

Retraction of articles by T. Liu *et al.*T. Liu,^{a*} Y.-X. Wang,^b Z.-W. Wang,^a Z.-P. Xie^{a,c} and J. Y. Zhu^d

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i>	Liu & Xie (2007a)	10.1107/S1600536807026852	EDUMAS
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807028255	EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNOF₂</i>	Liu Wang, Wang & Xie (2007a)	10.1107/S1600536807027195	ICSD 240891
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807031224	WIHJED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxy)acetato-κ²O:O']bis[(1,10-phenanthroline-κ²N,N')-(2-pyridyloxy)acetato-κO]neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')nickel(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')copper(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')cobalt(II)]-μ-acetamidato-κ²O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>Ethylenediammonium sulfate</i>	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
<i>Ethylenediammonium perchlorate</i>	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
<i>catena-Poly[[[nitrate-κO](1,10-phenanthroline-κ²N,N')manganese(II)]-μ-nitrate-κ²O:O']</i>	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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catena-Poly[[*(nitrate-κO)*(1,10-phenanthroline- κ^2N,N')copper(II)]- μ -acetamido- $\kappa^2O:N$]

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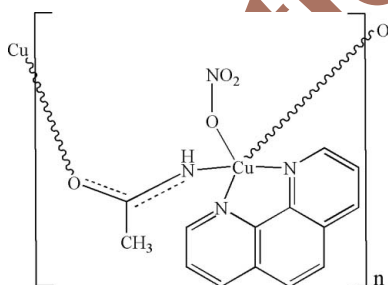
Received 11 November 2007; accepted 14 November 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.041; wR factor = 0.130; data-to-parameter ratio = 12.8.

In the crystal structure of the title compound, $[Cu(NO_3)(C_2H_4NO)(C_{12}H_8N_2)]_n$, the Cu^{II} atoms are linked by acetamidate ligands, forming a chain. Each Cu^{II} atom is five-coordinated by two N atoms of the 1,10-phenanthroline ligand, one nitrate O atom, and one N and one O atoms of acetamidate in a trigonal-bipyramidal geometry. In the crystal structure, the chains are linked by hydrogen bonds into a polymeric ribbon structure.

Related literature

For a related structure, see: Liu & Zhu (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(NO_3)(C_2H_4NO)(C_{12}H_8N_2)]_n$	$V = 1328.0 (6) \text{ \AA}^3$
$M_r = 363.82$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.680 (2) \text{ \AA}$	$\mu = 1.67 \text{ mm}^{-1}$
$b = 9.190 (3) \text{ \AA}$	$T = 273 (2) \text{ K}$
$c = 17.0137 (12) \text{ \AA}$	$0.41 \times 0.23 \times 0.22 \text{ mm}$
$\beta = 101.904 (2)^\circ$	

Data collection

Bruker APEXII area-detector diffractometer	8439 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	2679 independent reflections
$T_{\min} = 0.624$, $T_{\max} = 0.695$	2285 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$	209 parameters
$wR(F^2) = 0.130$	H-atom parameters constrained
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.80 \text{ e \AA}^{-3}$
2679 reflections	$\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.942 (2)	Cu1—N2	1.981 (2)
Cu1—O4 ⁱ	2.322 (2)	Cu1—N3	2.004 (2)
Cu1—N1	2.011 (3)		
O1—Cu1—O4 ⁱ	82.50 (9)	O4—Cu1—N2 ⁱ	125.47 (5)
O1—Cu1—N1	94.00 (11)	O4—Cu1—N3 ⁱ	141.73 (5)
O1—Cu1—N2	174.61 (10)	N1—Cu1—N2	82.97 (10)
O1—Cu1—N3	91.10 (10)	N1—Cu1—N3	165.98 (10)
O4—Cu1—N1 ⁱ	138.52 (4)	N2—Cu1—N3	92.87 (10)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O3 ⁱⁱ	0.93	2.50	3.319 (5)	147
C5—H5 \cdots O2 ⁱⁱⁱ	0.93	2.57	3.171 (5)	124

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); 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: AT2484).

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supplementary materials

Article retracted

Acta Cryst. (2007). E63, m3108 [doi:10.1107/S1600536807059077]

***catena*-Poly[[*(nitrate-κO)*(1,10-phenanthroline- κ^2N,N')copper(II)]- μ -acetamido- $\kappa^2O:N$]**

T. Liu and J. Y. Zhu

Comment

The crystal structure of *catena*-Poly[[*(nitrate-κO)*(1,10-phenanthroline- κ^2N,N')nickel(II)]- μ -acetamido- $\kappa^2O:N$], (II), has previously been reported (Liu & Zhu, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The title compound, $[\text{Cu}(\text{NO}_3)(\text{C}_2\text{H}_4\text{NO})(\text{C}_{12}\text{H}_8\text{N}_2)]_n$, which are linked by acetamidate ligands to form a chain. Each Cu^{II} atom is five-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand, one nitrate O atom, and one N and one O atoms of acetamidate within a bipyramidal coordination geometry (Table 1). The Cu—O and Cu—N bond are in the range [1.942 (2)–2.322 (2) Å] and [1.981 (2)–2.011 (3) Å], respectively (Table 1), as in (II).

In the crystal structure, no classic C—H \cdots O hydrogen bonds (Fig. 2 and Table 2) seem to be effective in the stabilization of the structure, resulting in the formation of a polymeric ribbon structure, as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Copper (II) nitrate hexahydrate (296.3 mg, 1 mmol), phen (180.2 mg, 1 mmol), acetamide (59.1 mg, 1 mmol) and distilled water (8 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small blue crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

The H atoms were positioned geometrically, with N—H = 0.86 Å (for NH), C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{N})$, where $x = 1.2$ for aromatic and NH H atoms and $x = 1.5$ for methyl H atoms.

Figures

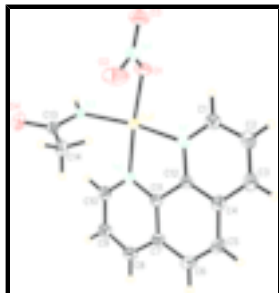


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2, y + 1/2, -z + 1/2$].

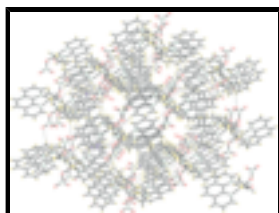


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[(nitrate- κ O)(1,10-phenanthroline- κ^2 N,N')copper(II)]- μ -acetamido- κ^2 O:N]

Crystal data

[Cu(NO₃)(C₂H₄NO)(C₁₂H₈N₂)]

$M_r = 363.82$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.680$ (2) Å

$b = 9.190$ (3) Å

$c = 17.0137$ (12) Å

$\beta = 101.904$ (2)°

$V = 1328.0$ (6) Å³

$Z = 4$

$F_{000} = 740$

$D_x = 1.820$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5781 reflections

$\theta = 2.3$ – 27.0 °

$\mu = 1.67$ mm⁻¹

$T = 273$ (2) K

Prism, blue

$0.41 \times 0.23 \times 0.22$ mm

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.624, T_{\max} = 0.695$

8439 measured reflections

2679 independent reflections

2285 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\text{max}} = 26.7$ °

$\theta_{\text{min}} = 2.5$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0915P)^2 + 0.5483P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
2679 reflections	$(\Delta/\sigma)_{\max} = 0.001$
209 parameters	$\Delta\rho_{\max} = 0.80 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.69 \text{ e } \text{\AA}^{-3}$
	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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.66503 (4)	0.92788 (4)	0.803179 (19)	0.03409 (17)
O1	0.5481 (3)	1.0048 (3)	0.70204 (13)	0.0470 (6)
O2	0.3259 (4)	0.9011 (4)	0.72922 (19)	0.0769 (10)
O3	0.3290 (3)	1.0282 (4)	0.62163 (17)	0.0623 (7)
O4	0.6206 (3)	0.5052 (3)	0.74795 (15)	0.0474 (6)
N1	0.6078 (3)	1.0941 (3)	0.86853 (16)	0.0356 (5)
N2	0.7951 (3)	0.8671 (3)	0.90775 (14)	0.0337 (5)
N3	0.6879 (3)	0.7347 (2)	0.75217 (13)	0.0281 (5)
H3A	0.7419	0.7239	0.7155	0.034*
N4	0.4025 (3)	0.9775 (3)	0.68377 (16)	0.0403 (6)
C1	0.5201 (4)	1.2102 (4)	0.8464 (2)	0.0441 (7)
H1	0.4813	1.2259	0.7919	0.053*
C2	0.4828 (4)	1.3112 (4)	0.9017 (2)	0.0486 (8)
H2	0.4225	1.3930	0.8840	0.058*
C3	0.5364 (4)	1.2873 (4)	0.9812 (2)	0.0474 (8)
H3	0.5094	1.3505	1.0189	0.057*
C4	0.6330 (4)	1.1664 (4)	1.00650 (19)	0.0386 (6)
C5	0.6977 (4)	1.1340 (4)	1.08823 (19)	0.0441 (7)

supplementary materials

H5	0.6726	1.1923	1.1285	0.053*
C6	0.7960 (4)	1.0188 (4)	1.10835 (19)	0.0443 (7)
H6	0.8381	1.0004	1.1622	0.053*
C7	0.8363 (4)	0.9251 (3)	1.04838 (18)	0.0364 (6)
C8	0.9427 (4)	0.8075 (4)	1.06354 (19)	0.0430 (7)
H8	0.9926	0.7856	1.1160	0.052*
C9	0.9725 (4)	0.7261 (4)	1.0016 (2)	0.0450 (7)
H9	1.0438	0.6494	1.0115	0.054*
C10	0.8963 (4)	0.7578 (3)	0.92368 (19)	0.0410 (7)
H10	0.9166	0.7012	0.8816	0.049*
C11	0.7675 (3)	0.9512 (3)	0.96854 (17)	0.0313 (6)
C12	0.6653 (3)	1.0726 (3)	0.94749 (18)	0.0319 (6)
C13	0.6164 (3)	0.6283 (3)	0.77790 (16)	0.0298 (5)
C14	0.5453 (4)	0.6522 (3)	0.83151 (19)	0.0384 (7)
H14A	0.4521	0.5932	0.8235	0.058*
H14B	0.5163	0.7531	0.8306	0.058*
H14C	0.6115	0.6292	0.8825	0.058*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0402 (3)	0.0328 (2)	0.0277 (2)	0.00245 (13)	0.00354 (16)	0.00106 (13)
O1	0.0436 (12)	0.0556 (15)	0.0381 (11)	-0.0051 (11)	-0.0004 (9)	0.0129 (11)
O2	0.0571 (16)	0.119 (3)	0.0546 (17)	-0.0216 (17)	0.0123 (14)	0.0260 (18)
O3	0.0540 (14)	0.0697 (17)	0.0541 (16)	-0.0053 (13)	-0.0104 (12)	0.0154 (14)
O4	0.0456 (12)	0.0372 (12)	0.0596 (14)	-0.0041 (10)	0.0115 (11)	-0.0154 (11)
N1	0.0387 (12)	0.0327 (12)	0.0354 (13)	0.0003 (10)	0.0078 (10)	0.0046 (10)
N2	0.0380 (12)	0.0302 (12)	0.0322 (11)	0.0023 (10)	0.0057 (10)	-0.0009 (10)
N3	0.0357 (11)	0.0277 (11)	0.0226 (10)	-0.0040 (9)	0.0097 (9)	-0.0034 (8)
N4	0.0415 (13)	0.0381 (13)	0.0384 (13)	0.0003 (11)	0.0018 (11)	0.0009 (12)
C1	0.0443 (16)	0.0401 (17)	0.0459 (17)	0.0061 (14)	0.0048 (14)	0.0030 (14)
C2	0.0476 (17)	0.0393 (17)	0.059 (2)	0.0113 (14)	0.0112 (15)	0.0014 (15)
C3	0.0483 (17)	0.0381 (17)	0.059 (2)	0.0077 (14)	0.0185 (15)	-0.0056 (15)
C4	0.0392 (14)	0.0383 (15)	0.0408 (15)	-0.0039 (12)	0.0141 (13)	-0.0049 (13)
C5	0.0510 (17)	0.0488 (18)	0.0362 (15)	-0.0016 (15)	0.0177 (14)	-0.0078 (14)
C6	0.0494 (17)	0.0536 (19)	0.0303 (14)	-0.0008 (15)	0.0096 (13)	-0.0018 (14)
C7	0.0408 (15)	0.0374 (16)	0.0311 (14)	-0.0032 (12)	0.0079 (12)	0.0029 (11)
C8	0.0479 (16)	0.0412 (16)	0.0365 (15)	0.0008 (14)	0.0009 (13)	0.0059 (13)
C9	0.0485 (17)	0.0356 (16)	0.0464 (17)	0.0089 (13)	-0.0007 (14)	0.0036 (14)
C10	0.0475 (16)	0.0332 (15)	0.0406 (16)	0.0062 (13)	0.0050 (13)	-0.0037 (12)
C11	0.0348 (13)	0.0288 (13)	0.0301 (13)	-0.0028 (11)	0.0061 (11)	0.0005 (10)
C12	0.0325 (13)	0.0292 (14)	0.0344 (14)	-0.0030 (10)	0.0081 (12)	0.0011 (11)
C13	0.0297 (12)	0.0270 (12)	0.0308 (13)	0.0024 (10)	0.0019 (11)	-0.0028 (10)
C14	0.0509 (16)	0.0299 (14)	0.0446 (15)	-0.0041 (12)	0.0337 (14)	-0.0055 (12)

Geometric parameters (\AA , $^\circ$)

Cu1—O1	1.942 (2)	C3—C4	1.405 (5)
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Cu1—O4 ⁱ	2.322 (2)	C3—H3	0.9300
Cu1—N1	2.011 (3)	C4—C12	1.395 (4)
Cu1—N2	1.981 (2)	C4—C5	1.420 (5)
Cu1—N3	2.004 (2)	C5—C6	1.359 (5)
O1—N4	1.263 (4)	C5—H5	0.9300
O2—N4	1.321 (4)	C6—C7	1.432 (4)
O3—N4	1.210 (4)	C6—H6	0.9300
O4—C13	1.244 (4)	C7—C11	1.387 (4)
O4—Cu1 ⁱⁱ	2.322 (2)	C7—C8	1.411 (5)
N1—C1	1.320 (4)	C8—C9	1.360 (5)
N1—C12	1.347 (4)	C8—H8	0.9300
N2—C10	1.325 (4)	C9—C10	1.385 (5)
N2—C11	1.352 (4)	C9—H9	0.9300
N3—C13	1.283 (4)	C10—H10	0.9300
N3—H3A	0.8600	C11—C12	1.425 (4)
C1—C2	1.406 (5)	C13—C14	1.222 (4)
C1—H1	0.9300	C14—H14A	0.9600
C2—C3	1.355 (5)	C14—H14B	0.9600
C2—H2	0.9300	C14—H14C	0.9600
O1—Cu1—O4 ⁱ	82.50 (9)	C3—C4—C5	123.8 (3)
O1—Cu1—N1	94.00 (11)	C6—C5—C4	120.8 (3)
O1—Cu1—N2	174.61 (10)	C6—C5—H5	119.6
O1—Cu1—N3	91.10 (10)	C4—C5—H5	119.6
O4—Cu1—N1 ⁱ	138.52 (4)	C5—C6—C7	121.4 (3)
O4—Cu1—N2 ⁱ	125.47 (5)	C5—C6—H6	119.3
O4—Cu1—N3 ⁱ	141.73 (5)	C7—C6—H6	119.3
N1—Cu1—N2	82.97 (10)	C11—C7—C8	116.4 (3)
N1—Cu1—N3	165.98 (10)	C11—C7—C6	118.4 (3)
N2—Cu1—N3	92.87 (10)	C8—C7—C6	125.2 (3)
N4—O1—Cu1	117.34 (19)	C9—C8—C7	120.1 (3)
C13—O4—Cu1 ⁱⁱ	121.63 (19)	C9—C8—H8	119.9
C1—N1—C12	118.4 (3)	C7—C8—H8	119.9
C1—N1—Cu1	130.6 (2)	C8—C9—C10	119.8 (3)
C12—N1—Cu1	110.93 (19)	C8—C9—H9	120.1
C10—N2—C11	119.5 (3)	C10—C9—H9	120.1
C10—N2—Cu1	128.9 (2)	N2—C10—C9	121.4 (3)
C11—N2—Cu1	111.59 (19)	N2—C10—H10	119.3
C13—N3—Cu1	115.46 (18)	C9—C10—H10	119.3
C13—N3—H3A	122.3	N2—C11—C7	122.9 (3)
Cu1—N3—H3A	122.3	N2—C11—C12	117.1 (3)
O3—N4—O2	118.6 (3)	C7—C11—C12	120.1 (3)
O3—N4—O1	117.3 (3)	N1—C12—C4	122.6 (3)
O2—N4—O1	124.1 (3)	N1—C12—C11	116.6 (3)
N1—C1—C2	122.9 (3)	C4—C12—C11	120.7 (3)
N1—C1—H1	118.6	C14—C13—O4	122.1 (3)
C2—C1—H1	118.6	C14—C13—N3	118.1 (3)
C3—C2—C1	118.8 (3)	O4—C13—N3	119.8 (3)

supplementary materials

C3—C2—H2	120.6	C13—C14—H14A	109.5
C1—C2—H2	120.6	C13—C14—H14B	109.5
C2—C3—C4	119.6 (3)	H14A—C14—H14B	109.5
C2—C3—H3	120.2	C13—C14—H14C	109.5
C4—C3—H3	120.2	H14A—C14—H14C	109.5
C12—C4—C3	117.7 (3)	H14B—C14—H14C	109.5
C12—C4—C5	118.5 (3)		

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

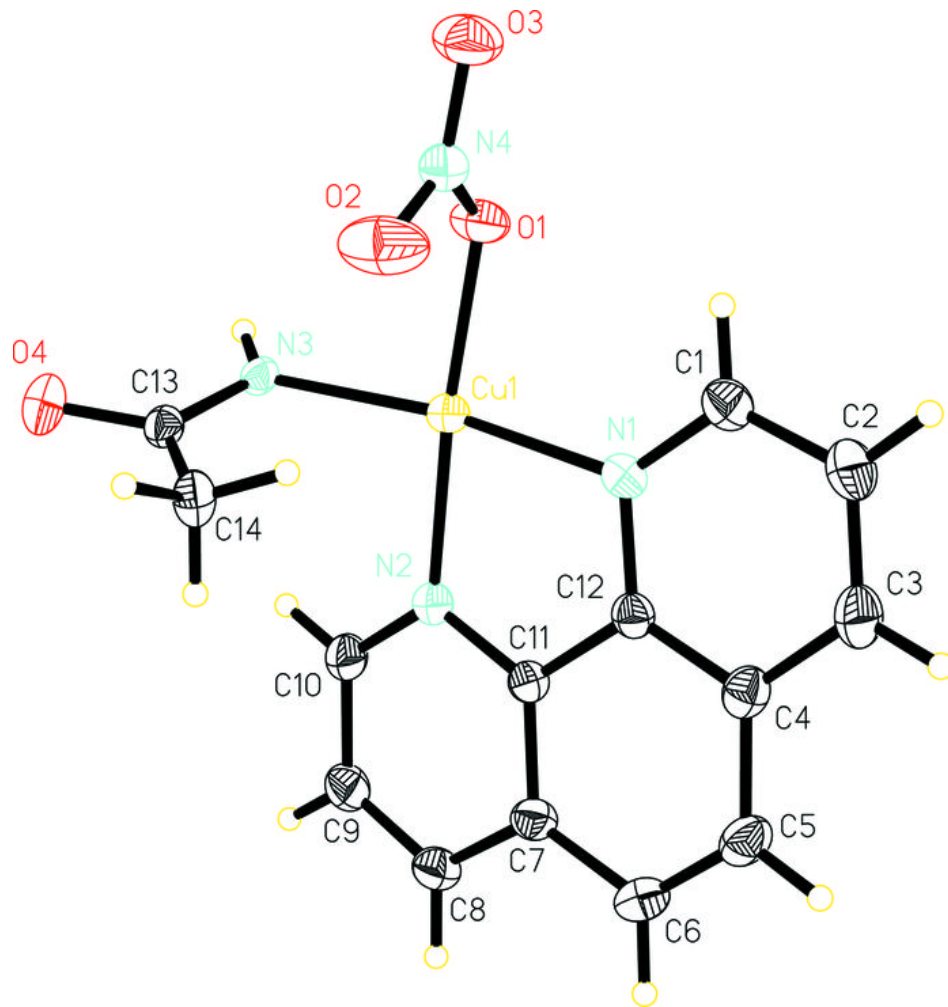
Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O3 ⁱⁱⁱ	0.93	2.50	3.319 (5)	147
C5—H5 \cdots O2 ^{iv}	0.93	2.57	3.171 (5)	124

Symmetry codes: (iii) $-x+1/2, y+1/2, -z+3/2$; (iv) $-x+1, -y+2, -z+2$.

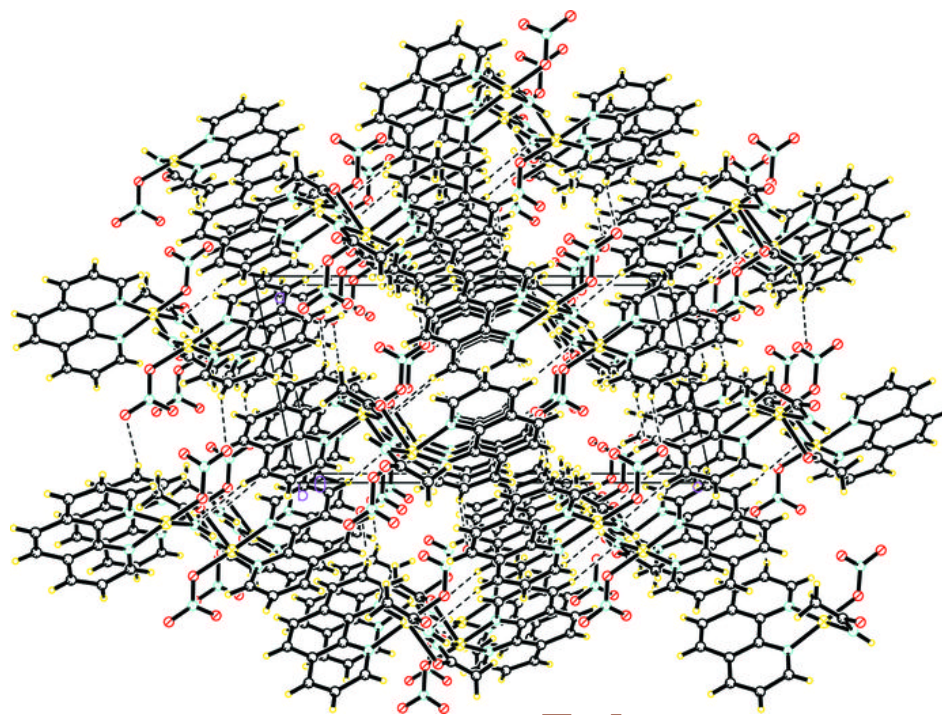
Article retracted

Fig. 1



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Fig. 2



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