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Bis(nitrato-κO)(5,7,12,14-tetramethyl-1,4,8,11-tetraazacyclotetradecane-6,13-diaminium-$\kappa^4N^1,N^4,N^8,N^{11}$)copper(II) dinitrate tetrahydrate

Xiang-Yun Liu[a]* and Hong-Ying Chu[b]

[a]Department of Chemistry and Chemical Engineering, Henan University of Urban Construction, Pingdingshan 467044, People's Republic of China, and [b]Department of Environment and Chemical Engineering, Yellow River Conservancy Technical Institute, Kaifeng 475004, People's Republic of China
Correspondence e-mail: tianlin1288@163.com

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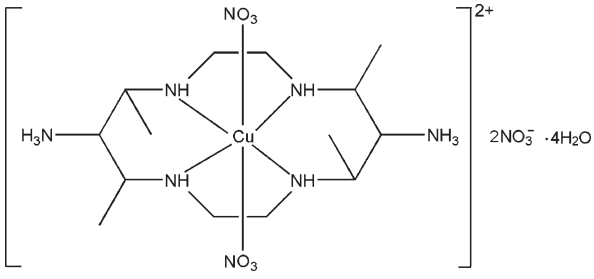
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.133; data-to-parameter ratio = 15.0.

In the title compound, $[Cu(NO_3)_2(C_{14}H_{36}N_6)](NO_3)_2\cdot 4H_2O$, the Cu^{II} atom, lying on an inversion center, is six-coordinated in a distorted octahedral environment by four N atoms from a centrosymmetric 14-membered tetraazacyclotetradecane macrocyclic ligand and two O atoms from two nitrate anions. The supramolecular network is consolidated by extensive O—H···O and N—H···O hydrogen-bonding interactions.

Related literature

For Cu(II) complexes of related macrocyclic ligands, see: Bernhardt (1999); Bernhardt & Sharpe (1998).



Experimental

Crystal data

$[Cu(NO_3)_2(C_{14}H_{36}N_6)](NO_3)_2\cdot 4H_2O$
M_r = 672.14
Monoclinic, $P2_1/n$
a = 9.201 (2) Å
b = 16.576 (4) Å
c = 9.278 (2) Å
β = 98.788 (4)°
V = 1398.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 123 K
0.37 × 0.34 × 0.31 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.739, T_{max} = 0.774
6071 measured reflections
3021 independent reflections
2269 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.133
S = 1.03
3021 reflections
202 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···O3	0.93	2.43	3.155 (4)	134
N1—H1C···O2W^{i}	0.93	2.28	3.096 (4)	146
N2—H2A···O3	0.93	2.52	3.244 (4)	135
N2—H2A···O4^{ii}	0.93	2.47	3.249 (4)	141
N3—H3D···O4	0.91	2.08	2.924 (4)	155
N3—H3E···O1W^{iii}	0.91	1.86	2.748 (4)	164
N3—H3F···O2^{i}	0.91	2.06	2.902 (4)	154
N3—H3F···O3^{i}	0.91	2.32	3.108 (4)	145
O1W—H1WA···O2^{i}	0.84 (4)	2.01 (3)	2.823 (4)	160 (5)
O1W—H1WB···O5^{iv}	0.84 (2)	1.97 (2)	2.795 (4)	168 (5)
O2W—H2WA···O6^{ii}	0.93 (5)	2.00 (5)	2.913 (5)	166 (5)
O2W—H2WB···O6^{v}	0.92 (2)	2.18 (2)	3.084 (5)	167 (5)

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x-1, y, z$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2316).

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supplementary materials

Acta Cryst. (2010). E**66**, m837 [**doi:10.1107/S1600536810023342**]

Bis(nitrato-κO)(5,7,12,14-tetramethyl-1,4,8,11-tetraazacyclotetradecane-6,13-diaminium-$\kappa^4N^1,N^4,N^8,N^{11}$)copper(II) dinitrate tetrahydrate

X.-Y. Liu and H.-Y. Chu

Comment

In the past, much attention has been given to the copper complexes of macrocyclic *trans*-5(*R*),7(*R*),12(*R*), 14(*R*)-tetramethyl-6, 13-dinitro-1,4,8,11-tetraazacyclotetradecane and related ligands (Bernhardt, 1999; Bernhardt & Sharpe, 1998). Recently, we have synthesized a Cu(II) complex based on 5,7,12,14-tetramethyl-6,13- diamino-1,4,8,11-tetraazacyclotetradecane and its structure is reported here.

The asymmetric unit of the title compound (Fig. 1) contains one Cu^{II} ion lying on an inversion center, one half of a 14-membered tetraazacyclotetradecane macrocyclic ligand, one coordinated nitrate anion, one uncoordinated nitrate anion and two solvent water molecules. The Cu^{II} ion has a slightly distorted octahedral coordination geometry, with two O atoms from two nitrate anions in the axial positions. The equatorial positions are occupied by four N atoms from the centrosymmetric 14-membered tetraazacyclotetradecane macrocyclic ligand [Cu1—N1 2.025 (2) and Cu1—N2 2.020 (2) Å]. The two uncoordinated nitrate anions are located above and below the 14-membered tetraazacyclotetradecane macrocycle and linked to the macrocycle *via* N—H···O hydrogen bonds (Table 1).

Experimental

An aqueous solution of 5,7,12,14-tetramethyl-6,13-diamino-1,4,8,11-tetraazacyclotetradecane (0.27 g, 1.0 mmol), $Cu(NO_3)_2$ (0.10 g, 0.5 mmol) and Na_2CO_3 (0.05 g, 0.5 mmol) was heated to reflux for 24 h. The reaction mixture was cooled to room temperature and red crystals of the title compound were obtained by slow evaporation of the solvent at room temperature.

Refinement

H atoms bound to C and N atoms were placed at calculated positions and were treated as riding on the parent atoms, with C—H = 1.00 (CH), 0.99 (CH_2) and 0.98 (CH_3) Å and N—H = 0.93 (NH) and 0.91 (NH_3) Å and with U_{iso}(H) = 1.2–1.5 U_{eq}(C, N). H atoms attached to water molecules were located in a difference Fourier map and refined with U_{iso}(H) = 1.2U_{eq}(O). The highest residual electron density was found 0.91 Å from O3 the deepest hole 0.52 Å from H2WA.

Figures

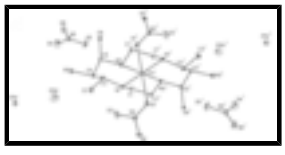


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are shown at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) 2-x, -y, 1-z.]

Bis(nitrato-κ*O*)(5,7,12,14-tetramethyl-1,4,8,11- tetraazacyclotetradecane-6,13-diaminium-$\kappa^4N^1,N^4,N^8,N^{11}$)copper(II) dinitrate tetrahydrate

Crystal data

$[Cu(NO_3)_2(C_{14}H_{36}N_6)](NO_3)_2{\cdot}4H_2O$	$F(000) = 710$
$M_r = 672.14$	$D_x = 1.596$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2543 reflections
$a = 9.201$ (2) Å	$\theta = 2.5$–$27.0°$
$b = 16.576$ (4) Å	$\mu = 0.87$ mm^{-1}
$c = 9.278$ (2) Å	$T = 123$ K
$\beta = 98.788$ (4)°	Block, red
$V = 1398.4$ (5) Å^3	0.37 × 0.34 × 0.31 mm
$Z = 2$	

Data collection

Bruker SMART 1000 CCD diffractometer	3021 independent reflections
Radiation source: fine-focus sealed tube	2269 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.027$
φ and ω scans	$\theta_{max} = 27.1°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -11 \rightarrow 11$
$T_{min} = 0.739$, $T_{max} = 0.774$	$k = -21 \rightarrow 17$
6071 measured reflections	$l = -10 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.133$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 2.4391P]$ where $P = (F_o^2 + 2F_c^2)/3$
3021 reflections	$(\Delta/\sigma)_{max} = 0.036$
202 parameters	$\Delta\rho_{max} = 1.24$ e Å^{-3}
6 restraints	$\Delta\rho_{min} = -0.81$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}

C1	0.8753 (4)	0.0883 (2)	0.2521 (3)	0.0169 (7)
H1A	0.9413	0.1356	0.2695	0.020*
H1B	0.7886	0.1039	0.1807	0.020*
C2	0.7676 (3)	0.13149 (18)	0.4684 (3)	0.0136 (6)
H2	0.8477	0.1722	0.4930	0.016*
C3	0.6400 (4)	0.1717 (2)	0.3687 (3)	0.0234 (8)
H3A	0.6749	0.1921	0.2809	0.035*
H3B	0.6019	0.2167	0.4205	0.035*
H3C	0.5616	0.1322	0.3408	0.035*
C4	0.7205 (3)	0.10160 (19)	0.6114 (3)	0.0129 (6)
H4	0.6574	0.0527	0.5888	0.016*
C5	0.8448 (3)	0.08013 (19)	0.7366 (3)	0.0137 (6)
H5	0.7973	0.0642	0.8224	0.016*
C6	0.9474 (3)	0.15076 (19)	0.7843 (3)	0.0167 (7)
H6A	1.0086	0.1378	0.8774	0.025*
H6B	0.8889	0.1991	0.7960	0.025*
H6C	1.0105	0.1608	0.7102	0.025*
C7	1.0453 (3)	−0.0192 (2)	0.8066 (3)	0.0170 (7)
H7A	1.0050	−0.0366	0.8947	0.020*
H7B	1.1144	0.0259	0.8342	0.020*
Cu1	1.0000	0.0000	0.5000	0.01124 (16)
N1	0.8274 (3)	0.06223 (16)	0.3922 (2)	0.0120 (5)
H1C	0.7509	0.0256	0.3683	0.014*
N2	0.9236 (3)	0.00785 (15)	0.6924 (3)	0.0128 (5)
H2A	0.8545	−0.0334	0.6882	0.015*
N3	0.6297 (3)	0.16570 (17)	0.6691 (3)	0.0173 (6)
H3D	0.6722	0.2147	0.6611	0.026*
H3E	0.6241	0.1555	0.7645	0.026*
H3F	0.5376	0.1657	0.6167	0.026*
N5	0.7860 (3)	0.36290 (18)	0.6169 (3)	0.0214 (6)
O4	0.6922 (3)	0.33861 (18)	0.6897 (3)	0.0377 (7)
O5	0.8513 (3)	0.31313 (17)	0.5511 (3)	0.0399 (7)
O6	0.8117 (3)	0.43623 (16)	0.6061 (4)	0.0402 (7)
O1W	0.1266 (3)	0.33514 (16)	0.4647 (3)	0.0236 (5)
O2W	0.4173 (4)	0.0272 (3)	0.8131 (4)	0.0592 (10)
H1WA	0.168 (5)	0.291 (2)	0.489 (6)	0.071*
H1WB	0.039 (3)	0.334 (3)	0.481 (6)	0.071*
H2WA	0.494 (5)	−0.008 (3)	0.846 (6)	0.071*
H2WB	0.396 (6)	0.045 (3)	0.901 (3)	0.071*
N4	0.7300 (3)	−0.14301 (18)	0.4733 (3)	0.0233 (6)
O1	0.8658 (2)	−0.13506 (15)	0.4843 (2)	0.0226 (5)
O2	0.6711 (3)	−0.21048 (15)	0.4441 (3)	0.0252 (6)
O3	0.6522 (3)	−0.08487 (18)	0.4963 (4)	0.0520 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0194 (16)	0.0188 (17)	0.0124 (14)	0.0044 (13)	0.0023 (11)	0.0043 (12)

C2	0.0175 (15)	0.0104 (15)	0.0122 (14)	0.0038 (12)	0.0004 (11)	0.0000 (11)
C3	0.0233 (18)	0.032 (2)	0.0150 (15)	0.0136 (15)	0.0039 (13)	0.0031 (14)
C4	0.0113 (14)	0.0153 (16)	0.0120 (13)	0.0026 (12)	0.0014 (11)	−0.0013 (11)
C5	0.0141 (15)	0.0155 (16)	0.0117 (13)	0.0025 (12)	0.0021 (11)	0.0011 (11)
C6	0.0171 (15)	0.0130 (16)	0.0192 (15)	0.0000 (12)	−0.0003 (12)	−0.0031 (12)
C7	0.0175 (15)	0.0232 (18)	0.0094 (13)	0.0068 (13)	−0.0009 (11)	0.0019 (11)
Cu1	0.0120 (3)	0.0135 (3)	0.0079 (2)	0.0030 (2)	0.00051 (17)	0.0002 (2)
N1	0.0121 (12)	0.0128 (13)	0.0112 (11)	0.0008 (10)	0.0022 (9)	−0.0003 (10)
N2	0.0123 (12)	0.0143 (14)	0.0113 (11)	0.0017 (10)	−0.0001 (9)	0.0009 (10)
N3	0.0161 (13)	0.0226 (16)	0.0134 (12)	0.0050 (11)	0.0030 (10)	−0.0006 (11)
N5	0.0167 (14)	0.0227 (16)	0.0244 (14)	0.0033 (12)	0.0021 (11)	0.0008 (12)
O4	0.0357 (16)	0.0389 (17)	0.0442 (16)	0.0024 (13)	0.0241 (13)	0.0093 (13)
O5	0.0442 (17)	0.0260 (15)	0.0558 (18)	−0.0001 (13)	0.0282 (14)	−0.0111 (13)
O6	0.0382 (16)	0.0149 (14)	0.071 (2)	−0.0009 (12)	0.0184 (14)	−0.0028 (13)
O1W	0.0252 (13)	0.0268 (14)	0.0192 (12)	−0.0001 (11)	0.0047 (10)	0.0005 (10)
O2W	0.051 (2)	0.068 (3)	0.056 (2)	0.0019 (19)	−0.0006 (17)	−0.0158 (19)
N4	0.0187 (14)	0.0206 (16)	0.0305 (16)	−0.0036 (12)	0.0031 (12)	−0.0016 (12)
O1	0.0153 (11)	0.0264 (14)	0.0268 (12)	−0.0057 (10)	0.0053 (9)	−0.0017 (10)
O2	0.0212 (12)	0.0197 (13)	0.0327 (13)	−0.0060 (10)	−0.0022 (10)	−0.0022 (10)
O3	0.0230 (15)	0.0230 (16)	0.111 (3)	0.0001 (12)	0.0151 (16)	−0.0074 (17)

Geometric parameters (Å, °)

C1—N1	1.499 (4)	C7—C1^{i}	1.505 (4)
C1—C7^{i}	1.505 (4)	C7—H7A	0.9900
C1—H1A	0.9900	C7—H7B	0.9900
C1—H1B	0.9900	Cu1—N2	2.020 (2)
C2—N1	1.496 (4)	Cu1—N1	2.025 (2)
C2—C3	1.532 (4)	Cu1—O1	2.550 (2)
C2—C4	1.539 (4)	N1—H1C	0.9300
C2—H2	1.0000	N2—H2A	0.9300
C3—H3A	0.9800	N3—H3D	0.9100
C3—H3B	0.9800	N3—H3E	0.9100
C3—H3C	0.9800	N3—H3F	0.9100
C4—N3	1.500 (4)	N5—O5	1.235 (4)
C4—C5	1.542 (4)	N5—O4	1.241 (4)
C4—H4	1.0000	N5—O6	1.245 (4)
C5—N2	1.491 (4)	O1W—H1WA	0.84 (4)
C5—C6	1.526 (4)	O1W—H1WB	0.84 (2)
C5—H5	1.0000	O2W—H2WA	0.93 (5)
C6—H6A	0.9800	O2W—H2WB	0.91 (2)
C6—H6B	0.9800	N4—O3	1.239 (4)
C6—H6C	0.9800	N4—O1	1.245 (4)
C7—N2	1.488 (3)	N4—O2	1.254 (4)
N1—C1—C7^{i}	108.5 (2)	N2—C7—H7A	109.9
N1—C1—H1A	110.0	C1^{i}—C7—H7A	109.9
C7^{i}—C1—H1A	110.0	N2—C7—H7B	109.9
N1—C1—H1B	110.0	C1^{i}—C7—H7B	109.9

C7^{i}—C1—H1B	110.0	H7A—C7—H7B	108.3
H1A—C1—H1B	108.4	N2^{i}—Cu1—N1	87.06 (10)
N1—C2—C3	110.6 (2)	N2—Cu1—N1	92.94 (10)
N1—C2—C4	109.4 (2)	O1—Cu1—N1	94.74 (9)
C3—C2—C4	111.7 (3)	O1—Cu1—N2	82.89 (8)
N1—C2—H2	108.3	O1—Cu1—N1^{i}	85.26 (9)
C3—C2—H2	108.3	O1—Cu1—N2^{i}	97.11 (8)
C4—C2—H2	108.3	C2—N1—C1	111.5 (2)
C2—C3—H3A	109.5	C2—N1—Cu1	118.36 (17)
C2—C3—H3B	109.5	C1—N1—Cu1	105.27 (18)
H3A—C3—H3B	109.5	C2—N1—H1C	107.1
C2—C3—H3C	109.5	C1—N1—H1C	107.1
H3A—C3—H3C	109.5	Cu1—N1—H1C	107.1
H3B—C3—H3C	109.5	C7—N2—C5	113.0 (2)
N3—C4—C2	109.0 (2)	C7—N2—Cu1	106.55 (18)
N3—C4—C5	106.5 (2)	C5—N2—Cu1	123.02 (18)
C2—C4—C5	116.8 (3)	C7—N2—H2A	104.1
N3—C4—H4	108.1	C5—N2—H2A	104.1
C2—C4—H4	108.1	Cu1—N2—H2A	104.1
C5—C4—H4	108.1	C4—N3—H3D	109.5
N2—C5—C6	113.0 (2)	C4—N3—H3E	109.5
N2—C5—C4	108.3 (2)	H3D—N3—H3E	109.5
C6—C5—C4	113.3 (3)	C4—N3—H3F	109.5
N2—C5—H5	107.3	H3D—N3—H3F	109.5
C6—C5—H5	107.3	H3E—N3—H3F	109.5
C4—C5—H5	107.3	O5—N5—O4	118.9 (3)
C5—C6—H6A	109.5	O5—N5—O6	120.0 (3)
C5—C6—H6B	109.5	O4—N5—O6	121.1 (3)
H6A—C6—H6B	109.5	H1WA—O1W—H1WB	109 (4)
C5—C6—H6C	109.5	H2WA—O2W—H2WB	99 (4)
H6A—C6—H6C	109.5	O3—N4—O1	120.2 (3)
H6B—C6—H6C	109.5	O3—N4—O2	119.3 (3)
N2—C7—C1^{i}	109.0 (2)	O1—N4—O2	120.5 (3)
N1—C2—C4—N3	−167.0 (2)	N2^{i}—Cu1—N1—C2	−142.1 (2)
C3—C2—C4—N3	−44.1 (3)	N2—Cu1—N1—C2	37.9 (2)
N1—C2—C4—C5	72.4 (3)	N2^{i}—Cu1—N1—C1	−16.78 (19)
C3—C2—C4—C5	−164.7 (3)	N2—Cu1—N1—C1	163.22 (19)
N3—C4—C5—N2	171.2 (2)	C1^{i}—C7—N2—C5	−175.9 (3)
C2—C4—C5—N2	−66.9 (3)	C1^{i}—C7—N2—Cu1	−37.9 (3)
N3—C4—C5—C6	−62.6 (3)	C6—C5—N2—C7	54.5 (3)
C2—C4—C5—C6	59.3 (3)	C4—C5—N2—C7	−179.2 (2)
C3—C2—N1—C1	56.7 (3)	C6—C5—N2—Cu1	−75.7 (3)
C4—C2—N1—C1	−179.9 (2)	C4—C5—N2—Cu1	50.7 (3)
C3—C2—N1—Cu1	178.9 (2)	N1^{i}—Cu1—N2—C7	11.4 (2)
C4—C2—N1—Cu1	−57.6 (3)	N1—Cu1—N2—C7	−168.6 (2)
C7^{i}—C1—N1—C2	171.5 (2)	N1^{i}—Cu1—N2—C5	144.2 (2)

C7^{i}—C1—N1—Cu1	42.0 (3)	N1—Cu1—N2—C5	−35.8 (2)

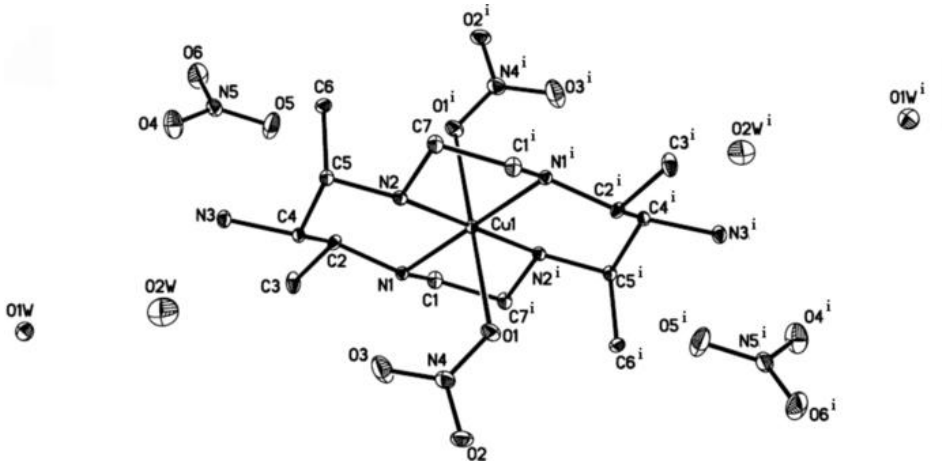
Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1C···O3	0.93	2.43	3.155 (4)	134
N1—H1C···O2W^{ii}	0.93	2.28	3.096 (4)	146
N2—H2A···O3	0.93	2.52	3.244 (4)	135
N2—H2A···O4^{iii}	0.93	2.47	3.249 (4)	141
N3—H3D···O4	0.91	2.08	2.924 (4)	155
N3—H3E···O1W^{iv}	0.91	1.86	2.748 (4)	164
N3—H3F···O2^{ii}	0.91	2.06	2.902 (4)	154
N3—H3F···O3^{ii}	0.91	2.32	3.108 (4)	145
O1W—H1WA···O2^{ii}	0.84 (4)	2.01 (3)	2.823 (4)	160 (5)
O1W—H1WB···O5^{v}	0.84 (2)	1.97 (2)	2.795 (4)	168 (5)
O2W—H2WA···O6^{iii}	0.93 (5)	2.00 (5)	2.913 (5)	166 (5)
O2W—H2WB···O6^{vi}	0.92 (2)	2.18 (2)	3.084 (5)	167 (5)

Symmetry codes: (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) *x*+1/2, −*y*+1/2, *z*+1/2; (v) *x*−1, *y*, *z*; (vi) *x*−1/2, −*y*+1/2, *z*+1/2.

Fig. 1


O2i
N4i
O3i
O6
N5
O5
C6
O1i
C7
C1i
N1i
C3i
O2Wi
O1Wi
O4
C5
N2
C2i
C4i
N3
C4
Cu1
N3i
C2
C3
N1
C1
N2i
C5i
O2W
O1W
C7i
O1
O5i
N5i
O4i
O3
N4
C6i
O6i
O2