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Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *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
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*d*)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*e*)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*f*)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*g*)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*a*)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*h*)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*b*)	10.1107/S1600536807056498	XIRJEO
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*i*)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-κ^2N,N')-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate

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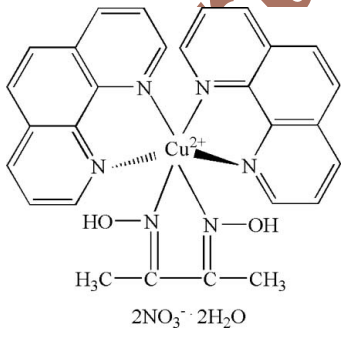
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.143; data-to-parameter ratio = 14.3.

In the cation of the title compound, $[Cu(C_{12}H_8N_2)_2(C_4H_8N_2O_2)](NO_3)_2{\cdot}2H_2O$, the Cu atom has a distorted octahedral coordination formed by six N atoms from one dimethylglyoxime and two 1,10-phenanthroline ligands. In the crystal structure, components are linked into a three-dimensional framework by O—H···O and C—H···O hydrogen bonds and π–π stacking interactions [centroid–centroid distance 3.592 (4) Å].

Related literature

For related structures, see: Zhong *et al.* (2007*a*,*b*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(C_{12}H_8N_2)_2(C_4H_8N_2O_2)](NO_3)_2{\cdot}2H_2O$
M_r = 700.13
Monoclinic, $P2_1/c$
a = 13.8102 (12) Å
b = 11.9816 (11) Å
c = 18.4018 (14) Å
β = 96.204 (2)°
V = 3027.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 273 (2) K
0.31 × 0.22 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.794, T_{max} = 0.867
20447 measured reflections
6368 independent reflections
3102 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.143
S = 1.01
6368 reflections
444 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.919 (3)	Cu1—N4	1.937 (3)
Cu1—N2	1.992 (3)	Cu1—N5	1.899 (3)
Cu1—N3	1.950 (3)	Cu1—N6	1.885 (3)
N1—Cu1—N2	84.03 (14)	N2—Cu1—N6	95.58 (13)
N1—Cu1—N3	92.68 (13)	N3—Cu1—N4	83.61 (13)
N1—Cu1—N4	175.34 (13)	N3—Cu1—N5	93.78 (14)
N1—Cu1—N5	92.83 (13)	N3—Cu1—N6	174.62 (13)
N1—Cu1—N6	90.22 (12)	N4—Cu1—N5	90.22 (12)
N2—Cu1—N3	89.24 (12)	N4—Cu1—N6	93.71 (12)
N2—Cu1—N4	93.09 (13)	N5—Cu1—N6	81.54 (14)
N2—Cu1—N5	175.75 (13)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C27—H27A···O2	0.96	2.40	2.806 (5)	105
C27—H27B···O8	0.96	2.50	3.225 (10)	132
C28—H28C···O1	0.96	2.41	2.769 (5)	102
O1—H1A···N2	0.82	2.84	3.006 (4)	94
C1—H1···N5	0.93	2.49	2.972 (5)	112
C13—H13···N1	0.93	2.57	3.027 (5)	111
C22—H22···N6	0.93	2.57	3.033 (5)	111
O1—H1A···O5^{i}	0.82	2.39	2.999 (4)	131
O1—H1A···O6^{i}	0.82	1.90	2.704 (4)	167
C3—H3···O5^{ii}	0.93	2.51	3.354 (5)	152
C5—H5···O1^{iii}	0.93	2.52	3.331 (5)	145
C18—H18···O2^{iv}	0.93	2.38	3.233 (5)	152
C22—H22···O6^{v}	0.93	2.53	3.279 (5)	137
C15—H15···O5^{vi}	0.93	2.54	3.357 (6)	147
C27—H27C···O7^{v}	0.96	2.59	3.356 (6)	137
C28—H28A···O7^{v}	0.96	2.63	3.316 (6)	128

Symmetry codes: (i) $x, y+1, z-1$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y+2, -z$; (iv) $-x+2, -y+1, -z$; (v) $-x+2, -y+1, -z+1$; (vi) $x, y, z-1$.

Data collection: *SMART* (Siemens, 1996); 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: HK2390).

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supplementary materials

Acta Cryst. (2007). E**63**, m3160-m3161 [**doi:10.1107/S1600536807061193**]

(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate

H. Zhong, X.-M. Yang, C.-J. Luo and M.-L. Li

Comment

The crystal structure of (dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline- κ^2N,N')nickel(II)dinitrate dihydrate, (II), (Zhong *et al.*, 2007*a*) and (dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II)dinitrate dihydrate, (III), (Zhong *et al.*, 2007*b*) have previously been reported. 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 those of (II) and (III). 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 six N atoms from one dimethylglyoxime and two 1,10-phenanthroline (phen) ligands are coordinated to the Cu atom in a distorted octahedral arrangement (Table 1). The dimethylglyoxime and two phen ligands are each planar, and the phen ligands are nearly perpendicular to each other, the dihedral angle of 86.04 (3)° being the same as in (II) and (III).

In the crystal structure, the molecules are linked into a three-dimensional framework by O—H···O and C—H···O hydrogen bonds (Table 2). There are π-π stacking interactions between adjacent phen ligands with a centroid-centroid distance of 3.592 (4) Å (symmetry code: $1-x, 2-y, 1-z$); this compares with 3.602 (3) and 3.5997 (7) Å in (II) and (III), respectively. These π-π stacking interactions and hydrogen bonds (Table 2) lead to a supramolecular network structure (Fig. 2), as in (II) and (III).

Compounds (I), (II) and (III) are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Copper (II) nitrate pentahydrate (295.5 mg, 1 mmol), phen (180.2 mg, 1 mmol), dimethyl glyoxime (116.2 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

H atoms (for H_2O) were located in a difference synthesis and refined isotropically [O—H = 0.811 (18)–0.880 (18) Å and U_{iso}(H) = 0.460 (7)–0.585 (10) Å^2]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*O*), where x = 1.2 for aromatic H, and x = 1.5 for all other H atoms.

Figures

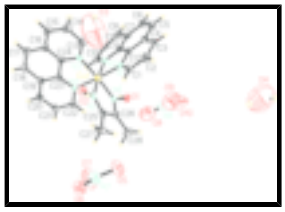

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

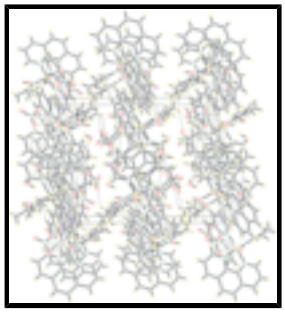

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

(Dimethylglyoxime-κ^2*N*,*N*')bis(1,10-phenanthroline-κ^2*N*,*N*')copper(II) dinitrate dihydrate

Crystal data

$[Cu(C_{12}H_8N_2)_2(C_4H_8N_2O_2)](NO_3)_2\cdot 2H_2O$	F_{000} = 1444
M_r = 700.13	D_x = 1.536 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6015 reflections
a = 13.8102 (12) Å	θ = 2.1–25.0°
b = 11.9816 (11) Å	μ = 0.79 mm^{-1}
c = 18.4018 (14) Å	T = 273 (2) K
β = 96.204 (2)°	Prism, blue
V = 3027.1 (4) Å^3	0.31 × 0.22 × 0.19 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	6368 independent reflections
Radiation source: fine-focus sealed tube	3102 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 273(2) K	θ_{max} = 27.0°
φ and ω scans	θ_{min} = 2.0°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→17
T_{min} = 0.794, T_{max} = 0.867	k = −15→15
20447 measured reflections	l = −22→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.143$	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.003$
6368 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
444 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
13 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.77578 (3)	0.75557 (4)	0.03822 (3)	0.04339 (18)
O1	0.7959 (2)	0.9963 (2)	0.04784 (15)	0.0477 (7)
H1A	0.8164	1.0029	0.0079	0.072*
O2	0.8348 (2)	0.6027 (2)	0.14811 (16)	0.0540 (8)
H2A	0.8278	0.5985	0.1917	0.081*
O3	0.5555 (11)	0.4274 (14)	0.1403 (10)	0.508 (12)
H3A	0.5564 (19)	0.4911 (16)	0.1554 (17)	0.460 (7)*
H3B	0.502 (2)	0.397 (2)	0.119 (2)	0.511 (11)*
O4	0.3053 (16)	0.665 (2)	0.7978 (7)	0.580 (18)
H4A	0.272 (2)	0.670 (3)	0.8355 (17)	0.585 (10)*
H4B	0.346 (9)	0.612 (11)	0.811 (6)	0.58 (8)*
O5	0.7740 (2)	0.1305 (3)	0.9095 (2)	0.0815 (11)
O6	0.8929 (2)	0.0157 (3)	0.92842 (18)	0.0651 (9)
O7	0.8888 (3)	0.1350 (4)	0.8436 (3)	0.1145 (16)
O8	0.7391 (5)	0.8777 (6)	0.2887 (3)	0.164 (2)
O9	0.6155 (6)	0.8839 (6)	0.3362 (4)	0.191 (3)

O10	0.6400 (7)	1.0072 (6)	0.2626 (5)	0.329 (9)
N1	0.6536 (2)	0.7798 (2)	0.07648 (19)	0.0366 (8)
N2	0.7070 (2)	0.8183 (2)	−0.05350 (18)	0.0356 (8)
N3	0.7386 (2)	0.6061 (2)	0.00380 (18)	0.0395 (8)
N4	0.8933 (2)	0.7246 (2)	−0.00692 (17)	0.0330 (7)
N5	0.8370 (2)	0.7042 (3)	0.12949 (18)	0.0383 (8)
N6	0.8219 (2)	0.8938 (2)	0.07669 (18)	0.0343 (8)
N7	0.8516 (3)	0.0927 (3)	0.8921 (2)	0.0582 (10)
N8	0.6663 (5)	0.9304 (8)	0.2888 (5)	0.132 (3)
C1	0.6306 (3)	0.7623 (3)	0.1435 (2)	0.0485 (11)
H1	0.6785	0.7366	0.1790	0.058*
C2	0.5363 (3)	0.7812 (4)	0.1628 (3)	0.0607 (13)
H2	0.5224	0.7687	0.2104	0.073*
C3	0.4661 (3)	0.8177 (4)	0.1117 (3)	0.0546 (12)
H3	0.4033	0.8292	0.1240	0.066*
C4	0.4875 (3)	0.8382 (3)	0.0407 (3)	0.0449 (11)
C5	0.4208 (3)	0.8803 (4)	−0.0175 (3)	0.0615 (14)
H5	0.3566	0.8935	−0.0090	0.074*
C6	0.4482 (3)	0.9016 (4)	−0.0850 (3)	0.0611 (13)
H6	0.4023	0.9284	−0.1216	0.073*
C7	0.5458 (3)	0.8837 (3)	−0.1006 (3)	0.0479 (11)
C8	0.5806 (4)	0.9062 (3)	−0.1657 (3)	0.0579 (13)
H8	0.5389	0.9352	−0.2042	0.069*
C9	0.6759 (4)	0.8867 (3)	−0.1750 (3)	0.0583 (13)
H9	0.6999	0.9039	−0.2189	0.070*
C10	0.7368 (3)	0.8403 (3)	−0.1170 (2)	0.0449 (11)
H10	0.8011	0.8245	−0.1239	0.054*
C11	0.6125 (3)	0.8403 (3)	−0.0440 (2)	0.0402 (10)
C12	0.5832 (3)	0.8181 (3)	0.0254 (2)	0.0367 (9)
C13	0.6603 (3)	0.5464 (4)	0.0144 (3)	0.0557 (12)
H13	0.6143	0.5757	0.0424	0.067*
C14	0.6465 (3)	0.4411 (4)	−0.0158 (3)	0.0693 (15)
H14	0.5902	0.4017	−0.0087	0.083*
C15	0.7126 (4)	0.3944 (4)	−0.0551 (3)	0.0630 (14)
H15	0.7025	0.3232	−0.0746	0.076*
C16	0.7965 (3)	0.4544 (3)	−0.0661 (2)	0.0454 (11)
C17	0.8721 (3)	0.4153 (4)	−0.1060 (2)	0.0518 (12)
H17	0.8656	0.3463	−0.1291	0.062*
C18	0.9519 (3)	0.4752 (4)	−0.1111 (2)	0.0518 (12)
H18	1.0005	0.4466	−0.1371	0.062*
C19	0.9649 (3)	0.5826 (3)	−0.0776 (2)	0.0413 (10)
C20	1.0478 (3)	0.6513 (4)	−0.0800 (2)	0.0485 (11)
H20	1.0997	0.6279	−0.1044	0.058*
C21	1.0503 (3)	0.7505 (4)	−0.0466 (2)	0.0483 (10)
H21	1.1046	0.7961	−0.0477	0.058*
C22	0.9718 (3)	0.7865 (3)	−0.0099 (2)	0.0425 (10)
H22	0.9753	0.8559	0.0128	0.051*
C23	0.8911 (3)	0.6242 (3)	−0.0406 (2)	0.0360 (9)
C24	0.8063 (3)	0.5595 (3)	−0.0345 (2)	0.0360 (9)

C25	0.8806 (3)	0.7818 (3)	0.1719 (2)	0.0404 (10)
C26	0.8678 (3)	0.8924 (3)	0.1411 (2)	0.0424 (10)
C27	0.9330 (3)	0.7564 (4)	0.2448 (2)	0.0625 (13)
H27A	0.9257	0.6786	0.2556	0.094*
H27B	0.9063	0.8005	0.2814	0.094*
H27C	1.0008	0.7736	0.2446	0.094*
C28	0.9050 (3)	0.9928 (4)	0.1832 (3)	0.0655 (14)
H28A	0.9691	0.9777	0.2069	0.098*
H28B	0.8622	1.0104	0.2193	0.098*
H28C	0.9078	1.0548	0.1505	0.098*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0398 (3)	0.0422 (3)	0.0474 (3)	0.0021 (2)	0.0012 (2)	−0.0023 (3)
O1	0.0571 (18)	0.0342 (15)	0.051 (2)	0.0071 (13)	0.0022 (15)	−0.0008 (14)
O2	0.0619 (19)	0.0469 (19)	0.052 (2)	0.0035 (14)	0.0016 (16)	0.0154 (15)
O3	0.43 (2)	0.68 (3)	0.48 (2)	0.07 (2)	0.37 (2)	0.14 (2)
O4	0.47 (3)	0.92 (5)	0.33 (2)	0.09 (3)	−0.065 (17)	−0.35 (2)
O5	0.059 (2)	0.082 (3)	0.105 (3)	0.0161 (19)	0.017 (2)	0.008 (2)
O6	0.064 (2)	0.0503 (19)	0.080 (3)	0.0093 (16)	0.0021 (18)	0.0147 (18)
O7	0.107 (3)	0.120 (4)	0.125 (4)	0.032 (3)	0.055 (3)	0.059 (3)
O8	0.158 (5)	0.171 (6)	0.158 (6)	−0.022 (5)	−0.004 (5)	−0.018 (4)
O9	0.243 (9)	0.178 (6)	0.150 (7)	−0.005 (6)	0.007 (6)	−0.012 (5)
O10	0.433 (15)	0.123 (5)	0.356 (13)	−0.061 (6)	−0.305 (11)	0.106 (6)
N1	0.0351 (18)	0.0340 (18)	0.040 (2)	0.0010 (13)	−0.0003 (15)	0.0014 (15)
N2	0.038 (2)	0.0291 (18)	0.039 (2)	0.0021 (14)	−0.0014 (15)	−0.0052 (15)
N3	0.0348 (18)	0.0357 (18)	0.047 (2)	0.0007 (15)	0.0007 (16)	0.0009 (16)
N4	0.0282 (17)	0.0293 (18)	0.040 (2)	0.0027 (13)	−0.0033 (14)	−0.0009 (14)
N5	0.0318 (18)	0.0396 (19)	0.044 (2)	0.0048 (15)	0.0046 (15)	0.0028 (17)
N6	0.0318 (17)	0.0326 (18)	0.038 (2)	0.0025 (14)	0.0020 (15)	−0.0013 (15)
N7	0.052 (3)	0.056 (3)	0.068 (3)	−0.008 (2)	0.010 (2)	0.009 (2)
N8	0.089 (5)	0.176 (9)	0.123 (7)	−0.005 (5)	−0.021 (5)	−0.079 (7)
C1	0.038 (2)	0.057 (3)	0.050 (3)	0.009 (2)	0.0039 (19)	0.004 (2)
C2	0.057 (3)	0.069 (3)	0.059 (3)	0.000 (2)	0.021 (3)	−0.001 (3)
C3	0.033 (2)	0.054 (3)	0.078 (4)	0.000 (2)	0.013 (2)	−0.016 (3)
C4	0.035 (2)	0.033 (2)	0.066 (3)	0.0021 (18)	−0.002 (2)	−0.006 (2)
C5	0.033 (2)	0.051 (3)	0.098 (5)	0.007 (2)	−0.005 (3)	−0.007 (3)
C6	0.052 (3)	0.048 (3)	0.077 (4)	0.010 (2)	−0.020 (3)	−0.004 (3)
C7	0.050 (3)	0.036 (2)	0.053 (3)	0.003 (2)	−0.015 (2)	−0.005 (2)
C8	0.072 (3)	0.046 (3)	0.051 (4)	0.008 (2)	−0.018 (3)	0.001 (2)
C9	0.091 (4)	0.042 (3)	0.039 (3)	−0.002 (2)	−0.007 (3)	0.000 (2)
C10	0.056 (3)	0.040 (2)	0.038 (3)	0.001 (2)	0.003 (2)	−0.006 (2)
C11	0.043 (3)	0.026 (2)	0.048 (3)	0.0012 (17)	−0.010 (2)	−0.0047 (19)
C12	0.035 (2)	0.028 (2)	0.046 (3)	−0.0028 (17)	0.0000 (19)	−0.0025 (19)
C13	0.042 (3)	0.042 (3)	0.084 (4)	−0.003 (2)	0.009 (2)	−0.007 (2)
C14	0.053 (3)	0.045 (3)	0.109 (5)	−0.017 (2)	0.004 (3)	−0.008 (3)
C15	0.066 (3)	0.035 (2)	0.085 (4)	−0.006 (2)	−0.005 (3)	−0.011 (2)

C16	0.051 (3)	0.034 (2)	0.048 (3)	0.006 (2)	−0.010 (2)	−0.001 (2)
C17	0.070 (3)	0.039 (3)	0.044 (3)	0.011 (2)	−0.005 (2)	−0.005 (2)
C18	0.069 (3)	0.050 (3)	0.035 (3)	0.029 (2)	0.003 (2)	−0.005 (2)
C19	0.046 (3)	0.045 (2)	0.032 (3)	0.013 (2)	−0.0020 (19)	0.002 (2)
C20	0.042 (3)	0.065 (3)	0.040 (3)	0.011 (2)	0.008 (2)	0.002 (2)
C21	0.036 (2)	0.057 (3)	0.052 (3)	−0.003 (2)	0.0042 (19)	0.004 (3)
C22	0.042 (3)	0.037 (2)	0.047 (3)	0.0025 (18)	−0.001 (2)	−0.0027 (19)
C23	0.037 (2)	0.038 (2)	0.032 (2)	0.0078 (18)	−0.0040 (18)	0.0026 (19)
C24	0.041 (2)	0.031 (2)	0.034 (3)	0.0058 (18)	−0.0033 (18)	−0.0009 (18)
C25	0.036 (2)	0.051 (3)	0.034 (3)	0.0035 (19)	0.0040 (18)	0.003 (2)
C26	0.038 (2)	0.042 (2)	0.047 (3)	−0.0004 (19)	0.007 (2)	−0.013 (2)
C27	0.058 (3)	0.078 (3)	0.048 (3)	−0.003 (3)	−0.011 (2)	0.006 (3)
C28	0.072 (3)	0.057 (3)	0.065 (4)	−0.006 (2)	−0.007 (3)	−0.022 (3)

Geometric parameters (Å, °)

Cu1—N1	1.919 (3)	C8—C9	1.365 (6)
Cu1—N2	1.992 (3)	C8—H8	0.9300
Cu1—N3	1.950 (3)	C9—C10	1.401 (6)
Cu1—N4	1.937 (3)	C9—H9	0.9300
Cu1—N5	1.899 (3)	C10—H10	0.9300
Cu1—N6	1.885 (3)	C11—C12	1.406 (5)
O1—N6	1.370 (4)	C13—C14	1.382 (6)
O1—H1A	0.8200	C13—H13	0.9300
O2—N5	1.265 (4)	C14—C15	1.346 (6)
O2—H2A	0.8200	C14—H14	0.9300
O5—N7	1.236 (4)	C15—C16	1.398 (6)
O6—N7	1.242 (4)	C15—H15	0.9300
O7—N7	1.190 (5)	C16—C24	1.386 (5)
O8—N8	1.188 (7)	C16—C17	1.419 (6)
O9—N8	1.303 (9)	C17—C18	1.326 (6)
O10—N8	1.083 (9)	C17—H17	0.9300
N1—C1	1.322 (5)	C18—C19	1.430 (5)
N1—C12	1.358 (5)	C18—H18	0.9300
N2—C10	1.307 (5)	C19—C23	1.379 (5)
N2—C11	1.360 (5)	C19—C20	1.415 (5)
N3—C13	1.328 (5)	C20—C21	1.336 (5)
N3—C24	1.352 (5)	C20—H20	0.9300
N4—C22	1.320 (5)	C21—C22	1.405 (5)
N4—C23	1.353 (4)	C21—H21	0.9300
N5—C25	1.317 (5)	C22—H22	0.9300
N6—C26	1.283 (5)	C23—C24	1.419 (5)
C1—C2	1.405 (5)	C25—C26	1.445 (5)
C1—H1	0.9300	C25—C27	1.485 (5)
C2—C3	1.347 (6)	C26—C28	1.492 (5)
C2—H2	0.9300	C27—H27A	0.9600
C3—C4	1.393 (6)	C27—H27B	0.9600
C3—H3	0.9300	C27—H27C	0.9600
C4—C12	1.401 (5)	C28—H28A	0.9600

C4—C5	1.426 (6)	C28—H28B	0.9600
C5—C6	1.362 (6)	C28—H28C	0.9600
C5—H5	0.9300	O3—H3A	0.811 (18)
C6—C7	1.425 (6)	O3—H3B	0.880 (18)
C6—H6	0.9300	O4—H4B	0.87 (13)
C7—C8	1.365 (6)	O4—H4A	0.876 (19)
C7—C11	1.413 (5)		
N1—Cu1—N2	84.03 (14)	C10—C9—H9	120.6
N1—Cu1—N3	92.68 (13)	N2—C10—C9	122.6 (4)
N1—Cu1—N4	175.34 (13)	N2—C10—H10	118.7
N1—Cu1—N5	92.83 (13)	C9—C10—H10	118.7
N1—Cu1—N6	90.22 (12)	N2—C11—C12	117.0 (3)
N2—Cu1—N3	89.24 (12)	N2—C11—C7	122.3 (4)
N2—Cu1—N4	93.09 (13)	C12—C11—C7	120.7 (4)
N2—Cu1—N5	175.75 (13)	N1—C12—C4	122.6 (4)
N2—Cu1—N6	95.58 (13)	N1—C12—C11	116.0 (3)
N3—Cu1—N4	83.61 (13)	C4—C12—C11	121.4 (4)
N3—Cu1—N5	93.78 (14)	N3—C13—C14	120.8 (4)
N3—Cu1—N6	174.62 (13)	N3—C13—H13	119.6
N4—Cu1—N5	90.22 (12)	C14—C13—H13	119.6
N4—Cu1—N6	93.71 (12)	C15—C14—C13	121.5 (4)
N5—Cu1—N6	81.54 (14)	C15—C14—H14	119.2
N6—O1—H1A	109.5	C13—C14—H14	119.2
N5—O2—H2A	109.5	C14—C15—C16	119.0 (4)
C1—N1—C12	118.2 (3)	C14—C15—H15	120.5
C1—N1—Cu1	128.8 (3)	C16—C15—H15	120.5
C12—N1—Cu1	112.9 (3)	C24—C16—C15	116.8 (4)
C10—N2—C11	118.4 (3)	C24—C16—C17	118.2 (4)
C10—N2—Cu1	131.7 (3)	C15—C16—C17	125.0 (4)
C11—N2—Cu1	109.9 (3)	C18—C17—C16	121.4 (4)
C13—N3—C24	118.3 (3)	C18—C17—H17	119.3
C13—N3—Cu1	129.6 (3)	C16—C17—H17	119.3
C24—N3—Cu1	112.1 (2)	C17—C18—C19	121.5 (4)
C22—N4—C23	117.3 (3)	C17—C18—H18	119.2
C22—N4—Cu1	129.9 (3)	C19—C18—H18	119.2
C23—N4—Cu1	112.9 (2)	C23—C19—C20	116.7 (4)
O2—N5—C25	122.7 (3)	C23—C19—C18	118.2 (4)
O2—N5—Cu1	122.0 (3)	C20—C19—C18	125.1 (4)
C25—N5—Cu1	115.3 (3)	C21—C20—C19	119.0 (4)
C26—N6—O1	116.9 (3)	C21—C20—H20	120.5
C26—N6—Cu1	116.6 (3)	C19—C20—H20	120.5
O1—N6—Cu1	125.4 (2)	C20—C21—C22	120.7 (4)
O7—N7—O5	119.6 (4)	C20—C21—H21	119.6
O7—N7—O6	120.6 (4)	C22—C21—H21	119.6
O5—N7—O6	119.6 (4)	N4—C22—C21	121.8 (4)
O10—N8—O8	133.9 (12)	N4—C22—H22	119.1
O10—N8—O9	118.9 (10)	C21—C22—H22	119.1
O8—N8—O9	106.9 (10)	N4—C23—C19	124.5 (4)
N1—C1—C2	122.2 (4)	N4—C23—C24	115.3 (3)

N1—C1—H1	118.9	C19—C23—C24	120.1 (4)
C2—C1—H1	118.9	N3—C24—C16	123.5 (4)
C3—C2—C1	119.5 (4)	N3—C24—C23	116.0 (3)
C3—C2—H2	120.2	C16—C24—C23	120.4 (4)
C1—C2—H2	120.2	N5—C25—C26	112.7 (4)
C2—C3—C4	120.1 (4)	N5—C25—C27	122.5 (4)
C2—C3—H3	120.0	C26—C25—C27	124.7 (4)
C4—C3—H3	120.0	N6—C26—C25	113.7 (3)
C3—C4—C12	117.3 (4)	N6—C26—C28	125.3 (4)
C3—C4—C5	125.5 (4)	C25—C26—C28	121.0 (4)
C12—C4—C5	117.2 (4)	C25—C27—H27A	109.5
C6—C5—C4	122.0 (4)	C25—C27—H27B	109.5
C6—C5—H5	119.0	H27A—C27—H27B	109.5
C4—C5—H5	119.0	C25—C27—H27C	109.5
C5—C6—C7	121.2 (4)	H27A—C27—H27C	109.5
C5—C6—H6	119.4	H27B—C27—H27C	109.5
C7—C6—H6	119.4	C26—C28—H28A	109.5
C8—C7—C11	117.2 (4)	C26—C28—H28B	109.5
C8—C7—C6	125.3 (4)	H28A—C28—H28B	109.5
C11—C7—C6	117.6 (5)	C26—C28—H28C	109.5
C9—C8—C7	120.7 (4)	H28A—C28—H28C	109.5
C9—C8—H8	119.6	H28B—C28—H28C	109.5
C7—C8—H8	119.6	H3A—O3—H3B	122 (3)
C8—C9—C10	118.7 (4)	H4B—O4—H4A	102 (8)
C8—C9—H9	120.6	H4A—O4—H4B	102 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C27—H27A···O2	0.96	2.40	2.806 (5)	105
C27—H27B···O8	0.96	2.50	3.225 (10)	132
C28—H28C···O1	0.96	2.41	2.769 (5)	102
O1—H1A···N2	0.82	2.84	3.006 (4)	94
C1—H1···N5	0.93	2.49	2.972 (5)	112
C13—H13···N1	0.93	2.57	3.027 (5)	111
C22—H22···N6	0.93	2.57	3.033 (5)	111
O1—H1A···O5^{i}	0.82	2.39	2.999 (4)	131
O1—H1A···O6^{i}	0.82	1.90	2.704 (4)	167
C3—H3···O5^{ii}	0.93	2.51	3.354 (5)	152
C5—H5···O1^{iii}	0.93	2.52	3.331 (5)	145
C18—H18···O2^{iv}	0.93	2.38	3.233 (5)	152
C22—H22···O6^{v}	0.93	2.53	3.279 (5)	137
C15—H15···O5^{vi}	0.93	2.54	3.357 (6)	147
C27—H27C···O7^{v}	0.96	2.59	3.356 (6)	137
C28—H28A···O7^{v}	0.96	2.63	3.316 (6)	128

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

Fig. 1

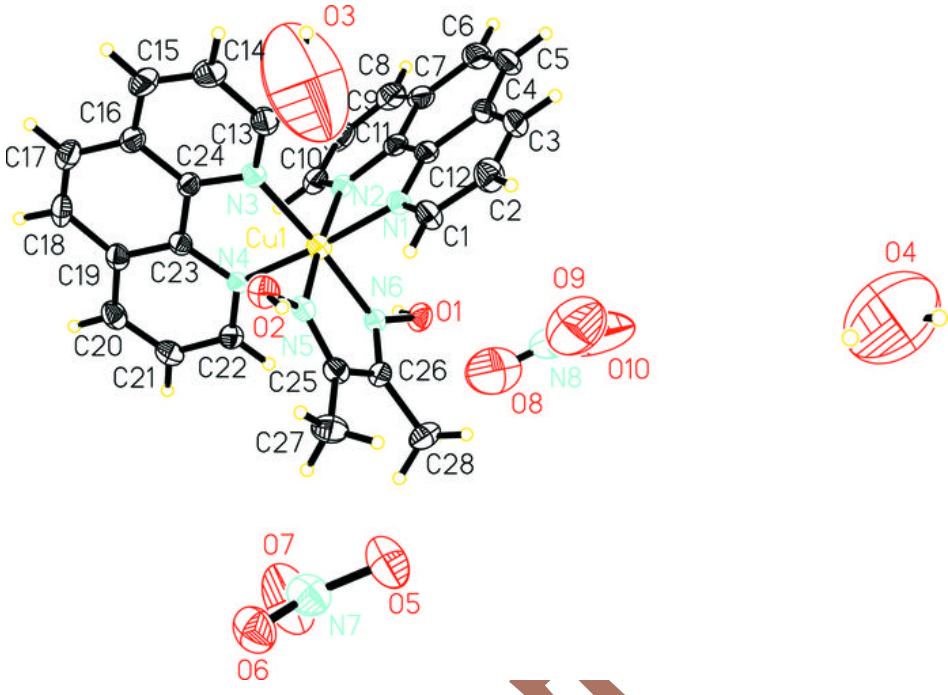

Fig. 2