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# Retraction of articles by T. Liu *et al.*

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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 |
|---|---|---|---|
| *Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)* | Liu & Xie (2007*a*) | 10.1107/S1600536807026852 | EDUMAS |
| *(Dihydroxyglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) dinitrate dihydrate* | Liu, Wang, Wang & Xie (2007*b*) | 10.1107/S1600536807028255 | EDUVAB |
| *Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)* | Liu & Xie (2007*b*) | 10.1107/S1600536807028735 | RIGQAA |
| *Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]* | Liu, Wang, Wang & Xie (2007*c*) | 10.1107/S1600536807030917 | UDUMIQ |
| *Polymeric $KNOF_2$* | Liu Wang, Wang & Xie (2007*a*) | 10.1107/S1600536807027195 | ICSD 240891 |
| *(Dihydroxyglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)cobalt(II) dinitrate dihydrate* | Liu, Wang, Wang & Xie (2007*d*) | 10.1107/S1600536807031224 | WIHJED |
| *Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]* | Liu, Wang, Wang & Xie (2007*e*) | 10.1107/S1600536807032679 | WIHQEK |
| *Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-$\kappa^2N,N'$)-[(2-pyridyloxy)acetato-κO]neodymium(III)}* | Liu, Wang, Wang & Xie (2007*f*) | 10.1107/S1600536807035349 | TIGDAP |
| *(Dihydroxyglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)manganese(II) dinitrate dihydrate* | Liu, Wang, Wang & Xie (2007*g*) | 10.1107/S1600536807035076 | TIGDET |
| *2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)* | Liu & Zhu (2007*j*) | 10.1107/S1600536807040068 | KIKQAX |
| *2-Hydroxy-3,5-dinitrobenzamide monohydrate* | Liu & Zhu (2007*k*) | 10.1107/S1600536807039712 | KIKQEB |
| *2-(1-Hydroxy-2-pyridyl)acetamide monohydrate* | Liu & Zhu (2007*l*) | 10.1107/S1600536807040652 | CIKQOD |
| *Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)* | Liu & Zhu (2007*a*) | 10.1107/S1600536807043486 | XIFXOA |
| *catena-Poly[hexakis($\mu_2$-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]* | Liu & Zhu (2007*b*) | 10.1107/S1600536807045485 | XILNAI |
| *3-Hydroxy-2,4,6-trinitropyridine monohydrate* | Liu & Zhu (2007*m*) | 10.1107/S1600536807045230 | PILNOO |
| *catena-Poly[hexakis($\mu_2$-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]* | Liu & Zhu (2007*c*) | 10.1107/S1600536807047733 | SILZET |
| *catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]* | Liu & Zhu (2007*d*) | 10.1107/S1600536807050969 | GIMZOS |
| *Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)* | Liu & Zhu (2007*e*) | 10.1107/S1600536807051756 | WINFAB |
| *2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate* | Liu & Zhu (2007*n*) | 10.1107/S1600536807048477 | GINFEP |
| *2-(Benzoylhydrazinocarbonyl)benzoic acid* | Liu & Zhu (2007*o*) | 10.1107/S160053680705204X | TINZIA |
| *Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)* | Liu & Zhu (2007*f*) | 10.1107/S1600536807054529 | HIPZIQ |
| *catena-Poly[[(nitrato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)nickel(II)]-μ-acetamido-$\kappa^2O:N$]* | Liu & Zhu (2007*g*) | 10.1107/S1600536807056504 | XIRGIP |
| *catena-Poly[[(nitrato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)copper(II)]-μ-acetamido-$\kappa^2O:N$]* | Liu & Zhu (2007*h*) | 10.1107/S1600536807059077 | HIQROP |
| *catena-Poly[[(nitrato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]* | Liu & Zhu (2007*i*) | 10.1107/S1600536807060631 | YIQMER |
| *N′-Benzoyl-4-nitronicotinohydrazide* | Liu & Zhu (2007*p*) | 10.1107/S1600536807053068 | CIPVON |
| *N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide* | Liu & Zhu (2007*q*) | 10.1107/S1600536807054876 | RIRWEV |

 doi:10.1107/S1600536809049976  

**Table 1 (continued)**

| Title | Reference | DOI | Refcode |
|---|---|---|---|
| *Ethylenediammonium sulfate* | Liu & Zhu (2007*r*) | 10.1107/S1600536807056280 | ETDAMS03 |
| *Ethylenediammonium perchlorate* | Liu & Zhu (2007*s*) | 10.1107/S1600536807059909 | HIRYEN |
| *catena-Poly[[(nitrato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)manganese(II)]-μ-nitrato-$\kappa^2O:O'$]* | Liu & Zhu (2008) | 10.1107/S160053680706254X | MIRROV |

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Liu, T. & Zhu, J. Y. (2007*a*). *Acta Cryst.* E**63**, m2506–m2507.
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Liu, T. & Zhu, J. Y. (2007*k*). *Acta Cryst.* E**63**, o3830.
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# (Dihydroxyglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) dinitrate dihydrate

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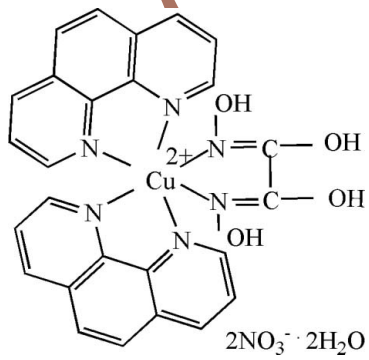
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.045; $wR$ factor = 0.167; data-to-parameter ratio = 13.6.

In the molecule of the title compound, $[Cu(C_{12}H_8N_2)_2(C_2H_4N_2O_4)](NO_3)_2\cdot 2H_2O$, the Cu atom has a distorted octahedral coordination formed by six N atoms from one dihydroxyglyoxime and two 1,10-phenanthroline ligands. In the crystal structure, molecules are linked into a three-dimensional framework by O—H···O and C—H···O hydrogen bonds and by $\pi$–$\pi$ stacking interactions, with a centroid–centroid distance of 3.5692 (5) Å (symmetry code: $1-x, 2-y, 1-z$).

## Related literature

For general background, see: Pope (1983); Pope & Müller (2001); Deisenhofer & Michel (1989); Wall *et al.* (1999); Allen *et al.* (1987). For related literature, see: Wu *et al.* (2003); Pan & Xu (2004); Liu *et al.* (2004); Li *et al.* (2005); Chaudhuri *et al.* (1991); Cervera *et al.* (1997).




## Experimental

### Crystal data

$[Cu(C_{12}H_8N_2)_2(C_2H_4N_2O_4)](NO_3)_2\cdot 2H_2O$
$M_r$ = 704.07
Monoclinic, $P2_1/c$
$a$ = 13.9108 (7) Å
$b$ = 12.011 (3) Å
$c$ = 18.338 (4) Å
$\beta$ = 95.897 (5)°
$V$ = 3047.8 (10) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.79 mm$^{-1}$
$T$ = 273 (2) K
0.30 × 0.23 × 0.18 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.798, $T_{max}$ = 0.871
19706 measured reflections
6028 independent reflections
3118 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.167
$S$ = 1.00
6028 reflections
444 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.79 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.61 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.933 (4) | Cu1—N4 | 1.950 (3) |
| Cu1—N2 | 1.999 (4) | Cu1—N5 | 1.906 (4) |
| Cu1—N3 | 1.959 (4) | Cu1—N6 | 1.889 (4) |
| N1—Cu1—N2 | 83.30 (16) | N2—Cu1—N6 | 95.51 (15) |
| N1—Cu1—N3 | 92.39 (15) | N3—Cu1—N4 | 83.97 (15) |
| N1—Cu1—N4 | 175.33 (15) | N3—Cu1—N5 | 93.86 (17) |
| N1—Cu1—N5 | 93.57 (16) | N3—Cu1—N6 | 174.47 (16) |
| N1—Cu1—N6 | 90.45 (15) | N4—Cu1—N5 | 89.60 (15) |
| N2—Cu1—N3 | 89.54 (15) | N4—Cu1—N6 | 93.42 (15) |
| N2—Cu1—N4 | 93.71 (15) | N5—Cu1—N6 | 81.23 (17) |
| N2—Cu1—N5 | 175.49 (15) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C22—H22···O6$^{i}$ | 0.93 | 2.55 | 3.289 (6) | 137 |
| C18—H18···O2$^{ii}$ | 0.93 | 2.42 | 3.269 (7) | 152 |
| C5—H5···O1$^{iii}$ | 0.93 | 2.55 | 3.354 (6) | 145 |
| C3—H3···O5$^{iv}$ | 0.93 | 2.54 | 3.387 (7) | 151 |
| O1—H1*A*···O6$^{v}$ | 0.82 | 2.00 | 2.697 (5) | 143 |
| O1—H1*A*···O5$^{v}$ | 0.82 | 2.36 | 2.991 (5) | 134 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; 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: HK2273).

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**supplementary materials**

*Acta Cryst.* (2007). E**63**, m1887-m1888 [ **doi:10.1107/S1600536807028255** ]

# (Dihydroxyglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) dinitrate dihydrate

**T. Liu, Z.-W. Wang, Y.-X. Wang and Z.-P. Xie**



## Comment

In recent years, interest in the chemistry of metal-oxygen clusters has grown because of their applications in areas including catalysis, materials chemistry and biochemistry (Pope, 1983; Pope & Müller, 2001). π-π Stacking between aromatic rings is related to the electron-transfer process in some biological systems (Deisenhofer & Michel, 1989; Wall *et al.*, 1999). Aromatic polycyclic compounds, such as phenanthroline, quinoline and benzimidazole, have commonly shown π-π stacking in metal complexes (Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005). As a bidentate flexible ligand, dihydroxyglyoxime is also a good ligand with excellent coordination capabilities for generating mono-, bi- or trinuclear complexes, which are commonly used as precursors for the formation of supramolecular architectures (Chaudhuri *et al.*, 1991; Cervera *et al.*, 1997). We report here the crystal structure of the title compound, (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 of one dihydroxyglyoxime and two 1,10-phenanthroline (phen) ligands are coordinated to the Cu atom, in a distorted octahedral arrangement (Table 1). The dihydroxyglyoxime and two phen ligands are each planar, and the phen ligands are nearly perpendicular to each other, with a dihedral angle of 87.21 (5)°.

In the crystal structure, there is a three-dimensional framework (Fig. 2) formed 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 3.543 (2) Å (symmetry code: $1-x, 2-y, 1-z$). These π-π stacking interactions and hydrogen bonds lead to a supramolecular network structure (Fig. 2).

## Experimental

Copper(II) dinitrate hexahydrate (296 mg, 1 mmol), phen (396 mg, 2 mmol) and dihydroxyglyoxime (120 mg, 1 mmol) were dissolved in ethanol (20 ml). The mixture was heated for 5 h under reflux with stirring. It was then filtered to give a clear solution, into which diethyl ether vapour was allowed to condense in a closed vessel. After being allowed to stand for a few days at room temperature, some blue single crystals suitable for X-ray diffraction analysis precipitated.

## Refinement

H atoms of the water molecules were located in a difference synthesis and refined isotropically [O—H = 0.84 (3)–0.86 (9) Å, $U_{iso}$(H) = 0.450 (8)–0.59 (5) Å$^2$]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}$(H) = $xU_{eq}$(C,*O*), where $x$ = 1.2 for aromatic H atoms and $x$ = 1.5 for OH H atoms.

## Figures

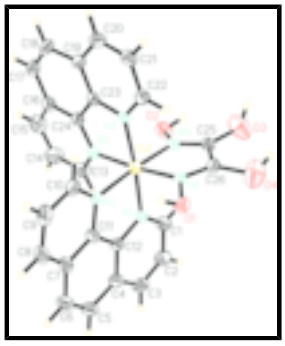

Fig. 1. The structure of the cationic complex of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Solvent molecules and nitrate anions have been omitted for clarity.

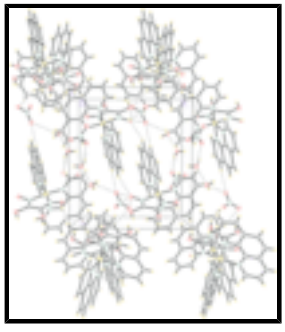

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.



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

### *Crystal data*

| | |
|---|---|
| $[Cu(C_{12}H_8N_2)_2(C_2H_4N_2O_4)](NO_3)_2·2H_2O$ | $F_{000}$ = 1444 |
| $M_r$ = 704.07 | $D_x$ = 1.534 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 5663 reflections |
| $a$ = 13.9108 (7) Å | θ = 2.2–24.9° |
| $b$ = 12.011 (3) Å | μ = 0.79 mm$^{-1}$ |
| $c$ = 18.338 (4) Å | $T$ = 273 (2) K |
| β = 95.897 (5)° | Prism, blue |
| $V$ = 3047.8 (10) Å$^3$ | 0.30 × 0.23 × 0.18 mm |
| $Z$ = 4 | |

### *Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 6028 independent reflections |
| Radiation source: fine-focus sealed tube | 3118 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.041 |
| $T$ = 273(2) K | $\theta_{max}$ = 26.4° |
| φ and ω scans | $\theta_{min}$ = 2.0° |
| Absorption correction: multi-scan | $h$ = −17→17 |

(SADABS; Sheldrick, 1996)
$T_{min}$ = 0.798, $T_{max}$ = 0.871
19706 measured reflections
$k = -15 \rightarrow 15$
$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.167
$S$ = 1.00
6028 reflections
444 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.79 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.61 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 | 0.77579 (4) | 0.75553 (5) | 0.03828 (3) | 0.0432 (2) |
| O1 | 0.7961 (3) | 0.9961 (3) | 0.04774 (18) | 0.0483 (9) |
| H1A | 0.8000 | 0.9954 | 0.0034 | 0.072* |
| O2 | 0.8338 (3) | 0.6031 (3) | 0.1481 (2) | 0.0563 (10) |
| H2A | 0.8712 | 0.5921 | 0.1850 | 0.085* |
| O3 | 0.9324 (4) | 0.7551 (5) | 0.2458 (3) | 0.1201 (19) |
| H3A | 0.9908 | 0.7545 | 0.2431 | 0.180* |
| O4 | 0.9039 (5) | 0.9954 (5) | 0.1835 (4) | 0.133 (2) |
| H4A | 0.9520 | 0.9796 | 0.2111 | 0.199* |
| O5 | 0.7739 (3) | 0.1302 (3) | 0.9096 (3) | 0.0814 (13) |
| O6 | 0.8930 (3) | 0.0159 (3) | 0.9283 (2) | 0.0641 (11) |
| O7 | 0.8887 (4) | 0.1343 (4) | 0.8437 (3) | 0.116 (2) |
| O8 | 0.7394 (6) | 0.8785 (7) | 0.2880 (4) | 0.166 (3) |

| | | | | |
|---|---|---|---|---|
| O9 | 0.6158 (7) | 0.8835 (7) | 0.3358 (5) | 0.184 (3) |
| O10 | 0.6387 (9) | 1.0077 (7) | 0.2627 (6) | 0.345 (11) |
| O11 | 0.5584 (13) | 0.4277 (14) | 0.1452 (12) | 0.497 (14) |
| O12 | 0.701 (2) | 0.340 (2) | 0.2000 (12) | 0.59 (2) |
| N1 | 0.6533 (3) | 0.7801 (3) | 0.0767 (2) | 0.0376 (9) |
| N2 | 0.7067 (3) | 0.8187 (3) | −0.0534 (2) | 0.0355 (9) |
| N3 | 0.7384 (3) | 0.6056 (3) | 0.0042 (2) | 0.0396 (9) |
| N4 | 0.8936 (2) | 0.7245 (3) | −0.0073 (2) | 0.0343 (9) |
| N5 | 0.8376 (3) | 0.7047 (3) | 0.1298 (2) | 0.0391 (9) |
| N6 | 0.8219 (2) | 0.8937 (3) | 0.0767 (2) | 0.0350 (9) |
| N7 | 0.8515 (3) | 0.0921 (4) | 0.8922 (3) | 0.0569 (12) |
| N8 | 0.6658 (6) | 0.9287 (9) | 0.2899 (5) | 0.130 (4) |
| C1 | 0.6305 (4) | 0.7620 (4) | 0.1432 (3) | 0.0491 (13) |
| H1 | 0.6778 | 0.7368 | 0.1789 | 0.059* |
| C2 | 0.5357 (4) | 0.7800 (5) | 0.1620 (3) | 0.0604 (15) |
| H2 | 0.5213 | 0.7658 | 0.2095 | 0.072* |
| C3 | 0.4666 (4) | 0.8173 (4) | 0.1120 (3) | 0.0557 (15) |
| H3 | 0.4044 | 0.8291 | 0.1248 | 0.067* |
| C4 | 0.4874 (3) | 0.8387 (4) | 0.0409 (3) | 0.0461 (13) |
| C5 | 0.4204 (4) | 0.8802 (4) | −0.0169 (4) | 0.0583 (15) |
| H5 | 0.3566 | 0.8924 | −0.0081 | 0.070* |
| C6 | 0.4477 (4) | 0.9023 (4) | −0.0846 (4) | 0.0615 (16) |
| H6 | 0.4025 | 0.9298 | −0.1211 | 0.074* |
| C7 | 0.5462 (4) | 0.8834 (4) | −0.1004 (3) | 0.0497 (13) |
| C8 | 0.5808 (4) | 0.9063 (4) | −0.1659 (3) | 0.0594 (15) |
| H8 | 0.5398 | 0.9356 | −0.2044 | 0.071* |
| C9 | 0.6761 (5) | 0.8862 (4) | −0.1748 (3) | 0.0598 (15) |
| H9 | 0.7001 | 0.9030 | −0.2190 | 0.072* |
| C10 | 0.7367 (4) | 0.8403 (4) | −0.1171 (3) | 0.0464 (13) |
| H10 | 0.8006 | 0.8247 | −0.1242 | 0.056* |
| C11 | 0.6124 (3) | 0.8403 (3) | −0.0443 (3) | 0.0398 (12) |
| C12 | 0.5832 (3) | 0.8180 (3) | 0.0253 (3) | 0.0371 (11) |
| C13 | 0.6609 (4) | 0.5462 (4) | 0.0146 (3) | 0.0554 (14) |
| H13 | 0.6147 | 0.5761 | 0.0422 | 0.066* |
| C14 | 0.6468 (4) | 0.4405 (5) | −0.0147 (4) | 0.0681 (18) |
| H14 | 0.5913 | 0.4008 | −0.0069 | 0.082* |
| C15 | 0.7131 (4) | 0.3945 (4) | −0.0545 (3) | 0.0674 (17) |
| H15 | 0.7034 | 0.3235 | −0.0741 | 0.081* |
| C16 | 0.7968 (4) | 0.4544 (4) | −0.0662 (3) | 0.0447 (12) |
| C17 | 0.8721 (4) | 0.4155 (4) | −0.1062 (3) | 0.0511 (14) |
| H17 | 0.8655 | 0.3468 | −0.1296 | 0.061* |
| C18 | 0.9512 (4) | 0.4742 (4) | −0.1111 (3) | 0.0533 (14) |
| H18 | 0.9997 | 0.4447 | −0.1366 | 0.064* |
| C19 | 0.9650 (3) | 0.5830 (4) | −0.0780 (3) | 0.0415 (12) |
| C20 | 1.0481 (4) | 0.6512 (4) | −0.0796 (3) | 0.0487 (13) |
| H20 | 1.1003 | 0.6273 | −0.1034 | 0.058* |
| C21 | 1.0500 (3) | 0.7503 (4) | −0.0464 (3) | 0.0479 (12) |
| H21 | 1.1040 | 0.7957 | −0.0474 | 0.057* |
| C22 | 0.9725 (3) | 0.7865 (4) | −0.0103 (3) | 0.0429 (12) |

| | | | | |
|---|---|---|---|---|
| H22 | 0.9758 | 0.8560 | 0.0122 | 0.051* |
| C23 | 0.8906 (3) | 0.6243 (4) | −0.0405 (2) | 0.0367 (11) |
| C24 | 0.8064 (3) | 0.5595 (4) | −0.0348 (2) | 0.0367 (11) |
| C25 | 0.8804 (3) | 0.7815 (4) | 0.1715 (3) | 0.0401 (11) |
| C26 | 0.8672 (3) | 0.8918 (4) | 0.1413 (3) | 0.0430 (12) |
| H11A | 0.514 (4) | 0.400 (3) | 0.116 (3) | 0.500 (16)* |
| H12A | 0.673 (10) | 0.286 (4) | 0.220 (6) | 0.59 (5)* |
| H11B | 0.557 (2) | 0.4964 (15) | 0.1531 (19) | 0.450 (8)* |
| H12B | 0.729 (3) | 0.317 (3) | 0.1644 (18) | 0.587 (12)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0397 (4) | 0.0421 (4) | 0.0469 (4) | 0.0020 (3) | 0.0012 (3) | −0.0024 (3) |
| O1 | 0.060 (2) | 0.0367 (18) | 0.047 (2) | 0.0085 (15) | 0.0012 (18) | −0.0016 (16) |
| O2 | 0.059 (2) | 0.050 (2) | 0.057 (3) | 0.0037 (17) | −0.0072 (18) | 0.0168 (18) |
| O3 | 0.106 (4) | 0.149 (5) | 0.097 (4) | 0.000 (4) | −0.027 (3) | 0.018 (3) |
| O4 | 0.148 (6) | 0.112 (4) | 0.133 (6) | −0.017 (4) | −0.010 (4) | −0.042 (4) |
| O5 | 0.059 (3) | 0.079 (3) | 0.107 (4) | 0.012 (2) | 0.016 (3) | 0.008 (3) |
| O6 | 0.064 (2) | 0.051 (2) | 0.076 (3) | 0.0083 (19) | 0.004 (2) | 0.014 (2) |
| O7 | 0.117 (4) | 0.116 (4) | 0.124 (5) | 0.031 (3) | 0.054 (4) | 0.053 (4) |
| O8 | 0.149 (6) | 0.189 (8) | 0.158 (7) | −0.025 (6) | 0.007 (6) | −0.034 (5) |
| O9 | 0.222 (10) | 0.186 (8) | 0.142 (7) | 0.006 (7) | 0.009 (6) | −0.017 (6) |
| O10 | 0.49 (2) | 0.122 (7) | 0.349 (15) | −0.081 (8) | −0.327 (14) | 0.109 (8) |
| O11 | 0.46 (3) | 0.62 (3) | 0.47 (3) | 0.05 (3) | 0.35 (3) | 0.10 (3) |
| O12 | 0.48 (3) | 0.94 (6) | 0.34 (3) | −0.12 (3) | 0.01 (2) | −0.40 (3) |
| N1 | 0.037 (2) | 0.034 (2) | 0.042 (3) | 0.0023 (16) | 0.0026 (18) | −0.0003 (18) |
| N2 | 0.040 (2) | 0.030 (2) | 0.035 (3) | 0.0036 (16) | −0.0011 (18) | −0.0033 (18) |
| N3 | 0.035 (2) | 0.034 (2) | 0.049 (3) | −0.0009 (17) | 0.0014 (19) | −0.0016 (19) |
| N4 | 0.031 (2) | 0.031 (2) | 0.040 (2) | 0.0034 (15) | −0.0023 (16) | −0.0020 (17) |
| N5 | 0.035 (2) | 0.040 (2) | 0.042 (3) | 0.0049 (18) | 0.0047 (18) | 0.006 (2) |
| N6 | 0.034 (2) | 0.031 (2) | 0.040 (3) | 0.0020 (16) | 0.0013 (18) | −0.0020 (18) |
| N7 | 0.051 (3) | 0.054 (3) | 0.067 (4) | −0.007 (2) | 0.011 (3) | 0.009 (3) |
| N8 | 0.084 (6) | 0.195 (11) | 0.108 (7) | −0.026 (6) | 0.003 (5) | −0.081 (8) |
| C1 | 0.043 (3) | 0.058 (3) | 0.046 (3) | 0.008 (2) | 0.005 (2) | 0.006 (3) |
| C2 | 0.053 (3) | 0.070 (4) | 0.060 (4) | 0.001 (3) | 0.016 (3) | −0.002 (3) |
| C3 | 0.037 (3) | 0.056 (3) | 0.077 (5) | −0.002 (2) | 0.016 (3) | −0.016 (3) |
| C4 | 0.037 (3) | 0.032 (3) | 0.068 (4) | −0.002 (2) | −0.002 (3) | −0.009 (3) |
| C5 | 0.036 (3) | 0.050 (3) | 0.087 (5) | 0.004 (2) | −0.003 (3) | −0.006 (3) |
| C6 | 0.051 (3) | 0.045 (3) | 0.084 (5) | 0.010 (3) | −0.020 (3) | −0.007 (3) |
| C7 | 0.053 (3) | 0.038 (3) | 0.054 (4) | 0.001 (2) | −0.014 (3) | −0.006 (3) |
| C8 | 0.075 (4) | 0.048 (3) | 0.050 (4) | 0.011 (3) | −0.016 (3) | −0.001 (3) |
| C9 | 0.092 (5) | 0.045 (3) | 0.040 (4) | −0.003 (3) | −0.004 (3) | −0.001 (3) |
| C10 | 0.060 (3) | 0.041 (3) | 0.038 (3) | 0.004 (2) | 0.003 (3) | −0.005 (2) |
| C11 | 0.043 (3) | 0.027 (2) | 0.047 (3) | 0.002 (2) | −0.009 (2) | −0.001 (2) |
| C12 | 0.034 (3) | 0.030 (2) | 0.047 (3) | 0.0008 (19) | 0.000 (2) | −0.005 (2) |
| C13 | 0.043 (3) | 0.045 (3) | 0.079 (4) | −0.004 (2) | 0.008 (3) | −0.005 (3) |
| C14 | 0.053 (4) | 0.045 (3) | 0.107 (5) | −0.013 (3) | 0.007 (3) | −0.011 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.070 (4) | 0.035 (3) | 0.093 (5) | −0.009 (3) | −0.008 (4) | −0.012 (3) |
| C16 | 0.052 (3) | 0.033 (3) | 0.046 (3) | 0.006 (2) | −0.010 (2) | −0.001 (2) |
| C17 | 0.072 (4) | 0.037 (3) | 0.042 (3) | 0.009 (3) | −0.003 (3) | −0.007 (2) |
| C18 | 0.075 (4) | 0.051 (3) | 0.033 (3) | 0.031 (3) | 0.001 (3) | −0.006 (3) |
| C19 | 0.046 (3) | 0.047 (3) | 0.031 (3) | 0.013 (2) | −0.002 (2) | 0.004 (2) |
| C20 | 0.043 (3) | 0.063 (4) | 0.041 (3) | 0.013 (3) | 0.008 (2) | 0.005 (3) |
| C21 | 0.037 (3) | 0.060 (3) | 0.047 (3) | −0.003 (3) | 0.004 (2) | 0.003 (3) |
| C22 | 0.042 (3) | 0.039 (3) | 0.047 (3) | 0.003 (2) | 0.000 (2) | −0.003 (2) |
| C23 | 0.038 (3) | 0.038 (3) | 0.033 (3) | 0.007 (2) | −0.005 (2) | 0.002 (2) |
| C24 | 0.042 (3) | 0.032 (2) | 0.034 (3) | 0.005 (2) | −0.004 (2) | 0.000 (2) |
| C25 | 0.039 (3) | 0.049 (3) | 0.032 (3) | 0.002 (2) | 0.001 (2) | 0.002 (2) |
| C26 | 0.042 (3) | 0.043 (3) | 0.043 (3) | −0.002 (2) | 0.005 (2) | −0.013 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.933 (4) | C3—C4 | 1.388 (7) |
| Cu1—N2 | 1.999 (4) | C3—H3 | 0.9300 |
| Cu1—N3 | 1.959 (4) | C4—C12 | 1.414 (6) |
| Cu1—N4 | 1.950 (3) | C4—C5 | 1.428 (7) |
| Cu1—N5 | 1.906 (4) | C5—C6 | 1.361 (8) |
| Cu1—N6 | 1.889 (4) | C5—H5 | 0.9300 |
| O1—N6 | 1.372 (4) | C6—C7 | 1.448 (7) |
| O1—H1A | 0.8200 | C6—H6 | 0.9300 |
| O2—N5 | 1.269 (5) | C7—C8 | 1.365 (7) |
| O2—H2A | 0.8200 | C7—C11 | 1.408 (7) |
| O3—C25 | 1.509 (6) | C8—C9 | 1.374 (7) |
| O3—H3A | 0.8200 | C8—H8 | 0.9300 |
| O4—C26 | 1.525 (6) | C9—C10 | 1.397 (7) |
| O4—H4A | 0.8200 | C9—H9 | 0.9300 |
| O5—N7 | 1.244 (5) | C10—H10 | 0.9300 |
| O6—N7 | 1.237 (5) | C11—C12 | 1.403 (6) |
| O7—N7 | 1.188 (6) | C13—C14 | 1.384 (7) |
| O8—N8 | 1.192 (9) | C13—H13 | 0.9300 |
| O9—N8 | 1.268 (9) | C14—C15 | 1.353 (7) |
| O10—N8 | 1.119 (10) | C14—H14 | 0.9300 |
| O11—H11A | 0.84 (5) | C15—C16 | 1.403 (7) |
| O11—H11B | 0.84 (3) | C15—H15 | 0.9300 |
| O12—H12A | 0.86 (9) | C16—C24 | 1.389 (6) |
| O12—H12B | 0.84 (4) | C16—C17 | 1.419 (7) |
| N1—C1 | 1.309 (6) | C17—C18 | 1.317 (7) |
| N1—C12 | 1.363 (6) | C17—H17 | 0.9300 |
| N2—C10 | 1.305 (6) | C18—C19 | 1.445 (7) |
| N2—C11 | 1.365 (5) | C18—H18 | 0.9300 |
| N3—C13 | 1.323 (6) | C19—C23 | 1.391 (6) |
| N3—C24 | 1.360 (5) | C19—C20 | 1.419 (7) |
| N4—C22 | 1.332 (6) | C20—C21 | 1.336 (6) |
| N4—C23 | 1.348 (5) | C20—H20 | 0.9300 |
| N5—C25 | 1.302 (6) | C21—C22 | 1.392 (6) |
| N6—C26 | 1.284 (6) | C21—H21 | 0.9300 |

| | | | |
|---|---|---|---|
| C1—C2 | 1.414 (7) | C22—H22 | 0.9300 |
| C1—H1 | 0.9300 | C23—C24 | 1.419 (6) |
| C2—C3 | 1.336 (8) | C25—C26 | 1.440 (6) |
| C2—H2 | 0.9300 | | |
| N1—Cu1—N2 | 83.30 (16) | C7—C6—H6 | 119.6 |
| N1—Cu1—N3 | 92.39 (15) | C8—C7—C11 | 117.0 (5) |
| N1—Cu1—N4 | 175.33 (15) | C8—C7—C6 | 124.8 (5) |
| N1—Cu1—N5 | 93.57 (16) | C11—C7—C6 | 118.2 (5) |
| N1—Cu1—N6 | 90.45 (15) | C7—C8—C9 | 120.0 (5) |
| N2—Cu1—N3 | 89.54 (15) | C7—C8—H8 | 120.0 |
| N2—Cu1—N4 | 93.71 (15) | C9—C8—H8 | 120.0 |
| N2—Cu1—N5 | 175.49 (15) | C8—C9—C10 | 119.6 (5) |
| N2—Cu1—N6 | 95.51 (15) | C8—C9—H9 | 120.2 |
| N3—Cu1—N4 | 83.97 (15) | C10—C9—H9 | 120.2 |
| N3—Cu1—N5 | 93.86 (17) | N2—C10—C9 | 122.1 (5) |
| N3—Cu1—N6 | 174.47 (16) | N2—C10—H10 | 118.9 |
| N4—Cu1—N5 | 89.60 (15) | C9—C10—H10 | 118.9 |
| N4—Cu1—N6 | 93.42 (15) | N2—C11—C12 | 116.5 (4) |
| N5—Cu1—N6 | 81.23 (17) | N2—C11—C7 | 123.0 (5) |
| N6—O1—H1A | 109.5 | C12—C11—C7 | 120.5 (5) |
| N5—O2—H2A | 109.5 | N1—C12—C11 | 116.1 (4) |
| C25—O3—H3A | 109.5 | N1—C12—C4 | 122.7 (5) |
| C26—O4—H4A | 109.5 | C11—C12—C4 | 121.1 (4) |
| H11A—O11—H11B | 118 (3) | N3—C13—C14 | 121.6 (5) |
| H12A—O12—H12B | 111 (7) | N3—C13—H13 | 119.2 |
| C1—N1—C12 | 118.4 (4) | C14—C13—H13 | 119.2 |
| C1—N1—Cu1 | 128.4 (3) | C15—C14—C13 | 120.4 (5) |
| C12—N1—Cu1 | 113.1 (3) | C15—C14—H14 | 119.8 |
| C10—N2—C11 | 118.2 (4) | C13—C14—H14 | 119.8 |
| C10—N2—Cu1 | 131.1 (3) | C14—C15—C16 | 119.7 (5) |
| C11—N2—Cu1 | 110.7 (3) | C14—C15—H15 | 120.1 |
| C13—N3—C24 | 118.5 (4) | C16—C15—H15 | 120.1 |
| C13—N3—Cu1 | 130.1 (3) | C24—C16—C15 | 116.7 (5) |
| C24—N3—Cu1 | 111.4 (3) | C24—C16—C17 | 118.0 (5) |
| C22—N4—C23 | 117.9 (4) | C15—C16—C17 | 125.3 (5) |
| C22—N4—Cu1 | 130.0 (3) | C18—C17—C16 | 121.6 (5) |
| C23—N4—Cu1 | 112.1 (3) | C18—C17—H17 | 119.2 |
| O2—N5—C25 | 123.7 (4) | C16—C17—H17 | 119.2 |
| O2—N5—Cu1 | 120.9 (3) | C17—C18—C19 | 122.2 (5) |
| C25—N5—Cu1 | 115.3 (3) | C17—C18—H18 | 118.9 |
| C26—N6—O1 | 117.2 (4) | C19—C18—H18 | 118.9 |
| C26—N6—Cu1 | 116.4 (3) | C23—C19—C20 | 117.0 (5) |
| O1—N6—Cu1 | 125.3 (3) | C23—C19—C18 | 117.1 (5) |
| O7—N7—O6 | 120.1 (5) | C20—C19—C18 | 125.9 (5) |
| O7—N7—O5 | 119.4 (5) | C21—C20—C19 | 118.9 (5) |
| O6—N7—O5 | 120.3 (5) | C21—C20—H20 | 120.6 |
| O10—N8—O8 | 131.8 (13) | C19—C20—H20 | 120.6 |
| O10—N8—O9 | 118.5 (11) | C20—C21—C22 | 121.0 (5) |
| O8—N8—O9 | 109.5 (11) | C20—C21—H21 | 119.5 |

| | | | |
|---|---|---|---|
| N1—C1—C2 | 121.5 (5) | C22—C21—H21 | 119.5 |
| N1—C1—H1 | 119.2 | N4—C22—C21 | 121.8 (4) |
| C2—C1—H1 | 119.2 | N4—C22—H22 | 119.1 |
| C3—C2—C1 | 120.4 (5) | C21—C22—H22 | 119.1 |
| C3—C2—H2 | 119.8 | N4—C23—C19 | 123.5 (4) |
| C1—C2—H2 | 119.8 | N4—C23—C24 | 116.3 (4) |
| C2—C3—C4 | 120.2 (5) | C19—C23—C24 | 120.2 (4) |
| C2—C3—H3 | 119.9 | N3—C24—C16 | 123.1 (4) |
| C4—C3—H3 | 119.9 | N3—C24—C23 | 116.1 (4) |
| C3—C4—C12 | 116.7 (5) | C16—C24—C23 | 120.8 (4) |
| C3—C4—C5 | 125.3 (5) | N5—C25—C26 | 113.1 (4) |
| C12—C4—C5 | 117.9 (5) | N5—C25—O3 | 121.9 (5) |
| C6—C5—C4 | 121.5 (5) | C26—C25—O3 | 124.8 (5) |
| C6—C5—H5 | 119.2 | N6—C26—C25 | 113.8 (4) |
| C4—C5—H5 | 119.2 | N6—C26—O4 | 124.0 (5) |
| C5—C6—C7 | 120.7 (5) | C25—C26—O4 | 122.2 (5) |
| C5—C6—H6 | 119.6 | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C22—H22···O6$^{i}$ | 0.93 | 2.55 | 3.289 (6) | 137 |
| C18—H18···O2$^{ii}$ | 0.93 | 2.42 | 3.269 (7) | 152 |
| C5—H5···O1$^{iii}$ | 0.93 | 2.55 | 3.354 (6) | 145 |
| C3—H3···O5$^{iv}$ | 0.93 | 2.54 | 3.387 (7) | 151 |
| O1—H1A···O6$^{v}$ | 0.82 | 2.00 | 2.697 (5) | 143 |
| O1—H1A···O5$^{v}$ | 0.82 | 2.36 | 2.991 (5) | 134 |

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

**Fig. 1**

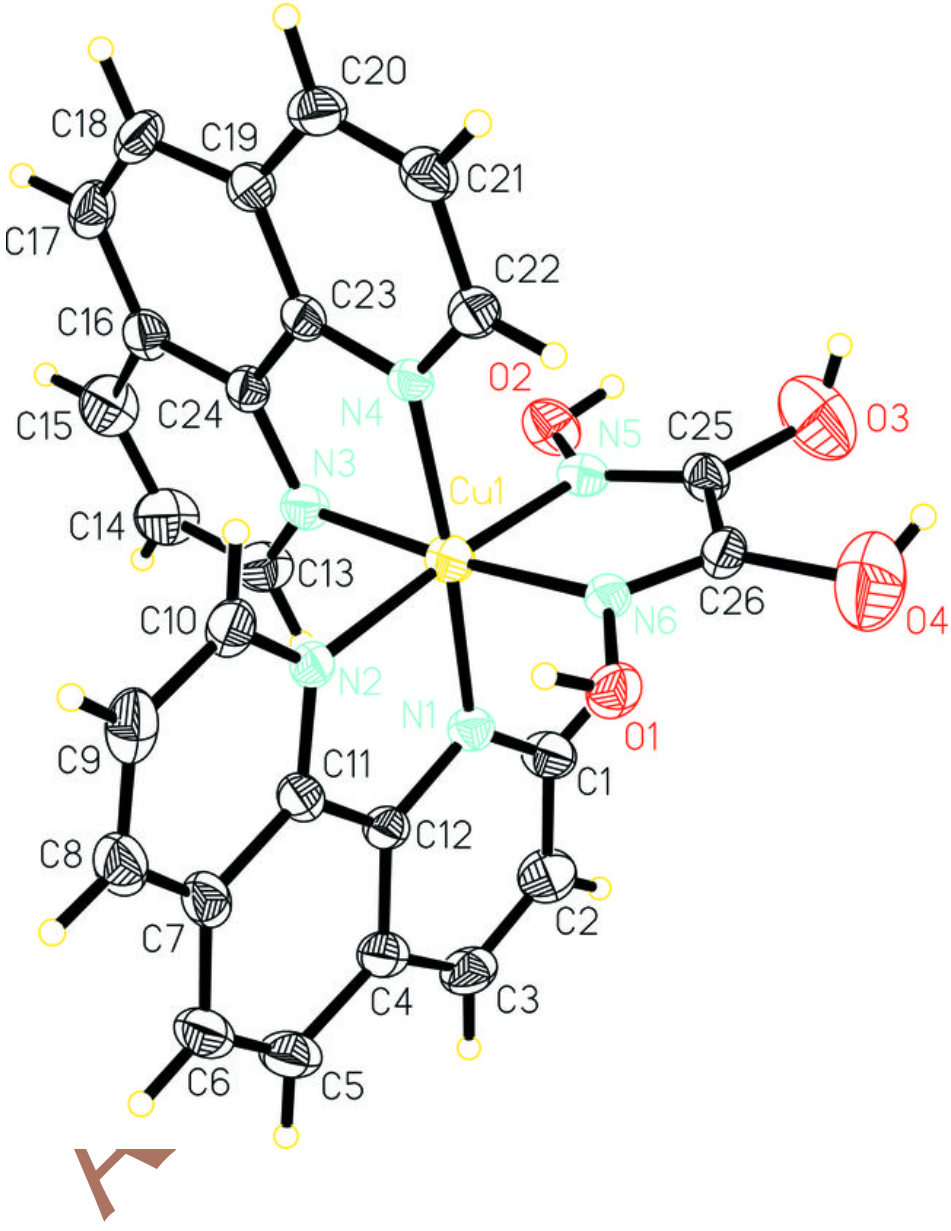
C20
C18
C19
C21
C17
C22
C23
C16
O2
N4
C24
N5
C25
O3
C15
N3
Cu1
C14
C13
C26
O4
C10
N6
N2
N1
O1
C9
C11
C1
C12
C8
C2
C7
C4
C3
C6
C5

**Fig. 2**