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Bis[bis(1*H*-benzimidazol-2-ylmethyl)amine]copper(II) dichloride methanol disolvate dihydrate

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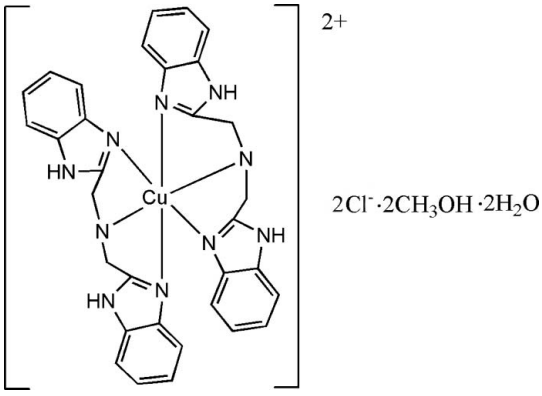
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.123; data-to-parameter ratio = 16.6.

In the title compound, $[Cu(C_{16}H_{14}N_5)_2]Cl_2\cdot 2CH_4O\cdot 2H_2O$, the cationic metal complex resides on a crystallographic centre of inversion, with the Cu^{2+} bonded to two bis(1*H*-benzimidazol-2-ylmethyl)amines (IDB). The coordination geometry of the Cu^{2+} ion is distorted octahedral with an N_6 ligand set. A three-dimensional framework structure is formed by means of hydrogen bonds and π–π interactions formed between imidazole and phenyl rings, and between phenyl and phenyl rings, with centroid-to-centroid distances of 3.690 (2)–3.977 (2) Å and interplanar spacings of 3.445 (2)–3.502 (2) Å.

Related literature

For related literature, see: Adams *et al.* (1990); Qin *et al.* (2005); Santoro *et al.* (2000); Suresh *et al.* (2006); Yan *et al.* (2004); Yu *et al.* (2006). For the treatment of disordered solvent, see: Spek (2003).



Experimental

Crystal data

$[Cu(C_{16}H_{14}N_5)_2]Cl_2\cdot 2CH_4O\cdot 2H_2O$
M_r = 725.13
Triclinic, $P\overline{1}$
a = 9.653 (3) Å
b = 9.921 (3) Å
c = 10.316 (3) Å
α = 82.095 (5)°
β = 88.441 (5)°
γ = 87.073 (5)°
V = 977.1 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 292 (2) K
0.23 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
9121 measured reflections
3799 independent reflections
2937 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.123
S = 0.97
3799 reflections
229 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1	0.860 (10)	2.027 (15)	2.839 (4)	157 (3)
O1—H1B···Cl1	0.81 (4)	2.59 (4)	3.206 (4)	134 (5)
N1—H1C···Cl1^{i}	0.855 (10)	2.455 (12)	3.296 (3)	168 (3)

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

Data collection: Bruker *SMART* CCD (Bruker, 2001); 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, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2050).

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Bis[bis(1*H*-benzimidazol-2-ylmethyl)amine]copper(II) dichloride methanol disolvate dihydrate

Xian-you Xia, Yong Zhang, Yuan Qu, Xue-mei Chen and Ting Liu

S1. Comment

Imidazole (Im) and benzimidazole (Bzim) are common species having biological and biochemical structure and function (Santoro *et al.*, 2000). Several compounds containing more than one benzimidazole moiety have been reported recently, *e.g.* Yan *et al.* (2004), Qin *et al.* (2005), and Yu *et al.* (2006). The title compound, (I), was prepared in a series of syntheses to produce new benzimidazole derivatives, and we report the crystal stucture herein.

The main geometric parameters of (I) are listed in Table 1, and the molecule structure is illustrated in Fig. 1. In (I), the Cu atom displays a distorted octahedral coordination geometry provided by two tridentate IDB ligands: one amine N atom and one benzimidazolyl N atom of each ligand make up the equatorial plane and another benzimidazolyl N atom of each ligand occupies the axial position. As shown in Table 2 and Fig. 2, the molecules are stablized by intermolecular Cl···H—N, Cl···H—O and O···H—N hydrogen bonds and $\pi\cdots\pi$ stacking, leading to the formation of a three dimension network.

S2. Experimental

All reagents and solvents were used as obtained without further purification. Bis(benzimidazol-2-yl-methyl)amine (IDB) was prepared according to the method described by Adams *et al.* (1990). Compound (I) was synthesized by reaction of IDB (0.54 g, 2 mmol) and copper(II) chloride dihydrate (0.17 g, 1 mmol) in methanol (40 ml) at 333 K for 8 h. The resulting solution was filtered and purple crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of the filtrate at room temperature after one week (yield 55%).

S3. Refinement

All H atoms bonded to C atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, with U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to N atoms were located in a difference map and were refined with distance restraints of N—H = 0.86 (1)Å and U_{iso}(H) = 1.2U_{eq}(N). Similarly located water H atoms were refined with distance restraints of O—H = 0.82 (1) Å, H···H = 1.35 (1)Å and U_{iso}(H) = 1.5U_{eq}(O). During the refinement of the structure, electron-density peaks were located that were believed to be highly disordered solvent molecule molecules (possibly methanol and water solvent). Attempts made to model the solvent molecules were not successful. The SQUEEZE option in *PLATON* (Spek, 2003) indicated there was a solvent cavity of volume 209 Å^3 containing approximately 18 electrons. In the final cycles of refinement, this contribution to the electron density was removed from the observed data. The density, the F(000) value, the molecular weight and the formula are given without taking into account the results obtained with the SQUEEZE option *PLATON* (Spek, 2003). Similar treatment of disordered solvent molecules were carried out by Suresh *et al.* (2006, and references therein).

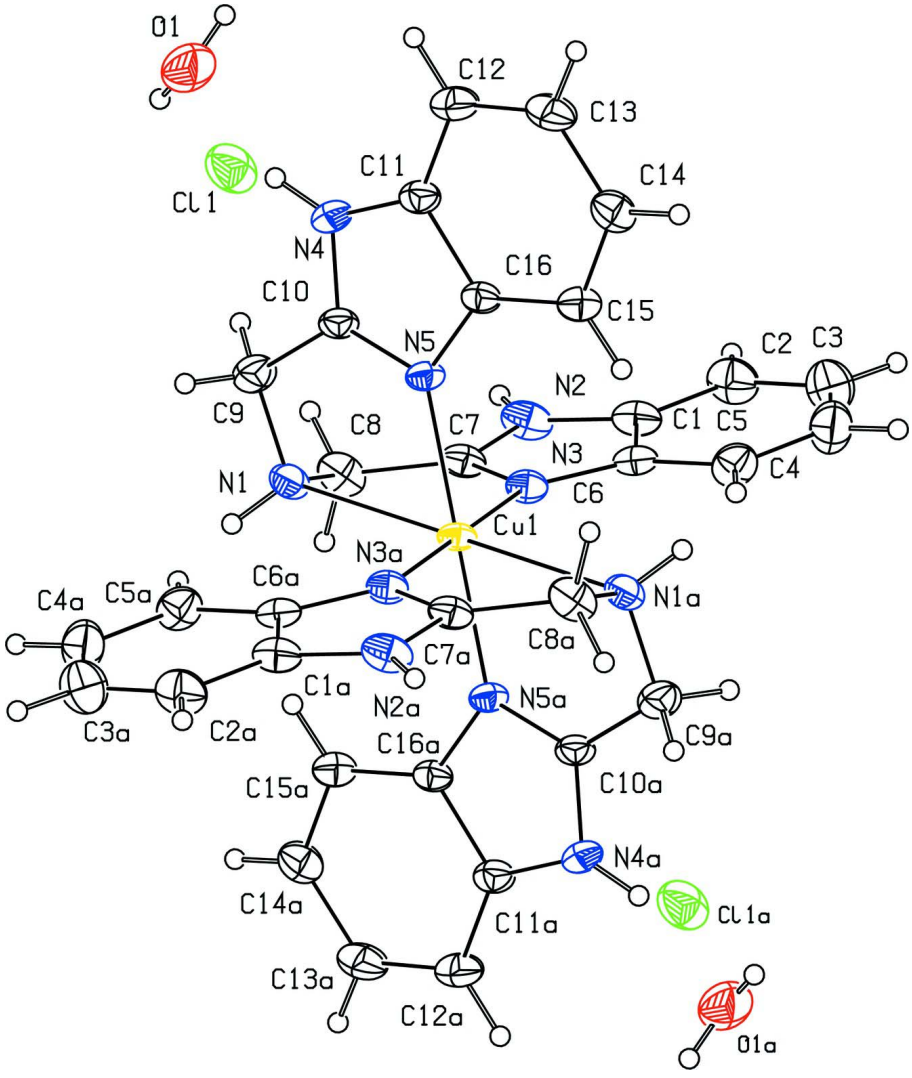

Figure 1

Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

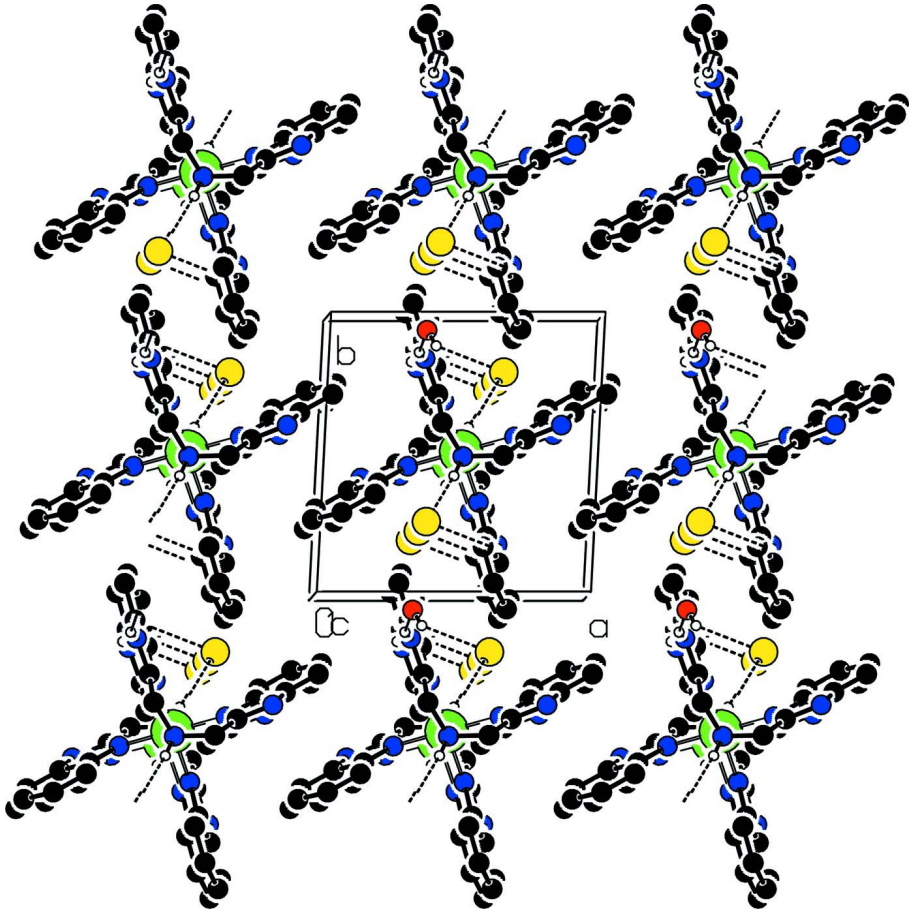

Figure 2

Plot of the crystal packing showing the linkage of the molecules by H-bonding and π–π interactions shown as dashed lines.

Bis[bis(1*H*-benzimidazol-2-ylmethyl)amine]copper(II) dichloride methanol disolvate dihydrate

Crystal data

$[Cu(C_{16}H_{14}N_5)_2]Cl_2\cdot 2CH_4O\cdot 2H_2O$
$M_r = 725.13$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.653\ (3)$ Å
$b = 9.921\ (3)$ Å
$c = 10.316\ (3)$ Å
$\alpha = 82.095\ (5)°$
$\beta = 88.441\ (5)°$
$\gamma = 87.073\ (5)°$
$V = 977.1\ (5)$ Å^3
$Z = 1$
$F(000) = 375$
$D_x = 1.232$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3239 reflections
$\theta = 1.6$–$25.5°$
$\mu = 0.74$ mm^{-1}
$T = 292$ K
Block, purple
0.23 × 0.22 × 0.20 mm

Data collection

CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
9121 measured reflections
3799 independent reflections
2937 reflections with $I > 2\sigma(I)$

R_{int} = 0.099
θ_{max} = 26.0°, θ_{min} = 2.0°
h = −11→11
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.123
S = 0.97
3799 reflections
229 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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}
Cu1	0.5000	0.5000	1.0000	0.02773 (17)
N1	0.4996 (3)	0.5259 (2)	0.7434 (2)	0.0378 (6)
H1C	0.530 (3)	0.597 (2)	0.696 (2)	0.045*
N2	0.1441 (3)	0.4115 (3)	0.8191 (3)	0.0434 (7)
H2	0.106 (3)	0.406 (4)	0.746 (2)	0.052*
N3	0.3091 (2)	0.4492 (2)	0.9528 (2)	0.0337 (6)
N4	0.6536 (3)	0.1732 (3)	0.8228 (3)	0.0384 (6)
H4	0.678 (3)	0.154 (3)	0.7466 (17)	0.046*
N5	0.5738 (2)	0.3203 (2)	0.9531 (2)	0.0308 (5)
C1	0.0971 (3)	0.3621 (3)	0.9427 (3)	0.0410 (8)
C2	−0.0207 (4)	0.2958 (4)	0.9870 (4)	0.0536 (10)
H2A	−0.0891	0.2804	0.9297	0.064*
C3	−0.0330 (4)	0.2534 (4)	1.1187 (4)	0.0652 (11)
H3	−0.1117	0.2092	1.1520	0.078*
C4	0.0712 (4)	0.2759 (4)	1.2042 (4)	0.0604 (10)
H4A	0.0607	0.2452	1.2930	0.072*
C5	0.1892 (4)	0.3426 (4)	1.1598 (3)	0.0467 (9)
H5	0.2577	0.3575	1.2172	0.056*
C6	0.2023 (3)	0.3866 (3)	1.0261 (3)	0.0351 (7)
C7	0.2717 (3)	0.4620 (3)	0.8288 (3)	0.0362 (7)
C8	0.3527 (4)	0.5231 (3)	0.7149 (3)	0.0467 (9)

H8A	0.3423	0.4713	0.6428	0.056*
H8B	0.3164	0.6154	0.6878	0.056*
C9	0.5817 (4)	0.4056 (3)	0.7148 (3)	0.0472 (9)
H9A	0.6722	0.4331	0.6808	0.057*
H9B	0.5365	0.3659	0.6472	0.057*
C10	0.6004 (3)	0.3008 (3)	0.8311 (3)	0.0332 (7)
C11	0.6591 (3)	0.1038 (3)	0.9456 (3)	0.0358 (7)
C12	0.7028 (4)	−0.0289 (3)	0.9947 (4)	0.0478 (9)
H12	0.7384	−0.0894	0.9394	0.057*
C13	0.6915 (4)	−0.0673 (3)	1.1271 (4)	0.0512 (9)
H13	0.7205	−0.1552	1.1623	0.061*
C14	0.6370 (4)	0.0231 (3)	1.2104 (3)	0.0465 (8)
H14	0.6298	−0.0062	1.2998	0.056*
C15	0.5939 (3)	0.1543 (3)	1.1627 (3)	0.0392 (7)
H15	0.5565	0.2135	1.2183	0.047*
C16	0.6075 (3)	0.1957 (3)	1.0300 (3)	0.0307 (6)
Cl1	0.37341 (12)	0.23380 (10)	0.47316 (9)	0.0656 (3)
O1	0.6586 (3)	0.0805 (3)	0.5743 (3)	0.0720 (9)
H1B	0.624 (5)	0.138 (3)	0.520 (4)	0.108*
H1A	0.628 (5)	0.009 (3)	0.588 (5)	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0332 (3)	0.0220 (3)	0.0305 (3)	−0.00342 (19)	−0.0075 (2)	−0.01034 (19)
N1	0.0506 (17)	0.0288 (13)	0.0344 (14)	−0.0086 (12)	−0.0034 (12)	−0.0028 (11)
N2	0.0460 (16)	0.0366 (14)	0.0493 (18)	−0.0054 (12)	−0.0220 (14)	−0.0071 (13)
N3	0.0357 (14)	0.0305 (13)	0.0373 (14)	−0.0051 (10)	−0.0075 (11)	−0.0104 (11)
N4	0.0492 (16)	0.0336 (14)	0.0354 (15)	−0.0016 (12)	0.0020 (13)	−0.0164 (12)
N5	0.0380 (14)	0.0249 (12)	0.0316 (13)	−0.0010 (10)	−0.0036 (11)	−0.0108 (10)
C1	0.0386 (18)	0.0319 (16)	0.054 (2)	0.0019 (13)	−0.0136 (16)	−0.0111 (14)
C2	0.039 (2)	0.054 (2)	0.070 (3)	−0.0086 (16)	−0.0110 (18)	−0.0128 (19)
C3	0.041 (2)	0.072 (3)	0.085 (3)	−0.0179 (19)	0.008 (2)	−0.015 (2)
C4	0.057 (2)	0.074 (3)	0.052 (2)	−0.015 (2)	0.0098 (18)	−0.013 (2)
C5	0.0430 (19)	0.055 (2)	0.046 (2)	−0.0066 (16)	−0.0051 (16)	−0.0175 (17)
C6	0.0345 (16)	0.0269 (14)	0.0467 (19)	0.0031 (12)	−0.0068 (14)	−0.0152 (13)
C7	0.0421 (18)	0.0271 (14)	0.0407 (17)	−0.0034 (13)	−0.0115 (14)	−0.0070 (13)
C8	0.057 (2)	0.0439 (19)	0.0391 (18)	−0.0100 (16)	−0.0185 (17)	0.0000 (15)
C9	0.069 (2)	0.0408 (18)	0.0341 (17)	−0.0025 (17)	0.0002 (16)	−0.0120 (14)
C10	0.0404 (17)	0.0268 (15)	0.0350 (16)	−0.0049 (12)	−0.0030 (13)	−0.0116 (12)
C11	0.0361 (17)	0.0305 (15)	0.0433 (18)	−0.0044 (13)	−0.0023 (14)	−0.0124 (14)
C12	0.054 (2)	0.0313 (17)	0.059 (2)	0.0059 (15)	−0.0006 (17)	−0.0131 (16)
C13	0.057 (2)	0.0276 (17)	0.067 (2)	0.0062 (15)	−0.0059 (19)	−0.0015 (16)
C14	0.052 (2)	0.0384 (18)	0.047 (2)	−0.0027 (15)	−0.0065 (17)	0.0012 (15)
C15	0.0443 (18)	0.0322 (16)	0.0427 (18)	−0.0009 (13)	−0.0058 (15)	−0.0106 (14)
C16	0.0293 (15)	0.0256 (14)	0.0387 (16)	−0.0028 (11)	−0.0048 (13)	−0.0082 (12)
Cl1	0.0962 (8)	0.0549 (6)	0.0461 (5)	−0.0196 (5)	−0.0092 (5)	−0.0009 (4)
O1	0.084 (2)	0.076 (2)	0.064 (2)	−0.0184 (18)	0.0032 (16)	−0.0355 (17)

Geometric parameters (Å, º)

Cu1—N1	2.624 (3)	C3—H3	0.9300
Cu1—N3^{i}	2.024 (2)	C4—C5	1.382 (5)
Cu1—N3	2.024 (2)	C4—H4A	0.9300
Cu1—N5^{i}	2.002 (2)	C5—C6	1.392 (5)
Cu1—N5	2.002 (2)	C5—H5	0.9300
N1—C9	1.459 (4)	C7—C8	1.470 (5)
N1—C8	1.459 (4)	C8—H8A	0.9700
N1—H1C	0.855 (10)	C8—H8B	0.9700
N2—C7	1.365 (4)	C9—C10	1.484 (5)
N2—C1	1.375 (4)	C9—H9A	0.9700
N2—H2	0.858 (10)	C9—H9B	0.9700
N3—C7	1.326 (4)	C11—C12	1.393 (4)
N3—C6	1.384 (4)	C11—C16	1.408 (4)
N4—C10	1.354 (4)	C12—C13	1.369 (5)
N4—C11	1.357 (4)	C12—H12	0.9300
N4—H4	0.860 (10)	C13—C14	1.400 (5)
N5—C10	1.316 (4)	C13—H13	0.9300
N5—C16	1.402 (4)	C14—C15	1.374 (4)
C1—C2	1.378 (5)	C14—H14	0.9300
C1—C6	1.400 (4)	C15—C16	1.379 (4)
C2—C3	1.370 (6)	C15—H15	0.9300
C2—H2A	0.9300	O1—H1A	0.778 (17)
C3—C4	1.401 (5)		

N5^{i}—Cu1—N5	180.00 (13)	C6—C5—H5	121.1
N5^{i}—Cu1—N3^{i}	88.03 (9)	N3—C6—C5	131.1 (3)
N5—Cu1—N3^{i}	91.97 (9)	N3—C6—C1	109.4 (3)
N5^{i}—Cu1—N3	91.97 (9)	C5—C6—C1	119.4 (3)
N5—Cu1—N3	88.03 (9)	N3—C7—N2	110.7 (3)
N3^{i}—Cu1—N3	180.00 (12)	N3—C7—C8	126.1 (3)
N5^{i}—Cu1—N1	105.57 (9)	N2—C7—C8	123.2 (3)
N5—Cu1—N1	74.43 (9)	N1—C8—C7	112.1 (3)
N3^{i}—Cu1—N1	105.76 (9)	N1—C8—H8A	109.2
N3—Cu1—N1	74.24 (9)	C7—C8—H8A	109.2
C9—N1—C8	114.0 (2)	N1—C8—H8B	109.2
C9—N1—Cu1	102.82 (18)	C7—C8—H8B	109.2
C8—N1—Cu1	102.97 (19)	H8A—C8—H8B	107.9
C9—N1—H1C	109 (2)	N1—C9—C10	113.0 (3)
C8—N1—H1C	106 (2)	N1—C9—H9A	109.0
Cu1—N1—H1C	122 (2)	C10—C9—H9A	109.0
C7—N2—C1	108.6 (2)	N1—C9—H9B	109.0
C7—N2—H2	124 (2)	C10—C9—H9B	109.0
C1—N2—H2	128 (2)	H9A—C9—H9B	107.8
C7—N3—C6	106.4 (2)	N5—C10—N4	112.0 (3)
C7—N3—Cu1	120.7 (2)	N5—C10—C9	125.3 (3)
C6—N3—Cu1	132.5 (2)	N4—C10—C9	122.7 (3)

C10—N4—C11	108.2 (2)	N4—C11—C12	133.0 (3)
C10—N4—H4	118 (2)	N4—C11—C16	106.0 (3)
C11—N4—H4	134 (2)	C12—C11—C16	120.9 (3)
C10—N5—C16	105.9 (2)	C13—C12—C11	117.7 (3)
C10—N5—Cu1	122.1 (2)	C13—C12—H12	121.2
C16—N5—Cu1	131.95 (19)	C11—C12—H12	121.2
N2—C1—C2	132.2 (3)	C12—C13—C14	121.3 (3)
N2—C1—C6	104.9 (3)	C12—C13—H13	119.3
C2—C1—C6	122.8 (3)	C14—C13—H13	119.3
C3—C2—C1	117.4 (3)	C15—C14—C13	121.3 (3)
C3—C2—H2A	121.3	C15—C14—H14	119.4
C1—C2—H2A	121.3	C13—C14—H14	119.4
C2—C3—C4	120.9 (4)	C14—C15—C16	118.2 (3)
C2—C3—H3	119.5	C14—C15—H15	120.9
C4—C3—H3	119.5	C16—C15—H15	120.9
C5—C4—C3	121.7 (4)	C15—C16—N5	131.6 (3)
C5—C4—H4A	119.1	C15—C16—C11	120.6 (3)
C3—C4—H4A	119.1	N5—C16—C11	107.8 (3)
C4—C5—C6	117.8 (3)	H1B—O1—H1A	120 (3)
C4—C5—H5	121.1		

N5^{i}—Cu1—N1—C9	167.82 (19)	C6—N3—C7—N2	0.6 (3)
N5—Cu1—N1—C9	−12.18 (19)	Cu1—N3—C7—N2	174.94 (19)
N3^{i}—Cu1—N1—C9	75.4 (2)	C6—N3—C7—C8	179.9 (3)
N3—Cu1—N1—C9	−104.6 (2)	Cu1—N3—C7—C8	−5.8 (4)
N5^{i}—Cu1—N1—C8	−73.47 (19)	C1—N2—C7—N3	−0.7 (4)
N5—Cu1—N1—C8	106.53 (19)	C1—N2—C7—C8	179.9 (3)
N3^{i}—Cu1—N1—C8	−165.85 (18)	C9—N1—C8—C7	90.9 (3)
N3—Cu1—N1—C8	14.15 (18)	Cu1—N1—C8—C7	−19.7 (3)
N5^{i}—Cu1—N3—C7	100.4 (2)	N3—C7—C8—N1	20.5 (5)
N5—Cu1—N3—C7	−79.6 (2)	N2—C7—C8—N1	−160.3 (3)
N1—Cu1—N3—C7	−5.3 (2)	C8—N1—C9—C10	−95.4 (3)
N5^{i}—Cu1—N3—C6	−87.1 (3)	Cu1—N1—C9—C10	15.3 (3)
N5—Cu1—N3—C6	92.9 (3)	C16—N5—C10—N4	−2.0 (3)
N1—Cu1—N3—C6	167.3 (3)	Cu1—N5—C10—N4	178.00 (18)
N3^{i}—Cu1—N5—C10	−99.2 (2)	C16—N5—C10—C9	−179.4 (3)
N3—Cu1—N5—C10	80.8 (2)	Cu1—N5—C10—C9	0.7 (4)
N1—Cu1—N5—C10	6.6 (2)	C11—N4—C10—N5	1.6 (3)
N3^{i}—Cu1—N5—C16	80.8 (2)	C11—N4—C10—C9	179.0 (3)
N3—Cu1—N5—C16	−99.2 (2)	N1—C9—C10—N5	−13.7 (4)
N1—Cu1—N5—C16	−173.3 (3)	N1—C9—C10—N4	169.2 (3)
C7—N2—C1—C2	−176.6 (4)	C10—N4—C11—C12	179.4 (3)
C7—N2—C1—C6	0.5 (3)	C10—N4—C11—C16	−0.4 (3)
N2—C1—C2—C3	176.8 (4)	N4—C11—C12—C13	−178.7 (3)
C6—C1—C2—C3	0.2 (5)	C16—C11—C12—C13	1.1 (5)
C1—C2—C3—C4	−0.6 (6)	C11—C12—C13—C14	0.5 (5)
C2—C3—C4—C5	0.7 (7)	C12—C13—C14—C15	−0.6 (5)
C3—C4—C5—C6	−0.4 (6)	C13—C14—C15—C16	−0.9 (5)

C7—N3—C6—C5	176.4 (3)	C14—C15—C16—N5	180.0 (3)
Cu1—N3—C6—C5	3.0 (5)	C14—C15—C16—C11	2.5 (4)
C7—N3—C6—C1	−0.3 (3)	C10—N5—C16—C15	−176.0 (3)
Cu1—N3—C6—C1	−173.7 (2)	Cu1—N5—C16—C15	3.9 (5)
C4—C5—C6—N3	−176.5 (3)	C10—N5—C16—C11	1.7 (3)
C4—C5—C6—C1	−0.1 (5)	Cu1—N5—C16—C11	−178.31 (18)
N2—C1—C6—N3	−0.1 (3)	N4—C11—C16—C15	177.2 (3)
C2—C1—C6—N3	177.3 (3)	C12—C11—C16—C15	−2.6 (4)
N2—C1—C6—C5	−177.2 (3)	N4—C11—C16—N5	−0.8 (3)
C2—C1—C6—C5	0.2 (5)	C12—C11—C16—N5	179.3 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1	0.86 (1)	2.03 (2)	2.839 (4)	157 (3)
O1—H1*B*···Cl1	0.81 (4)	2.59 (4)	3.206 (4)	134 (5)
N1—H1*C*···Cl1^{ii}	0.86 (1)	2.46 (1)	3.296 (3)	168 (3)

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