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μ-4,4′-Bipyridine-κ^2N:N'-bis[aqua(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)] dinitrate

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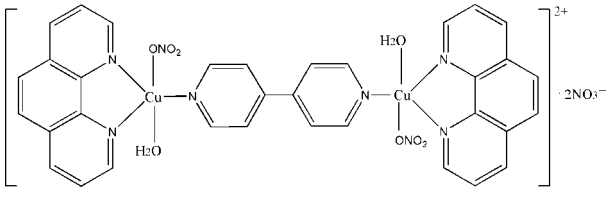
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.009 Å; R factor = 0.050; wR factor = 0.227; data-to-parameter ratio = 11.8.

The title compound, $[Cu_2(NO_3)_2(C_{10}H_8N_2)(C_{12}H_8N_2)_2(H_2O)_2](NO_3)_2$, comprises a binuclear copper complex cation and two nitrate anions. In the doubly-charged bridged dicopper cation, each Cu atom is five-coordinated in a distorted square-pyramidal geometry, formed by one O atom of the coordinated water molecule, one O atom of a coordinated nitrate anion, two N atoms from the bidentate 1,10-phenanthroline (phen) ligand and another N atom from the 4,4′-bipyridine (bipy) ligand. The bipy ligand bridges the Cu atoms to give a centrosymmetric binuclear structure. The complex is stabilized by hydrogen bonds and aromatic ring-stacking interactions [average interplanar distance 3.3139 (2) Å and ring-centroid separation 3.7971 (9) Å.

Related literature

For related literature, see: Blake *et al.* (1998); Wu *et al.* (2002); Lin *et al.* (2005).



Experimental

Crystal data

$[Cu_2(NO_3)_2(C_{10}H_8N_2)(C_{12}H_8N_2)_2(H_2O)_2](NO_3)_2$
M_r = 927.76
Triclinic, $P\overline{1}$
a = 7.3754 (18) Å
b = 8.925 (2) Å
c = 13.812 (3) Å
α = 92.347 (2)°
β = 97.596 (2)°
γ = 96.311 (3)°
V = 894.3 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 291 (2) K
0.37 × 0.27 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.647, T_{max} = 0.776
6155 measured reflections
3200 independent reflections
2909 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.227
S = 1.02
3200 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.992 (5)	Cu1—N1	2.030 (4)
Cu1—O1	2.000 (4)	Cu1—O7	2.230 (4)
Cu1—N2	2.025 (4)		
N3—Cu1—O1	93.23 (18)	N2—Cu1—N1	81.49 (17)
O1—Cu1—N2	91.76 (17)	O1—Cu1—O7	92.06 (18)
N3—Cu1—N1	92.10 (18)	N1—Cu1—O7	104.49 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H2W···O3^{i}	0.83	2.07	2.886 (6)	172

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: AT2361).

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supplementary materials

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μ-4,4'-Bipyridine-κ^2N:N'-bis[aqua(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)] dinitrate

Z.-X. Du and J.-X. Li

Comment

In the previous literatures, binuclear copper complexes containing (phen-Cu-bipy-Cu-phen) subunit (Blake *et al.*, 1998; Wu *et al.*, 2002; Lin *et al.*, 2005) have been reported. In our paper, we describe another new compound containing (phen-Cu-bipy-Cu-phen) subunit, (I), (Fig.1).

Compound (I) is comprised of a binuclear copper complex cation and two nitrate anions. In the doubly charged bridged dicopper cation, each Cu center has distorted square-pyramidal geometry, formed by one O atom of the coordinated water molecule, one O atom of coordinated nitrate anion, two N atoms from bidentate 1,10-phenanthroline (phen) ligand and another N atom from 4,4'-bipyridine (bipy) (Table 1). The plane N1/N2/O1/N3 defines the base of the pyramid while water O7 occupies the apex. The distance from Cu1 to the least-squares plane N1/N2/O1/N3 is 0.1924 (4)Å towards O7. The bipy ligand bridge the Cu atoms to give this binuclear structure.

The water molecules and coordinated nitrate O atoms take part in intermolecular hydrogen bonds interactions and they join complex cations into a one-dimensional chain structure along *a* axis (Fig. 2 and Table 2). The chains are further expanded into two-dimensional network *via* the π-π stacking between 1,10-phenanthroline rings of adjacent chains of (I) (Fig. 3). The dihedral angle of aromatics involved in stacking is 0.0002 (3)°. Interplanar average distance and ring-centroid separation distance are 3.3139 (2) Å, 3.7971 (9) Å, respectively.

Experimental

A 10 ml water solution of $Cu(NO)_3{\cdot}3H_2O$ (0.242 g,1 mmol) was dropped into 10 ml me thanol solution of 4,4'-bipyridine (0.078 g, 0.5 mmol) and 1,10-phenanthroline (0.18 g,1 mmol) to be stirred for 4 h at 333 K. The filtrate stayed in air for about one week to obtain blue block-shaped crystals. Analysis, found (%): C 43.85, H 3.05, N 15.16. $C_{34}H_{28}Cu_2N_{10}O_{14}$ requires (%): C 43.98, H 3.02, N 15.09.

Refinement

H atoms were positioned geometrically with C—H = 0.93 Å, O—H = 0.82 Å, and treated as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Figures

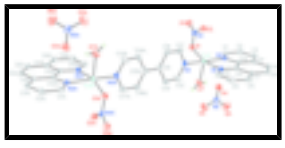


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Atoms with the suffix A are are at the symmetry position (−*x* + 1, −*y* + 2, −*z* + 1).

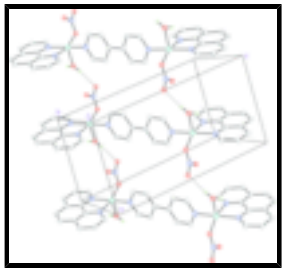


Fig. 2. Packing diagram, showing the one-dimensional chain structure of (I), linked *via* hydrogen bonds (dashed lines). H atoms on C atoms and uncoordinated nitrate anions have been omitted for clarity.

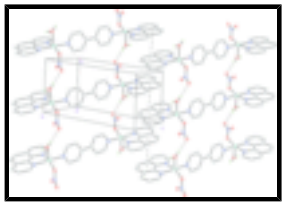


Fig. 3. The π–π stacking diagram between 1,10-phenanthroline rings of adjacent chains of (I). H atoms on C atoms and uncoordinated nitrate anions have been omitted.

μ-4,4'-Bipyridine-κ^2*N*:*N*'-bis[aqua(nitrato-κ*O*)(1,10- phenanthroline-κ^2*N*,*N*')copper(II)] dinitrate

Crystal data

$[Cu_2(NO_3)_2(C_{10}H_8N_2)(C_{12}H_8N_2)_2(H_2O)_2](NO_3)_2$	$Z = 1$
$M_r = 927.76$	$F_{000} = 472$
Triclinic, $P\overline{1}$	$D_x = 1.723$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3754$ (18) Å	Cell parameters from 3225 reflections
$b = 8.925$ (2) Å	$\theta = 2.7$–27.0°
$c = 13.812$ (3) Å	$\mu = 1.28$ mm^{-1}
$\alpha = 92.347$ (2)°	$T = 291$ (2) K
$\beta = 97.596$ (2)°	Block, blue
$\gamma = 96.311$ (3)°	0.37 × 0.27 × 0.21 mm
$V = 894.3$ (4) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	3200 independent reflections
Radiation source: fine-focus sealed tube	2909 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.021$
$T = 291$(2) K	$\theta_{max} = 25.5^\circ$
φ and ω scans	$\theta_{min} = 2.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.647$, $T_{max} = 0.776$	$k = -10 \rightarrow 10$
6155 measured reflections	$l = -16 \rightarrow 16$

Refinement

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

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.227$

$S = 1.02$

3200 reflections

271 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.183P)^2 + 1.6705P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.89$ e Å^{-3}

$\Delta\rho_{min} = -0.76$ e Å^{-3}

Extinction correction: none

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	0.69132 (8)	0.51338 (6)	0.71023 (4)	0.0247 (3)
O1	0.8055 (5)	0.4093 (5)	0.6066 (3)	0.0350 (9)
O2	1.0496 (6)	0.5437 (6)	0.6817 (3)	0.0462 (11)
O3	1.0720 (6)	0.3763 (6)	0.5659 (3)	0.0506 (12)
O4	0.4104 (7)	0.0751 (6)	0.7586 (4)	0.0540 (12)
O5	0.1351 (9)	0.0598 (9)	0.6823 (5)	0.082 (2)
O6	0.1944 (10)	−0.0793 (7)	0.8020 (5)	0.0754 (18)
O7	0.4292 (6)	0.3593 (5)	0.6762 (4)	0.0452 (11)
H1W	0.4431	0.2774	0.6993	0.068*
H2W	0.3303	0.3587	0.6404	0.068*
N1	0.6613 (6)	0.6354 (5)	0.8332 (3)	0.0260 (9)
N2	0.7736 (6)	0.3662 (5)	0.8101 (3)	0.0255 (9)
N3	0.6235 (7)	0.6792 (5)	0.6252 (3)	0.0321 (10)
N4	0.9803 (6)	0.4446 (5)	0.6181 (3)	0.0322 (10)
N5	0.2454 (8)	0.0181 (6)	0.7465 (4)	0.0423 (12)
C1	0.8307 (8)	0.2313 (6)	0.7951 (4)	0.0328 (12)
H1	0.8363	0.1960	0.7314	0.039*
C2	0.8818 (8)	0.1423 (7)	0.8717 (5)	0.0381 (13)
H2A	0.9207	0.0487	0.8589	0.046*
C3	0.8750 (8)	0.1918 (7)	0.9661 (5)	0.0397 (14)
H3A	0.9084	0.1318	1.0174	0.048*
C4	0.8170 (7)	0.3343 (6)	0.9852 (4)	0.0293 (11)

C5	0.8056 (8)	0.3986 (7)	1.0814 (4)	0.0358 (13)
H5A	0.8374	0.3448	1.1361	0.043*
C6	0.7489 (8)	0.5364 (7)	1.0925 (4)	0.0370 (13)
H6A	0.7435	0.5761	1.1552	0.044*
C7	0.6971 (7)	0.6229 (6)	1.0106 (4)	0.0314 (12)
C8	0.6355 (8)	0.7680 (7)	1.0179 (4)	0.0371 (13)
H8	0.6265	0.8132	1.0786	0.044*
C9	0.5897 (8)	0.8397 (6)	0.9341 (5)	0.0379 (13)
H9	0.5496	0.9347	0.9379	0.045*
C10	0.6025 (8)	0.7715 (6)	0.8425 (4)	0.0323 (12)
H10	0.5693	0.8221	0.7865	0.039*
C11	0.7076 (7)	0.5630 (6)	0.9160 (4)	0.0244 (10)
C12	0.7669 (7)	0.4173 (6)	0.9032 (4)	0.0249 (10)
C13	0.4474 (9)	0.6993 (7)	0.5978 (5)	0.0449 (15)
H13	0.3561	0.6266	0.6122	0.054*
C14	0.3950 (9)	0.8222 (7)	0.5495 (5)	0.0401 (14)
H14	0.2706	0.8314	0.5325	0.048*
C15	0.5268 (8)	0.9328 (6)	0.5258 (4)	0.0295 (11)
C16	0.7091 (10)	0.9111 (8)	0.5549 (6)	0.0521 (18)
H16	0.8029	0.9818	0.5407	0.063*
C17	0.7528 (9)	0.7864 (8)	0.6044 (5)	0.0480 (17)
H17	0.8761	0.7760	0.6241	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0303 (4)	0.0238 (4)	0.0218 (4)	0.0077 (3)	0.0047 (3)	0.0055 (3)
O1	0.029 (2)	0.047 (2)	0.0290 (19)	0.0074 (17)	0.0032 (15)	−0.0030 (16)
O2	0.040 (2)	0.055 (3)	0.043 (2)	0.001 (2)	0.0053 (19)	0.000 (2)
O3	0.047 (3)	0.072 (3)	0.041 (2)	0.033 (2)	0.015 (2)	0.009 (2)
O4	0.050 (3)	0.050 (3)	0.060 (3)	0.002 (2)	0.001 (2)	0.008 (2)
O5	0.059 (3)	0.100 (5)	0.083 (4)	0.008 (3)	−0.011 (3)	0.036 (4)
O6	0.085 (4)	0.057 (3)	0.090 (4)	0.010 (3)	0.027 (3)	0.039 (3)
O7	0.033 (2)	0.035 (2)	0.064 (3)	0.0007 (18)	−0.007 (2)	0.014 (2)
N1	0.028 (2)	0.024 (2)	0.027 (2)	0.0036 (17)	0.0069 (17)	0.0044 (16)
N2	0.025 (2)	0.022 (2)	0.030 (2)	0.0051 (17)	0.0061 (17)	0.0044 (17)
N3	0.041 (3)	0.031 (2)	0.027 (2)	0.009 (2)	0.0051 (19)	0.0078 (18)
N4	0.033 (2)	0.040 (3)	0.026 (2)	0.010 (2)	0.0070 (18)	0.0111 (19)
N5	0.054 (3)	0.031 (3)	0.045 (3)	0.010 (2)	0.014 (2)	0.004 (2)
C1	0.032 (3)	0.026 (3)	0.042 (3)	0.004 (2)	0.006 (2)	0.007 (2)
C2	0.038 (3)	0.025 (3)	0.053 (4)	0.008 (2)	0.003 (3)	0.008 (2)
C3	0.033 (3)	0.037 (3)	0.050 (4)	0.006 (3)	0.002 (2)	0.023 (3)
C4	0.023 (2)	0.032 (3)	0.032 (3)	0.000 (2)	0.002 (2)	0.011 (2)
C5	0.032 (3)	0.047 (3)	0.025 (3)	−0.003 (3)	−0.003 (2)	0.014 (2)
C6	0.032 (3)	0.053 (4)	0.024 (3)	−0.006 (3)	0.003 (2)	−0.002 (2)
C7	0.025 (3)	0.037 (3)	0.032 (3)	−0.003 (2)	0.008 (2)	−0.001 (2)
C8	0.037 (3)	0.038 (3)	0.035 (3)	−0.002 (2)	0.009 (2)	−0.011 (2)
C9	0.038 (3)	0.027 (3)	0.051 (4)	0.004 (2)	0.015 (3)	−0.005 (2)

C10	0.038 (3)	0.023 (3)	0.037 (3)	0.007 (2)	0.007 (2)	0.002 (2)
C11	0.020 (2)	0.027 (3)	0.026 (2)	−0.0016 (19)	0.0067 (18)	0.0010 (19)
C12	0.020 (2)	0.028 (3)	0.028 (2)	0.004 (2)	0.0020 (18)	0.0089 (19)
C13	0.037 (3)	0.032 (3)	0.061 (4)	−0.005 (3)	−0.009 (3)	0.016 (3)
C14	0.035 (3)	0.034 (3)	0.047 (3)	−0.001 (2)	−0.010 (2)	0.014 (2)
C15	0.042 (3)	0.027 (3)	0.021 (2)	0.008 (2)	0.004 (2)	0.003 (2)
C16	0.040 (4)	0.054 (4)	0.073 (5)	0.016 (3)	0.026 (3)	0.038 (4)
C17	0.038 (3)	0.052 (4)	0.063 (4)	0.020 (3)	0.019 (3)	0.028 (3)

Geometric parameters (Å, °)

Cu1—N3	1.992 (5)	C3—H3A	0.9300
Cu1—O1	2.000 (4)	C4—C12	1.410 (7)
Cu1—N2	2.025 (4)	C4—C5	1.441 (8)
Cu1—N1	2.030 (4)	C5—C6	1.351 (9)
Cu1—O7	2.230 (4)	C5—H5A	0.9300
O1—N4	1.280 (6)	C6—C7	1.430 (8)
O2—N4	1.239 (7)	C6—H6A	0.9300
O3—N4	1.238 (6)	C7—C11	1.406 (7)
O4—N5	1.253 (8)	C7—C8	1.423 (8)
O5—N5	1.220 (8)	C8—C9	1.367 (9)
O6—N5	1.243 (8)	C8—H8	0.9300
O7—H1W	0.8200	C9—C10	1.400 (8)
O7—H2W	0.8251	C9—H9	0.9300
N1—C10	1.341 (7)	C10—H10	0.9300
N1—C11	1.359 (7)	C11—C12	1.429 (7)
N2—C1	1.336 (7)	C13—C14	1.372 (8)
N2—C12	1.355 (7)	C13—H13	0.9300
N3—C13	1.338 (8)	C14—C15	1.387 (9)
N3—C17	1.343 (9)	C14—H14	0.9300
C1—C2	1.386 (8)	C15—C16	1.388 (9)
C1—H1	0.9300	C15—C15^{i}	1.485 (10)
C2—C3	1.368 (10)	C16—C17	1.376 (9)
C2—H2A	0.9300	C16—H16	0.9300
C3—C4	1.412 (8)	C17—H17	0.9300
N3—Cu1—O1	93.23 (18)	C3—C4—C5	124.7 (5)
N3—Cu1—N2	172.57 (18)	C6—C5—C4	120.5 (5)
O1—Cu1—N2	91.76 (17)	C6—C5—H5A	119.8
N3—Cu1—N1	92.10 (18)	C4—C5—H5A	119.8
O1—Cu1—N1	161.67 (18)	C5—C6—C7	121.9 (5)
N2—Cu1—N1	81.49 (17)	C5—C6—H6A	119.1
N3—Cu1—O7	98.37 (19)	C7—C6—H6A	119.1
O1—Cu1—O7	92.06 (18)	C11—C7—C8	116.8 (5)
N2—Cu1—O7	86.94 (17)	C11—C7—C6	118.8 (5)
N1—Cu1—O7	104.49 (18)	C8—C7—C6	124.3 (5)
N4—O1—Cu1	111.1 (3)	C9—C8—C7	118.9 (5)
Cu1—O7—H1W	109.5	C9—C8—H8	120.5
Cu1—O7—H2W	136.7	C7—C8—H8	120.5
H1W—O7—H2W	113.0	C8—C9—C10	120.6 (5)

C10—N1—C11	118.0 (5)	C8—C9—H9	119.7
C10—N1—Cu1	129.5 (4)	C10—C9—H9	119.7
C11—N1—Cu1	112.5 (3)	N1—C10—C9	121.9 (5)
C1—N2—C12	118.7 (5)	N1—C10—H10	119.0
C1—N2—Cu1	128.6 (4)	C9—C10—H10	119.0
C12—N2—Cu1	112.6 (3)	N1—C11—C7	123.7 (5)
C13—N3—C17	117.3 (5)	N1—C11—C12	116.5 (4)
C13—N3—Cu1	121.4 (4)	C7—C11—C12	119.9 (5)
C17—N3—Cu1	120.7 (4)	N2—C12—C4	123.0 (5)
O3—N4—O2	123.2 (5)	N2—C12—C11	116.9 (4)
O3—N4—O1	118.3 (5)	C4—C12—C11	120.1 (5)
O2—N4—O1	118.5 (4)	N3—C13—C14	123.2 (6)
O5—N5—O6	120.3 (7)	N3—C13—H13	118.4
O5—N5—O4	120.5 (6)	C14—C13—H13	118.4
O6—N5—O4	119.2 (6)	C13—C14—C15	120.3 (6)
N2—C1—C2	122.0 (5)	C13—C14—H14	119.8
N2—C1—H1	119.0	C15—C14—H14	119.8
C2—C1—H1	119.0	C14—C15—C16	116.1 (5)
C3—C2—C1	120.1 (5)	C14—C15—C15^{i}	121.2 (7)
C3—C2—H2A	119.9	C16—C15—C15^{i}	122.7 (7)
C1—C2—H2A	119.9	C17—C16—C15	120.8 (6)
C2—C3—C4	119.8 (5)	C17—C16—H16	119.6
C2—C3—H3A	120.1	C15—C16—H16	119.6
C4—C3—H3A	120.1	N3—C17—C16	122.3 (6)
C12—C4—C3	116.5 (5)	N3—C17—H17	118.9
C12—C4—C5	118.8 (5)	C16—C17—H17	118.9
N3—Cu1—O1—N4	97.0 (4)	C5—C6—C7—C11	−0.7 (8)
N2—Cu1—O1—N4	−77.5 (4)	C5—C6—C7—C8	179.6 (5)
N1—Cu1—O1—N4	−9.7 (7)	C11—C7—C8—C9	0.3 (8)
O7—Cu1—O1—N4	−164.5 (4)	C6—C7—C8—C9	−180.0 (5)
N3—Cu1—N1—C10	4.4 (5)	C7—C8—C9—C10	0.2 (9)
O1—Cu1—N1—C10	111.3 (6)	C11—N1—C10—C9	0.6 (8)
N2—Cu1—N1—C10	−179.4 (5)	Cu1—N1—C10—C9	179.8 (4)
O7—Cu1—N1—C10	−94.8 (5)	C8—C9—C10—N1	−0.7 (9)
N3—Cu1—N1—C11	−176.3 (4)	C10—N1—C11—C7	0.1 (8)
O1—Cu1—N1—C11	−69.4 (7)	Cu1—N1—C11—C7	−179.3 (4)
N2—Cu1—N1—C11	−0.1 (3)	C10—N1—C11—C12	179.1 (4)
O7—Cu1—N1—C11	84.5 (4)	Cu1—N1—C11—C12	−0.3 (6)
N3—Cu1—N2—C1	−148.8 (13)	C8—C7—C11—N1	−0.5 (8)
O1—Cu1—N2—C1	−16.6 (5)	C6—C7—C11—N1	179.8 (5)
N1—Cu1—N2—C1	−179.5 (5)	C8—C7—C11—C12	−179.5 (5)
O7—Cu1—N2—C1	75.4 (5)	C6—C7—C11—C12	0.8 (8)
N3—Cu1—N2—C12	31.2 (15)	C1—N2—C12—C4	−0.3 (8)
O1—Cu1—N2—C12	163.4 (4)	Cu1—N2—C12—C4	179.8 (4)
N1—Cu1—N2—C12	0.5 (3)	C1—N2—C12—C11	179.1 (5)
O7—Cu1—N2—C12	−104.6 (4)	Cu1—N2—C12—C11	−0.9 (6)
O1—Cu1—N3—C13	115.9 (5)	C3—C4—C12—N2	−0.3 (8)
N2—Cu1—N3—C13	−112.0 (14)	C5—C4—C12—N2	179.9 (5)

N1—Cu1—N3—C13	−81.6 (5)	C3—C4—C12—C11	−179.7 (5)
O7—Cu1—N3—C13	23.4 (5)	C5—C4—C12—C11	0.5 (8)
O1—Cu1—N3—C17	−73.1 (5)	N1—C11—C12—N2	0.8 (7)
N2—Cu1—N3—C17	59.0 (15)	C7—C11—C12—N2	179.9 (4)
N1—Cu1—N3—C17	89.3 (5)	N1—C11—C12—C4	−179.8 (4)
O7—Cu1—N3—C17	−165.7 (5)	C7—C11—C12—C4	−0.7 (8)
Cu1—O1—N4—O3	172.2 (4)	C17—N3—C13—C14	0.6 (10)
Cu1—O1—N4—O2	−6.7 (6)	Cu1—N3—C13—C14	171.9 (5)
C12—N2—C1—C2	0.5 (8)	N3—C13—C14—C15	0.5 (11)
Cu1—N2—C1—C2	−179.5 (4)	C13—C14—C15—C16	−0.7 (9)
N2—C1—C2—C3	−0.1 (9)	C13—C14—C15—C15^{i}	−179.6 (7)
C1—C2—C3—C4	−0.5 (9)	C14—C15—C16—C17	−0.1 (10)
C2—C3—C4—C12	0.6 (8)	C15^{i}—C15—C16—C17	178.7 (7)
C2—C3—C4—C5	−179.5 (5)	C13—N3—C17—C16	−1.5 (11)
C12—C4—C5—C6	−0.4 (8)	Cu1—N3—C17—C16	−172.8 (6)
C3—C4—C5—C6	179.8 (6)	C15—C16—C17—N3	1.3 (12)
C4—C5—C6—C7	0.5 (9)		

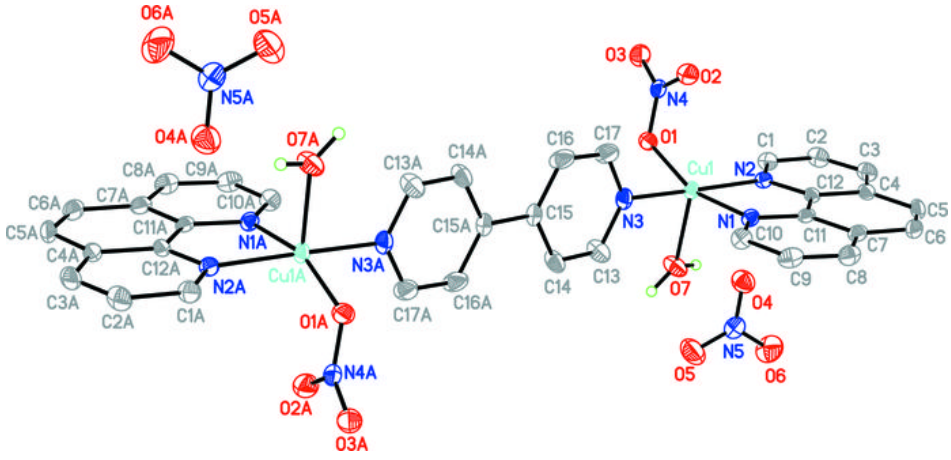
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H2W···O3^{ii}	0.83	2.07	2.886 (6)	172

Symmetry codes: (ii) *x*−1, *y*, *z*.

Fig. 1


O6A
O5A
N5A
O4A
O7A
C8A
C9A
C6A
C7A
C10A
C5A
C11A
N1A
C4A
C12A
N2A
C3A
C2A
C1A
Cu1A
O1A
N4A
O2A
O3A
N3A
C13A
C14A
C15A
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O3
O2
N4
O1
C16
C17
C15
N3
C14
C13
Cu1
N2
C1
C2
C3
C12
C4
N1
C10
C11
C7
C5
C6
C9
C8
O7
O4
N5
O5
O6

Fig. 2

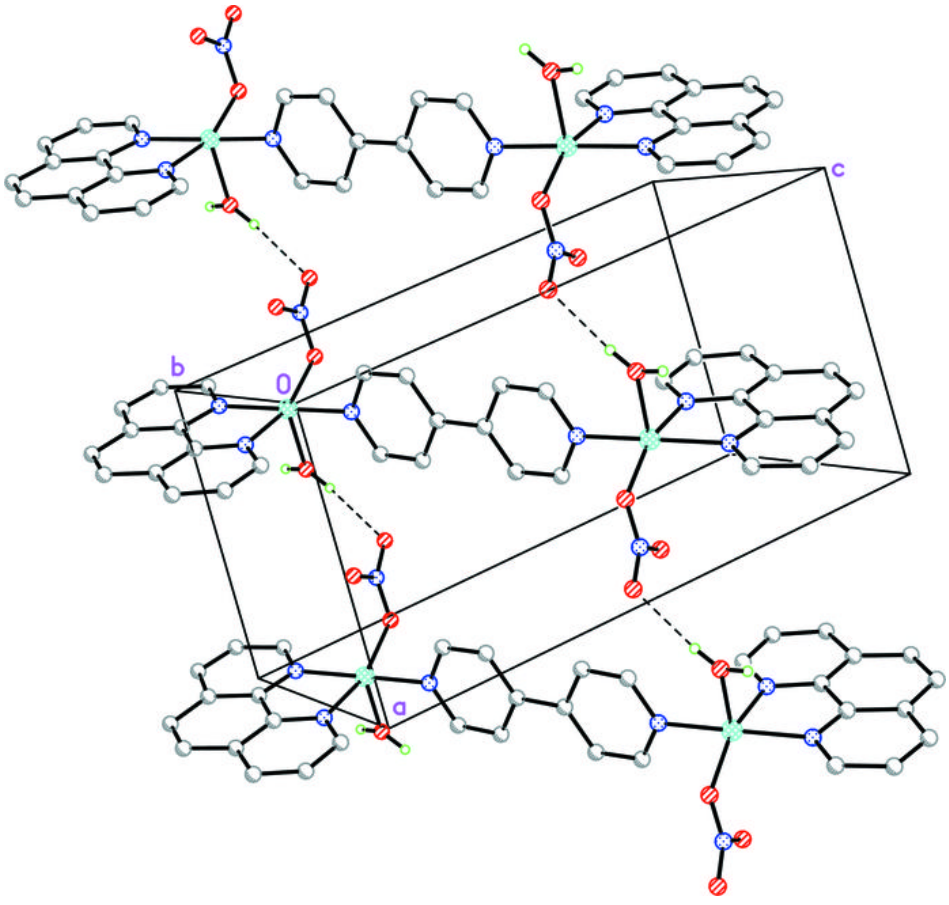

Fig. 3