C3	0.053 (3)	0.055 (3)	0.038 (2)	−0.001 (2)	−0.012 (2)	0.0102 (19)
C4	0.042 (2)	0.038 (2)	0.034 (2)	0.0002 (18)	−0.0023 (18)	−0.0021 (16)
C5	0.034 (2)	0.031 (2)	0.031 (2)	−0.0009 (16)	0.0002 (16)	0.0023 (15)
C6	0.033 (2)	0.045 (2)	0.032 (2)	−0.0050 (18)	0.0061 (17)	0.0036 (16)
C7	0.045 (3)	0.065 (3)	0.037 (2)	−0.003 (2)	0.0028 (19)	0.000 (2)
C8	0.036 (2)	0.084 (3)	0.041 (3)	−0.003 (2)	0.0043 (19)	0.006 (2)
C11	0.067 (3)	0.049 (3)	0.033 (2)	−0.001 (2)	0.005 (2)	0.0013 (18)
C12	0.054 (3)	0.097 (4)	0.072 (3)	−0.035 (3)	0.002 (2)	0.015 (3)

Geometric parameters (Å, °)

C9—C10	1.513 (9)	C15'—H15F	0.9600
C9—C2	1.538 (19)	Cu1—N2	1.930 (3)
C9—H9A	0.9700	Cu1—O4	1.944 (2)
C9—H9B	0.9700	Cu1—N1	2.041 (3)
C10—H10A	0.9600	Cu1—Cl1	2.2301 (11)
C10—H10B	0.9600	Cu1—Cl1^{i}	2.7249 (11)
C10—H10C	0.9600	Cl1—Cu1^{i}	2.7249 (11)
C9'—C10'	1.501 (9)	N1—C1	1.325 (4)
C9'—C2	1.51 (2)	N1—C5	1.345 (4)
C9'—H9'1	0.9700	N2—C6	1.338 (4)
C9'—H9'2	0.9700	N2—C7	1.364 (4)
C10'—H10D	0.9600	N3—C6	1.287 (4)
C10'—H10E	0.9600	N3—C8	1.472 (4)
C10'—H10F	0.9600	N3—H3A	0.8600
C13—C14	1.511 (6)	O1—C11	1.237 (4)
C13—C15	1.532 (7)	O2—C11	1.227 (5)
C13—C8	1.540 (15)	O3—C7	1.220 (4)
C13—H13	0.9800	O4—H4A	0.8257
C14—H14A	0.9600	O4—H4B	0.8371
C14—H14B	0.9600	C1—C2	1.384 (5)
C14—H14C	0.9600	C1—H1	0.9300

C15—H15A	0.9600	C2—C3	1.362 (5)
C15—H15B	0.9600	C3—C4	1.387 (5)
C15—H15C	0.9600	C3—H3	0.9300
C13'—C8	1.42 (4)	C4—C5	1.398 (4)
C13'—C14'	1.533 (10)	C4—C11	1.531 (5)
C13'—C15'	1.536 (10)	C5—C6	1.467 (4)
C13'—H13'	0.9800	C7—C8	1.530 (5)
C14'—H14D	0.9600	C8—C12	1.544 (5)
C14'—H14E	0.9600	C12—H12A	0.9600
C14'—H14F	0.9600	C12—H12B	0.9600
C15'—H15D	0.9600	C12—H12C	0.9600
C15'—H15E	0.9600		
C10—C9—C2	104.8 (10)	C1—N1—C5	119.9 (3)
C10—C9—H9A	110.8	C1—N1—Cu1	123.7 (3)
C2—C9—H9A	110.8	C5—N1—Cu1	116.4 (2)
C10—C9—H9B	110.8	C6—N2—C7	107.1 (3)
C2—C9—H9B	110.8	C6—N2—Cu1	115.9 (2)
H9A—C9—H9B	108.9	C7—N2—Cu1	137.0 (3)
C10'—C9'—C2	113.3 (13)	C6—N3—C8	109.5 (3)
C10'—C9'—H9'1	108.9	C6—N3—H3A	125.2
C2—C9'—H9'1	108.9	C8—N3—H3A	125.2
C10'—C9'—H9'2	108.9	Cu1—O4—H4A	109.5
C2—C9'—H9'2	108.9	Cu1—O4—H4B	126.0
H9'1—C9'—H9'2	107.7	H4A—O4—H4B	121.4
C9'—C10'—H10D	109.5	N1—C1—C2	122.5 (4)
C9'—C10'—H10E	109.5	N1—C1—H1	118.8
H10D—C10'—H10E	109.5	C2—C1—H1	118.8
C9'—C10'—H10F	109.5	C3—C2—C1	116.7 (4)
H10D—C10'—H10F	109.5	C3—C2—C9'	130.1 (6)
H10E—C10'—H10F	109.5	C1—C2—C9'	113.0 (6)
C14—C13—C15	111.2 (6)	C3—C2—C9	117.1 (7)
C14—C13—C8	111.3 (9)	C1—C2—C9	125.8 (7)
C15—C13—C8	110.9 (10)	C2—C3—C4	123.5 (4)
C14—C13—H13	107.8	C2—C3—H3	118.3
C15—C13—H13	107.8	C4—C3—H3	118.3
C8—C13—H13	107.8	C3—C4—C5	115.3 (4)
C8—C13'—C14'	116 (3)	C3—C4—C11	116.9 (3)
C8—C13'—C15'	116 (3)	C5—C4—C11	127.8 (3)
C14'—C13'—C15'	110.7 (10)	N1—C5—C4	122.1 (3)
C8—C13'—H13'	104.0	N1—C5—C6	109.8 (3)
C14'—C13'—H13'	104.0	C4—C5—C6	128.0 (3)
C15'—C13'—H13'	104.0	N3—C6—N2	115.2 (3)
C13'—C14'—H14D	109.5	N3—C6—C5	127.0 (3)
C13'—C14'—H14E	109.5	N2—C6—C5	117.8 (3)
H14D—C14'—H14E	109.5	O3—C7—N2	126.0 (4)
C13'—C14'—H14F	109.5	O3—C7—C8	125.2 (4)
H14D—C14'—H14F	109.5	N2—C7—C8	108.8 (3)
H14E—C14'—H14F	109.5	C13'—C8—N3	114 (2)
C13'—C15'—H15D	109.5	C13'—C8—C7	115.5 (13)

C13'—C15'—H15E	109.5	N3—C8—C7	99.4 (3)
H15D—C15'—H15E	109.5	N3—C8—C13	110.4 (7)
C13'—C15'—H15F	109.5	C7—C8—C13	109.4 (5)
H15D—C15'—H15F	109.5	C13'—C8—C12	107.2 (11)
H15E—C15'—H15F	109.5	N3—C8—C12	111.2 (3)
N2—Cu1—O4	89.01 (11)	C7—C8—C12	109.1 (3)
N2—Cu1—N1	79.86 (12)	C13—C8—C12	116.0 (6)
O4—Cu1—N1	166.85 (11)	O2—C11—O1	125.1 (4)
N2—Cu1—Cl1	172.96 (9)	O2—C11—C4	121.9 (3)
O4—Cu1—Cl1	92.56 (9)	O1—C11—C4	113.0 (4)
N1—Cu1—Cl1	97.67 (9)	C8—C12—H12A	109.5
N2—Cu1—Cl1^{i}	93.48 (9)	C8—C12—H12B	109.5
O4—Cu1—Cl1^{i}	99.06 (9)	H12A—C12—H12B	109.5
N1—Cu1—Cl1^{i}	88.66 (8)	C8—C12—H12C	109.5
Cl1—Cu1—Cl1^{i}	93.06 (3)	H12A—C12—H12C	109.5
Cu1—Cl1—Cu1^{i}	86.94 (3)	H12B—C12—H12C	109.5
O4—Cu1—Cl1—Cu1^{i}	−99.22 (9)	Cu1—N2—C6—N3	−178.5 (2)
N1—Cu1—Cl1—Cu1^{i}	89.06 (8)	C7—N2—C6—C5	−179.0 (3)
Cl1^{i}—Cu1—Cl1—Cu1^{i}	0.0	Cu1—N2—C6—C5	2.8 (4)
N2—Cu1—N1—C1	−178.6 (3)	N1—C5—C6—N3	−177.8 (3)
O4—Cu1—N1—C1	−146.0 (5)	C4—C5—C6—N3	1.7 (6)
Cl1—Cu1—N1—C1	−5.2 (3)	N1—C5—C6—N2	0.8 (4)
Cl1^{i}—Cu1—N1—C1	87.7 (3)	C4—C5—C6—N2	−179.7 (3)
N2—Cu1—N1—C5	4.3 (2)	C6—N2—C7—O3	−179.8 (4)
O4—Cu1—N1—C5	36.9 (6)	Cu1—N2—C7—O3	−2.2 (7)
Cl1—Cu1—N1—C5	177.6 (2)	C6—N2—C7—C8	0.1 (4)
Cl1^{i}—Cu1—N1—C5	−89.4 (2)	Cu1—N2—C7—C8	177.8 (3)
O4—Cu1—N2—C6	−176.7 (3)	C14'—C13'—C8—N3	−56 (3)
N1—Cu1—N2—C6	−3.7 (2)	C15'—C13'—C8—N3	77 (3)
Cl1^{i}—Cu1—N2—C6	84.3 (2)	C14'—C13'—C8—C7	59 (4)
O4—Cu1—N2—C7	5.9 (4)	C15'—C13'—C8—C7	−169 (3)
N1—Cu1—N2—C7	178.8 (4)	C14'—C13'—C8—C13	10 (14)
Cl1^{i}—Cu1—N2—C7	−93.2 (4)	C15'—C13'—C8—C13	143 (19)
C5—N1—C1—C2	−0.5 (5)	C14'—C13'—C8—C12	−180 (3)
Cu1—N1—C1—C2	−177.5 (3)	C15'—C13'—C8—C12	−47 (4)
N1—C1—C2—C3	0.8 (6)	C6—N3—C8—C13'	123.5 (10)
N1—C1—C2—C9'	−175.0 (7)	C6—N3—C8—C7	−0.1 (4)
N1—C1—C2—C9	173.5 (6)	C6—N3—C8—C13	114.7 (4)
C10'—C9'—C2—C3	−29.3 (16)	C6—N3—C8—C12	−115.0 (4)
C10'—C9'—C2—C1	145.7 (9)	O3—C7—C8—C13'	57 (2)
C10'—C9'—C2—C9	−70 (3)	N2—C7—C8—C13'	−123 (2)
C10—C9—C2—C3	−110.5 (10)	O3—C7—C8—N3	180.0 (4)
C10—C9—C2—C1	76.7 (12)	N2—C7—C8—N3	0.0 (4)
C10—C9—C2—C9'	36 (3)	O3—C7—C8—C13	64.3 (8)
C1—C2—C3—C4	0.0 (6)	N2—C7—C8—C13	−115.7 (7)
C9'—C2—C3—C4	174.9 (8)	O3—C7—C8—C12	−63.6 (5)

C9—C2—C3—C4	−173.4 (6)	N2—C7—C8—C12	116.4 (3)
C2—C3—C4—C5	−1.0 (5)	C14—C13—C8—C13'	−179 (17)
C2—C3—C4—C11	179.2 (3)	C15—C13—C8—C13'	−55 (16)
C1—N1—C5—C4	−0.6 (5)	C14—C13—C8—N3	−62.2 (10)
Cu1—N1—C5—C4	176.6 (2)	C15—C13—C8—N3	62.2 (10)
C1—N1—C5—C6	178.9 (3)	C14—C13—C8—C7	46.3 (12)
Cu1—N1—C5—C6	−3.9 (3)	C15—C13—C8—C7	170.6 (8)
C3—C4—C5—N1	1.3 (5)	C14—C13—C8—C12	170.2 (8)
C11—C4—C5—N1	−178.9 (3)	C15—C13—C8—C12	−65.5 (12)
C3—C4—C5—C6	−178.1 (3)	C3—C4—C11—O2	−175.5 (4)
C11—C4—C5—C6	1.7 (6)	C5—C4—C11—O2	4.7 (6)
C8—N3—C6—N2	0.3 (5)	C3—C4—C11—O1	5.0 (5)
C8—N3—C6—C5	178.9 (3)	C5—C4—C11—O1	−174.8 (3)
C7—N2—C6—N3	−0.2 (4)		

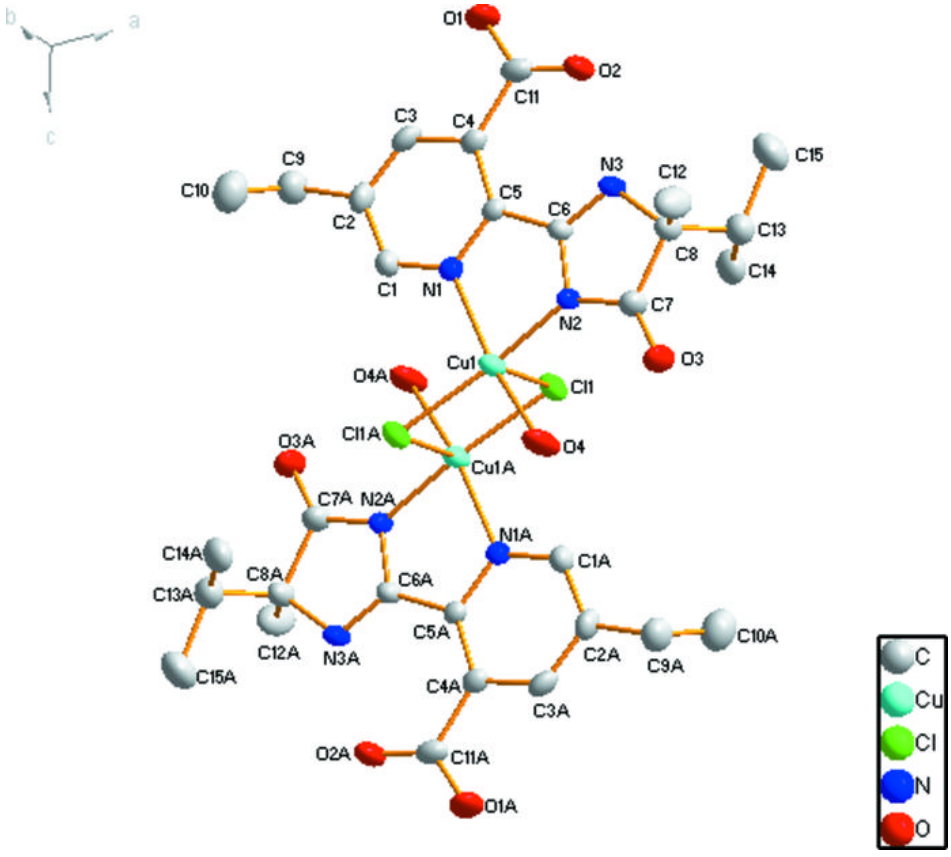
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4B···O1^{ii}	0.84	1.70	2.537 (4)	174
O4—H4A···O3	0.83	1.97	2.759 (4)	159
N3—H3A···O2	0.86	1.72	2.493 (4)	148

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

Fig. 1


b
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C2A
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Fig. 2