Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraimidazolebis(trichloroacetato)-copper(II)

Li-Min Li,[a] Huan-Mei Guo,[a] Fang-Fang Jian,[b]* Zeng-Hui Zhang[c] and Ning Zhang[c]

[a]Microscale Science Institute, Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, [b]Microscale Science Institute, Weifang University, Weifang 261061, People's Republic of China, and [c]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: ffjian2008@163.com

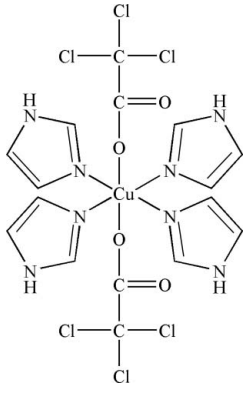
Received 22 April 2010; accepted 12 May 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.055; wR factor = 0.168; data-to-parameter ratio = 18.4.

The title compound, $[Cu(C_2Cl_3O_2)_2(C_3H_4N_2)_4]$, was prepared by the reaction of imidazole and trichloroacetatocopper(II). The Cu^{II} atom adopts a distorted octahedral coordination geometry, binding the N atoms of four imidazole ligands and the carboxylate O atoms of two trichloroacetate anions. The molecular structure and packing are stabilized by N—H···O hydrogen-bonding interactions. Close intermolecular Cl···Cl contacts [3.498 (3) Å] are also found in the structure.

Related literature

For background to work on metal-organic frameworks, see: Chen *et al.* (2001); Fang *et al.* (2005). For a related structure, see: Moncol *et al.* (2007).



Experimental

Crystal data

$[Cu(C_2Cl_3O_2)_2(C_3H_4N_2)_4]$
M_r = 660.61
Triclinic, $P\overline{1}$
a = 10.054 (2) Å
b = 10.539 (2) Å
c = 12.959 (3) Å
α = 108.12 (3)°
β = 92.93 (3)°
γ = 95.18 (3)°
V = 1295.2 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
12377 measured reflections
5823 independent reflections
5048 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.168
S = 1.05
5823 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N7	1.997 (2)	Cu1—N5	2.022 (3)
Cu1—N3	2.001 (2)	Cu1—O3	2.479 (2)
Cu1—N1	2.011 (3)	Cu1—O2	2.618 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8A···O1^{i}	0.86	2.03	2.885 (3)	177
N6—H6A···O4^{ii}	0.86	2.02	2.854 (3)	164
N2—H2A···O1^{iii}	0.86	1.96	2.790 (3)	162
N4—H4B···O4^{iv}	0.86	1.93	2.764 (3)	162

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors would like to thank the Natural Science Foundation of Shandong Province for financial support (No. Y2008B30).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2779).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, B., Eddaoudi, M., Hyde, S. T., OKeeffe, M. & Yaghi, O. M. (2001). *Science*, **291**, 1021–1023.
Fang, Q. R., Zhu, G. S., Xue, M., Sun, J. Y., Wei, Y., Qiu, S. & Xu, R. R. (2005). *Angew. Chem. Int. Ed.* **44**, 3845–3848.
Moncol, J., Maroszova, J., Peter, L., Mark, H., Marian, V., Morris, H., Svorec, J., Melnik, M., Mazur, M. & Koman, M. (2007). *Inorg. Chim. Acta*, **360**, 3213–3225.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, m682 [https://doi.org/10.1107/S1600536810017459]

Tetraimidazolebis(trichloroacetato)copper(II)

Li-Min Li, Huan-Mei Guo, Fang-Fang Jian, Zeng-Hui Zhang and Ning Zhang

S1. Comment

Metal-organic framework coordination polymers have attracted tremendous attention because of their molecular topologies and their potentially useful ion exchange, adsorption, catalytic and magnetic properties (Chen *et al.*, 2001; Fang *et al.*, 2005). In order to search for new complexes of this type, we synthesized the title compound and report its crystal structure here.

The title structure contains one copper(II) cation, four imidazole ligands and two trichloroacetate anions. The coordination sphere of the copper(II) ion is best described as a slightly distorted octahedron. The Cu—N bond lengths are in agreement with those reported recently (Moncol *et al.*, 2007). The crystal packing is stabilized by C—H···O and N—H···O hydrogen interaction (Table 1).

S2. Experimental

The title compound was obtained by adding imidazole(4 mmol) dropwise to a solution of copper(II) trichloroacetate acid (1 mmol) in ethanol (30 ml) with stirring for 1 hour at room temperature. A blue solution formed and after a few days rod-like crystals precipitated.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C-H) = 0.93Å, U_{iso}=1.2U_{eq} (C) for aromatic H atoms and 0.86Å, U_{iso} = 1.2U_{eq} (N) for the NH groups.

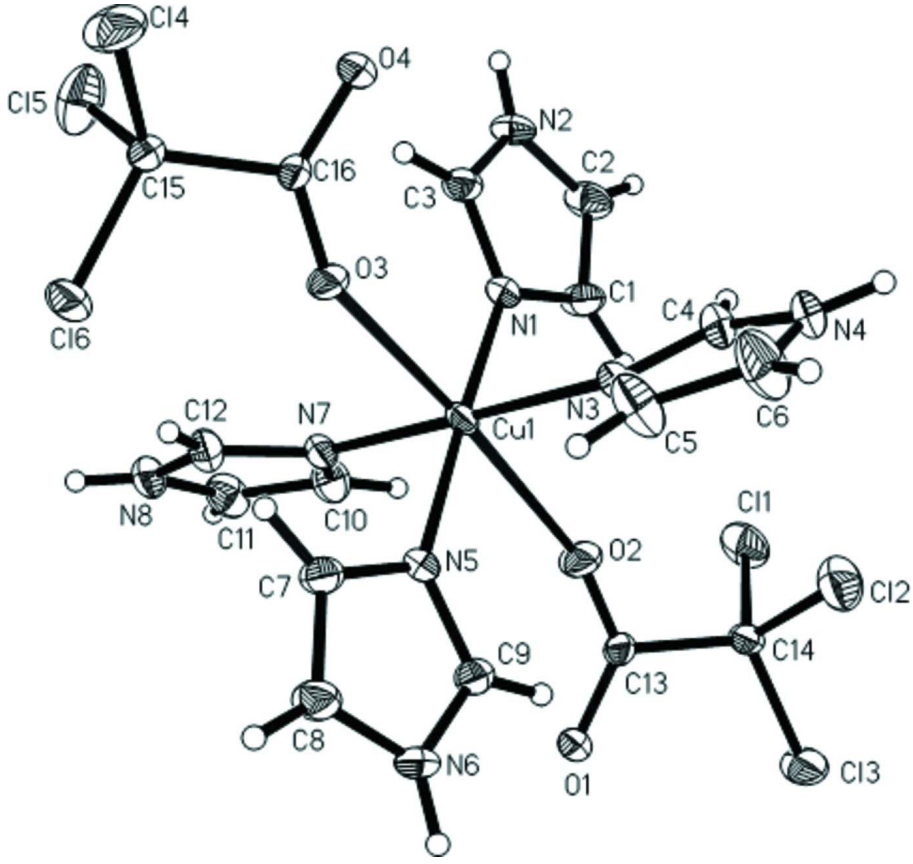


Figure 1

The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

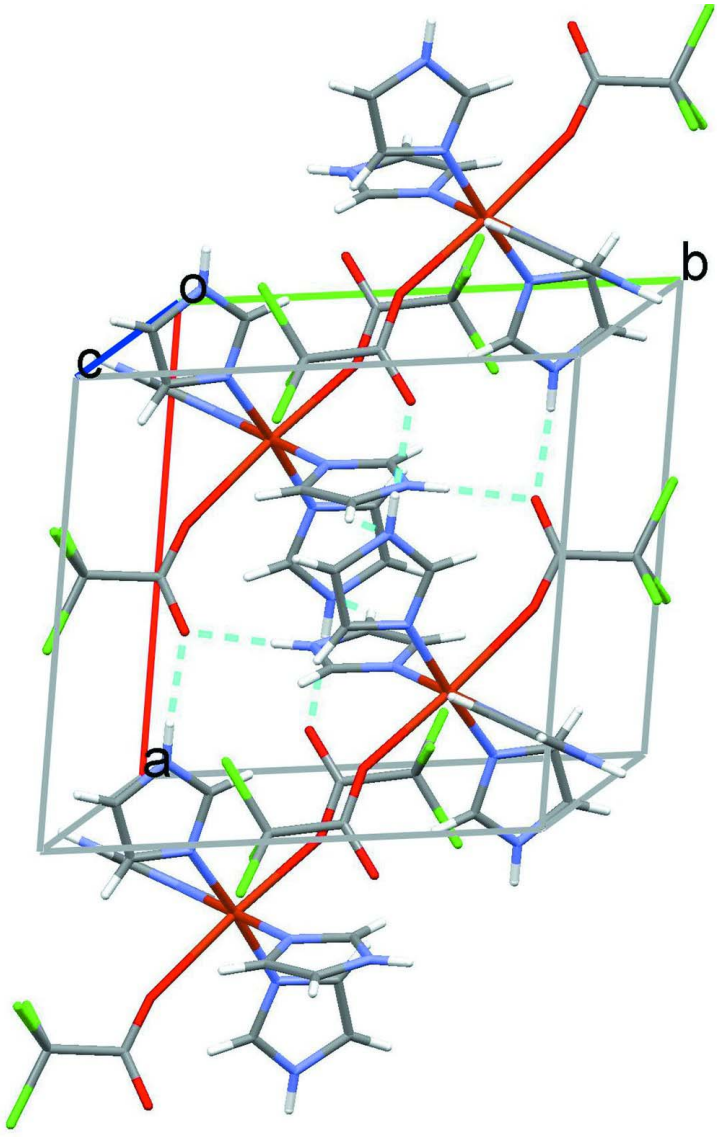


Figure 2

Crystal packing of the title compound viewed down the *c* axis.

Tetraimidazolebis(trichloroacetato)copper(II)

Crystal data

$[Cu(C_2Cl_3O_2)_2(C_3H_4N_2)_4]$
$M_r = 660.61$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.054\ (2)$ Å
$b = 10.539\ (2)$ Å
$c = 12.959\ (3)$ Å
$\alpha = 108.12\ (3)°$
$\beta = 92.93\ (3)°$
$\gamma = 95.18\ (3)°$
$V = 1295.2\ (4)$ Å^3
$Z = 2$
$F(000) = 662$
$D_x = 1.694$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2238 reflections
$\theta = 2.1–26.3°$
$\mu = 1.50$ mm^{-1}
$T = 293$ K
Rod, blue
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
12377 measured reflections
5823 independent reflections
5048 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -13 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.168$
$S = 1.05$
5823 reflections
316 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.1013P)^2 + 0.8989P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.43$ e Å^{-3}
$\Delta\rho_{min} = -0.86$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.26177 (3)	0.25376 (3)	0.24476 (3)	0.02655 (14)
Cl1	0.41741 (11)	−0.13876 (10)	0.38566 (9)	0.0542 (3)
Cl4	−0.12008 (10)	0.61045 (11)	0.09196 (10)	0.0593 (3)
Cl6	0.14287 (9)	0.67968 (9)	0.19926 (13)	0.0687 (4)
Cl2	0.44972 (12)	−0.16467 (11)	0.16082 (9)	0.0619 (3)
Cl3	0.67814 (10)	−0.15040 (9)	0.30617 (13)	0.0744 (4)
Cl5	−0.08098 (15)	0.63279 (11)	0.31833 (10)	0.0716 (4)
N7	0.2999 (2)	0.3951 (2)	0.3900 (2)	0.0290 (5)
N3	0.2209 (2)	0.1099 (2)	0.1006 (2)	0.0296 (5)
N1	0.1157 (2)	0.1667 (2)	0.3089 (2)	0.0294 (5)
O1	0.6441 (2)	0.1316 (2)	0.3576 (2)	0.0412 (6)
O3	0.1177 (2)	0.4023 (2)	0.1870 (2)	0.0390 (5)
C16	0.0052 (3)	0.4292 (3)	0.1668 (2)	0.0271 (6)
N5	0.4180 (2)	0.3358 (2)	0.1859 (2)	0.0269 (5)
C14	0.5229 (3)	−0.0894 (3)	0.2966 (3)	0.0349 (7)
N8	0.3302 (3)	0.5850 (3)	0.5243 (2)	0.0424 (7)
H8A	0.3349	0.6695	0.5591	0.051*

C15	−0.0107 (3)	0.5819 (3)	0.1915 (3)	0.0357 (7)
C4	0.1621 (3)	−0.0146 (3)	0.0788 (3)	0.0377 (7)
H4A	0.1307	−0.0507	0.1311	0.045*
C3	−0.0074 (3)	0.1991 (3)	0.3191 (3)	0.0335 (6)
H3A	−0.0390	0.2708	0.3018	0.040*
N6	0.6185 (2)	0.3773 (3)	0.1383 (2)	0.0337 (6)
H6A	0.7006	0.3686	0.1245	0.040*
O2	0.4247 (2)	0.1096 (2)	0.3115 (2)	0.0460 (6)
C12	0.2979 (4)	0.5269 (3)	0.4173 (3)	0.0394 (7)
H12A	0.2769	0.5727	0.3689	0.047*
N2	−0.0805 (3)	0.1150 (3)	0.3579 (2)	0.0376 (6)
H2A	−0.1633	0.1184	0.3713	0.045*
C13	0.5316 (3)	0.0686 (3)	0.3258 (3)	0.0294 (6)
C9	0.5368 (3)	0.2938 (3)	0.1716 (3)	0.0313 (6)
H9A	0.5608	0.2159	0.1833	0.038*
C1	0.1205 (3)	0.0559 (3)	0.3430 (3)	0.0399 (7)
H1A	0.1957	0.0112	0.3454	0.048*
N4	0.1536 (3)	−0.0808 (3)	−0.0272 (3)	0.0433 (7)
H4B	0.1195	−0.1626	−0.0581	0.052*
C8	0.5480 (3)	0.4792 (3)	0.1302 (3)	0.0424 (8)
H8B	0.5789	0.5522	0.1086	0.051*
C2	−0.0014 (3)	0.0224 (4)	0.3726 (3)	0.0438 (8)
H2B	−0.0262	−0.0491	0.3978	0.053*
C7	0.4245 (3)	0.4526 (3)	0.1596 (3)	0.0381 (7)
H7A	0.3546	0.5052	0.1618	0.046*
C11	0.3542 (4)	0.4870 (4)	0.5681 (3)	0.0456 (8)
H11A	0.3785	0.4980	0.6409	0.055*
C6	0.2081 (5)	0.0029 (5)	−0.0779 (3)	0.0653 (13)
H6B	0.2160	−0.0161	−0.1523	0.078*
C5	0.2490 (5)	0.1207 (4)	0.0017 (3)	0.0543 (10)
H5A	0.2902	0.1974	−0.0095	0.065*
C10	0.3354 (4)	0.3696 (3)	0.4845 (3)	0.0405 (7)
H10A	0.3452	0.2852	0.4904	0.049*
O4	−0.1012 (2)	0.3534 (2)	0.1345 (2)	0.0390 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0222 (2)	0.0225 (2)	0.0301 (2)	−0.00600 (13)	0.00312 (13)	0.00353 (15)
Cl1	0.0542 (6)	0.0461 (5)	0.0682 (6)	−0.0106 (4)	0.0040 (4)	0.0314 (4)
Cl4	0.0390 (5)	0.0648 (6)	0.0921 (8)	0.0136 (4)	−0.0025 (5)	0.0498 (6)
Cl6	0.0311 (5)	0.0322 (5)	0.1425 (12)	−0.0079 (3)	−0.0069 (5)	0.0329 (5)
Cl2	0.0673 (7)	0.0517 (6)	0.0537 (6)	−0.0014 (5)	0.0007 (5)	0.0010 (4)
Cl3	0.0299 (5)	0.0347 (5)	0.1577 (13)	0.0097 (4)	−0.0054 (6)	0.0295 (6)
Cl5	0.0955 (9)	0.0523 (6)	0.0649 (7)	0.0291 (6)	0.0273 (6)	0.0068 (5)
N7	0.0274 (12)	0.0239 (12)	0.0307 (12)	−0.0021 (9)	0.0016 (9)	0.0032 (9)
N3	0.0265 (12)	0.0227 (12)	0.0352 (13)	−0.0011 (9)	0.0000 (9)	0.0045 (9)
N1	0.0220 (12)	0.0265 (12)	0.0366 (13)	−0.0031 (9)	0.0016 (9)	0.0072 (10)

O1	0.0255 (11)	0.0243 (11)	0.0680 (16)	−0.0004 (8)	0.0045 (10)	0.0072 (10)
O3	0.0243 (11)	0.0312 (11)	0.0648 (16)	0.0079 (9)	−0.0020 (10)	0.0193 (10)
C16	0.0235 (13)	0.0207 (13)	0.0377 (15)	0.0043 (10)	0.0042 (10)	0.0096 (10)
N5	0.0215 (11)	0.0241 (11)	0.0319 (12)	−0.0026 (9)	0.0001 (9)	0.0059 (9)
C14	0.0225 (14)	0.0250 (14)	0.056 (2)	0.0005 (11)	−0.0017 (12)	0.0128 (13)
N8	0.0403 (16)	0.0304 (14)	0.0435 (16)	−0.0018 (11)	0.0021 (12)	−0.0050 (12)
C15	0.0238 (14)	0.0259 (14)	0.058 (2)	0.0039 (11)	0.0032 (13)	0.0142 (13)
C4	0.0408 (18)	0.0237 (14)	0.0433 (18)	−0.0025 (12)	0.0015 (13)	0.0049 (12)
C3	0.0240 (14)	0.0353 (16)	0.0424 (17)	0.0007 (11)	0.0042 (11)	0.0144 (13)
N6	0.0193 (12)	0.0384 (14)	0.0436 (15)	0.0014 (10)	0.0066 (10)	0.0132 (11)
O2	0.0285 (12)	0.0370 (13)	0.0778 (19)	0.0111 (10)	0.0030 (11)	0.0239 (12)
C12	0.0413 (18)	0.0271 (15)	0.0458 (19)	0.0002 (13)	−0.0012 (14)	0.0075 (13)
N2	0.0210 (12)	0.0474 (16)	0.0459 (15)	−0.0026 (11)	0.0043 (10)	0.0184 (12)
C13	0.0260 (14)	0.0209 (13)	0.0437 (16)	0.0048 (10)	0.0085 (11)	0.0121 (11)
C9	0.0257 (14)	0.0303 (14)	0.0398 (16)	0.0050 (11)	0.0042 (11)	0.0132 (12)
C1	0.0252 (15)	0.0426 (18)	0.059 (2)	0.0046 (13)	0.0035 (13)	0.0259 (15)
N4	0.0420 (16)	0.0270 (14)	0.0465 (17)	−0.0031 (11)	−0.0039 (12)	−0.0062 (12)
C8	0.0301 (16)	0.0394 (18)	0.067 (2)	0.0030 (13)	0.0102 (15)	0.0290 (16)
C2	0.0341 (18)	0.049 (2)	0.056 (2)	−0.0062 (14)	0.0003 (14)	0.0309 (17)
C7	0.0255 (15)	0.0341 (16)	0.062 (2)	0.0053 (12)	0.0068 (13)	0.0243 (15)
C11	0.049 (2)	0.048 (2)	0.0307 (16)	−0.0056 (16)	0.0007 (13)	0.0033 (14)
C6	0.087 (3)	0.059 (3)	0.0338 (19)	−0.020 (2)	0.0015 (19)	−0.0010 (18)
C5	0.073 (3)	0.047 (2)	0.0355 (18)	−0.0206 (19)	−0.0033 (17)	0.0105 (15)
C10	0.048 (2)	0.0372 (17)	0.0346 (16)	0.0008 (14)	0.0011 (13)	0.0101 (13)
O4	0.0229 (10)	0.0261 (11)	0.0637 (16)	−0.0024 (8)	−0.0011 (9)	0.0102 (10)

Geometric parameters (Å, º)

Cu1—N7	1.997 (2)	N8—H8A	0.8600
Cu1—N3	2.001 (2)	C4—N4	1.327 (4)
Cu1—N1	2.011 (3)	C4—H4A	0.9300
Cu1—N5	2.022 (3)	C3—N2	1.333 (4)
Cu1—O3	2.479 (2)	C3—H3A	0.9300
Cu1—O2	2.618 (2)	N6—C9	1.333 (4)
Cl1—C14	1.768 (4)	N6—C8	1.367 (4)
Cl4—C15	1.767 (4)	N6—H6A	0.8600
Cl6—C15	1.757 (3)	O2—C13	1.220 (4)
Cl2—C14	1.778 (4)	C12—H12A	0.9300
Cl3—C14	1.754 (3)	N2—C2	1.364 (5)
Cl5—C15	1.768 (4)	N2—H2A	0.8600
N7—C12	1.325 (4)	C9—H9A	0.9300
N7—C10	1.370 (4)	C1—C2	1.353 (5)
N3—C4	1.328 (4)	C1—H1A	0.9300
N3—C5	1.362 (5)	N4—C6	1.350 (6)
N1—C3	1.316 (4)	N4—H4B	0.8600
N1—C1	1.375 (4)	C8—C7	1.348 (5)
O1—C13	1.240 (4)	C8—H8B	0.9300
O3—C16	1.226 (4)	C2—H2B	0.9300

C16—O4	1.245 (4)	C7—H7A	0.9300
C16—C15	1.565 (4)	C11—C10	1.358 (5)
N5—C9	1.312 (4)	C11—H11A	0.9300
N5—C7	1.372 (4)	C6—C5	1.357 (5)
C14—C13	1.582 (4)	C6—H6B	0.9300
N8—C12	1.339 (5)	C5—H5A	0.9300
N8—C11	1.358 (5)	C10—H10A	0.9300

N7—Cu1—N3	178.78 (10)	N3—C4—H4A	124.3
N7—Cu1—N1	87.99 (10)	N1—C3—N2	110.6 (3)
N3—Cu1—N1	90.80 (11)	N1—C3—H3A	124.7
N7—Cu1—N5	91.08 (10)	N2—C3—H3A	124.7
N3—Cu1—N5	90.11 (10)	C9—N6—C8	107.4 (3)
N1—Cu1—N5	175.95 (10)	C9—N6—H6A	126.3
N7—Cu1—O3	88.90 (10)	C8—N6—H6A	126.3
N3—Cu1—O3	91.37 (9)	N7—C12—N8	110.6 (3)
N1—Cu1—O3	95.17 (9)	N7—C12—H12A	124.7
N5—Cu1—O3	88.70 (9)	N8—C12—H12A	124.7
N7—Cu1—O2	88.42 (10)	C3—N2—C2	108.2 (3)
N3—Cu1—O2	91.36 (10)	C3—N2—H2A	125.9
N1—Cu1—O2	87.03 (9)	C2—N2—H2A	125.9
N5—Cu1—O2	89.06 (9)	O2—C13—O1	129.8 (3)
O3—Cu1—O2	176.47 (7)	O2—C13—C14	113.8 (3)
C12—N7—C10	105.8 (3)	O1—C13—C14	116.3 (2)
C12—N7—Cu1	130.0 (2)	N5—C9—N6	111.3 (3)
C10—N7—Cu1	124.2 (2)	N5—C9—H9A	124.4
C4—N3—C5	104.8 (3)	N6—C9—H9A	124.4
C4—N3—Cu1	129.0 (2)	C2—C1—N1	109.2 (3)
C5—N3—Cu1	126.2 (2)	C2—C1—H1A	125.4
C3—N1—C1	106.1 (3)	N1—C1—H1A	125.4
C3—N1—Cu1	126.4 (2)	C4—N4—C6	107.9 (3)
C1—N1—Cu1	127.3 (2)	C4—N4—H4B	126.0
O3—C16—O4	129.6 (3)	C6—N4—H4B	126.0
O3—C16—C15	116.0 (3)	C7—C8—N6	106.1 (3)
O4—C16—C15	114.3 (2)	C7—C8—H8B	126.9
C9—N5—C7	105.8 (3)	N6—C8—H8B	126.9
C9—N5—Cu1	127.4 (2)	C1—C2—N2	105.9 (3)
C7—N5—Cu1	126.8 (2)	C1—C2—H2B	127.0
C13—C14—Cl3	114.2 (2)	N2—C2—H2B	127.0
C13—C14—Cl1	108.4 (2)	C8—C7—N5	109.4 (3)
Cl3—C14—Cl1	108.81 (19)	C8—C7—H7A	125.3
C13—C14—Cl2	108.8 (2)	N5—C7—H7A	125.3
Cl3—C14—Cl2	107.99 (19)	C10—C11—N8	106.2 (3)
Cl1—C14—Cl2	108.56 (17)	C10—C11—H11A	126.9
C12—N8—C11	108.0 (3)	N8—C11—H11A	126.9
C12—N8—H8A	126.0	N4—C6—C5	105.9 (4)
C11—N8—H8A	126.0	N4—C6—H6B	127.0
C16—C15—Cl6	112.6 (2)	C5—C6—H6B	127.0

C16—C15—Cl4	111.9 (2)	C6—C5—N3	110.0 (4)
Cl6—C15—Cl4	107.7 (2)	C6—C5—H5A	125.0
C16—C15—Cl5	106.0 (2)	N3—C5—H5A	125.0
Cl6—C15—Cl5	109.80 (19)	C11—C10—N7	109.4 (3)
Cl4—C15—Cl5	108.70 (17)	C11—C10—H10A	125.3
N4—C4—N3	111.3 (3)	N7—C10—H10A	125.3
N4—C4—H4A	124.3		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8*A*···O1^{i}	0.86	2.03	2.885 (3)	177
N6—H6*A*···O4^{ii}	0.86	2.02	2.854 (3)	164
N2—H2*A*···O1^{iii}	0.86	1.96	2.790 (3)	162
N4—H4*B*···O4^{iv}	0.86	1.93	2.764 (3)	162

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