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# Poly[[($\mu_3$-2,4,6-tri-4-pyridyl-1,3,5-triazine)copper(I)] nitrate monohydrate]

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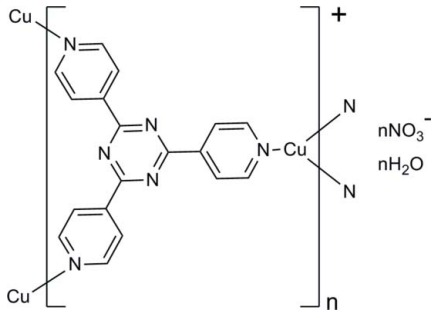
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.070; $wR$ factor = 0.125; data-to-parameter ratio = 15.7.

In the title compound, $\{[Cu(C_{18}H_{12}N_6)]NO_3\cdot H_2O\}_n$, the $Cu^I$ ion is coordinated by three N atoms [Cu—N 1.962 (3)–2.019 (3) Å] from three 2,4,6-tri-4-pyridyl-1,3,5-triazine ($L$) ligands. Each $L$ ligand bridges three $Cu^I$ atoms, generating a positively charged three-dimensional polymeric network with voids propagated along the $b$ axis. These voids are filled with $NO_3^-$ anions with a shortest Cu···O distance of 2.645 (3) Å and water molecules, which are linked into negatively charged helical chains *via* intermolecular O—H···O hydrogen bonds.

## Related literature

For metal complexes with 2,4,6-tri(4-pyridyl)-1,3,5-triazine ligands, see: Abrahams *et al.* (1999); Dybtsev *et al.* (2004); Barrios *et al.* (2007).




## Experimental

### Crystal data

$[Cu(C_{18}H_{12}N_6)]NO_3\cdot H_2O$
$M_r$ = 455.90
Monoclinic, $P2_1/c$
$a$ = 9.917 (2) Å
$b$ = 8.7409 (17) Å
$c$ = 22.499 (6) Å
$\beta$ = 107.43 (3)°
$V$ = 1860.7 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.22 mm$^{-1}$
$T$ = 293 K
0.10 × 0.10 × 0.10 mm

### Data collection

Rigaku SCX-mini diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.736, $T_{max}$ = 1.000
18394 measured reflections
4262 independent reflections
2717 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.097

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.125
$S$ = 1.09
4262 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4$W$—H4$WA$···O2 | 0.91 | 2.23 | 3.057 (7) | 151 |
| O4$W$—H4$WB$···O2$^{i}$ | 0.92 | 2.23 | 3.082 (7) | 155 |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5064).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m515 [ **doi:10.1107/S1600536811011445** ]

# Poly[[($\mu_3$-2,4,6-tri-4-pyridyl-1,3,5-triazine)copper(I)] nitrate monohydrate]

**M. Feng, H.-J. Tian, H.-F. Mi and T.-L. Hu**

## Comment

As an interesting polydentate nitrogen donor ligand, 2,4,6-tris(4-pyridyl)-1,3,5-triazine(*L*) has attracted increasing attention in the synthesis of novel transition metal complexes with novel topology and properties (Abrahams *et al.* 1999; Dybtsev *et al.* 2004; Barrios *et al.* 2007). Our interest in 2,4,6-tris(4-pyridyl)-1,3,5-triazine transition metal complexes prompts us to report here the crystal structure of the title compound (1).

In 1 (Fig. 1), each $Cu^{I}$ ion is coordinated by three N atoms [Cu—N 1.962 (3)–2.019 (3) Å] from three ligands *L*, and each ligand *L* bridge three $Cu^{I}$ centers generating positively charged three-dimensional polymeric network with the voids propagated along axis *b*. These voids are filled with $NO_3^-$ anions with the shortest Cu···O distance of 2.645 (3) Å and crystalline water molecules, which are linked into negatively charged helical chains *via* intermolecular O—H···O hydrogen bonds.

## Experimental

In a typical synthesis, a mixture of $Cu(NO_3)_2.6H_2O$ (1 mmol), 2,4,6-tris(4-pyridyl)-1,3,5-triazine (1 mmol) and methanol (10 ml), was added to a 20 ml Teflon-lined reactor under autogenous pressure at 140 °C for 3 days.

## Refinement

C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C). The H atoms of the water molecules were located on a difference map, and refined as riding in their as-found relative positions with $U_{iso}$(H) = 1.2$U_{eq}$(O).

## Figures

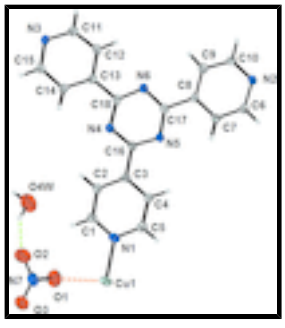


Fig. 1. A content of the asymmetric unit of 1 showing the atomic numbering and displacement ellipsoids drawn at the 30% probability level. The O—H···O hydrogen bond is shown by the dashed green line, and the shortest Cu···O distance is shown by the dotted red line.

## Poly[[(μ3-2,4,6-tri-4-pyridyl-1,3,5-triazine)copper(I)] nitrate monohydrate]

*Crystal data*

| | |
|---|---|
| $[Cu(C_{18}H_{12}N_6)]NO_3·H_2O$ | $F(000) = 928$ |
| $M_r = 455.90$ | $D_x = 1.627$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 14882 reflections |
| $a = 9.917$ (2) Å | $\theta = 3.0$–$27.7°$ |
| $b = 8.7409$ (17) Å | $\mu = 1.22$ mm$^{-1}$ |
| $c = 22.499$ (6) Å | $T = 293$ K |
| $\beta = 107.43$ (3)° | Block, red |
| $V = 1860.7$ (7) Å$^3$ | 0.10 × 0.10 × 0.10 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Rigaku SCX-mini diffractometer | 4262 independent reflections |
| Radiation source: fine-focus sealed tube | 2717 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.097$ |
| ω scans | $\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$ |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | $h = -12 \rightarrow 12$ |
| $T_{min} = 0.736$, $T_{max} = 1.000$ | $k = -11 \rightarrow 11$ |
| 18394 measured reflections | $l = -28 \rightarrow 29$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.070$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.125$ | H-atom parameters constrained |
| $S = 1.09$ | $w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 2.1056P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4262 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 271 parameters | $\Delta\rho_{max} = 0.36$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.1691 (5) | 0.5154 (5) | 0.27731 (19) | 0.0411 (12) |
| H1 | −0.2584 | 0.5537 | 0.2569 | 0.049* |
| C2 | −0.1040 (4) | 0.5629 (5) | 0.33689 (19) | 0.0380 (11) |
| H2 | −0.1487 | 0.6318 | 0.3563 | 0.046* |
| C3 | 0.0293 (4) | 0.5073 (5) | 0.36812 (18) | 0.0296 (9) |
| C4 | 0.0904 (4) | 0.4047 (5) | 0.33735 (18) | 0.0344 (10) |
| H4 | 0.1795 | 0.3642 | 0.3568 | 0.041* |
| C5 | 0.0177 (4) | 0.3635 (5) | 0.27772 (19) | 0.0383 (11) |
| H5 | 0.0600 | 0.2945 | 0.2573 | 0.046* |
| C6 | 0.5691 (4) | 0.2273 (5) | 0.55716 (19) | 0.0379 (11) |
| H6 | 0.5981 | 0.1474 | 0.5366 | 0.046* |
| C7 | 0.4531 (4) | 0.3104 (5) | 0.52532 (18) | 0.0321 (10) |
| H7 | 0.4053 | 0.2872 | 0.4840 | 0.039* |
| C8 | 0.4077 (4) | 0.4293 (5) | 0.55511 (18) | 0.0276 (9) |
| C9 | 0.4827 (4) | 0.4592 (5) | 0.61641 (19) | 0.0398 (11) |
| H9 | 0.4557 | 0.5381 | 0.6382 | 0.048* |
| C10 | 0.5983 (4) | 0.3696 (5) | 0.64455 (19) | 0.0407 (11) |
| H10 | 0.6482 | 0.3904 | 0.6858 | 0.049* |
| C11 | 0.0496 (4) | 0.9682 (5) | 0.6342 (2) | 0.0388 (11) |
| H11 | 0.0994 | 1.0111 | 0.6722 | 0.047* |
| C12 | 0.1191 (4) | 0.8664 (5) | 0.60714 (18) | 0.0354 (10) |
| H12 | 0.2124 | 0.8393 | 0.6271 | 0.042* |
| C13 | 0.0474 (4) | 0.8050 (5) | 0.54967 (17) | 0.0270 (9) |
| C14 | −0.0906 (4) | 0.8507 (5) | 0.52211 (18) | 0.0310 (10) |
| H14 | −0.1408 | 0.8143 | 0.4829 | 0.037* |
| C15 | −0.1526 (4) | 0.9498 (5) | 0.55297 (19) | 0.0360 (10) |
| H15 | −0.2462 | 0.9775 | 0.5342 | 0.043* |
| C16 | 0.1021 (4) | 0.5523 (5) | 0.43321 (17) | 0.0281 (9) |
| C17 | 0.2806 (4) | 0.5165 (5) | 0.52141 (18) | 0.0276 (9) |
| C18 | 0.1122 (4) | 0.6898 (5) | 0.51893 (18) | 0.0278 (9) |
| Cu1 | −0.19856 (5) | 0.38069 (7) | 0.15691 (2) | 0.03757 (18) |
| N1 | −0.1108 (4) | 0.4169 (4) | 0.24703 (15) | 0.0364 (9) |
| N2 | 0.6432 (3) | 0.2554 (4) | 0.61653 (15) | 0.0321 (8) |
| N3 | −0.0852 (3) | 1.0091 (4) | 0.60904 (15) | 0.0329 (8) |
| N4 | 0.0422 (3) | 0.6577 (4) | 0.45964 (15) | 0.0313 (8) |
| N5 | 0.2221 (3) | 0.4792 (4) | 0.46175 (14) | 0.0290 (8) |
| N6 | 0.2306 (3) | 0.6215 (4) | 0.55228 (14) | 0.0308 (8) |
| N7 | −0.4795 (5) | 0.6084 (6) | 0.1312 (2) | 0.0619 (12) |

| | | | | |
|---|---|---|---|---|
| O1 | −0.3565 (4) | 0.6301 (5) | 0.13251 (19) | 0.0806 (12) |
| O2 | −0.5122 (4) | 0.6217 (6) | 0.18018 (19) | 0.1031 (17) |
| O3 | −0.5691 (4) | 0.5721 (6) | 0.0832 (2) | 0.0948 (15) |
| O4W | −0.3407 (5) | 0.8630 (5) | 0.2697 (2) | 0.1142 (17) |
| H4WA | −0.4160 | 0.8171 | 0.2417 | 0.142* |
| H4WB | −0.3653 | 0.9580 | 0.2804 | 0.142* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.033 (2) | 0.058 (3) | 0.026 (2) | 0.007 (2) | −0.002 (2) | 0.001 (2) |
| C2 | 0.031 (2) | 0.047 (3) | 0.034 (2) | 0.010 (2) | 0.006 (2) | −0.007 (2) |
| C3 | 0.029 (2) | 0.033 (2) | 0.024 (2) | −0.0004 (19) | 0.0058 (18) | 0.0032 (18) |
| C4 | 0.030 (2) | 0.041 (3) | 0.029 (2) | 0.008 (2) | 0.0042 (19) | −0.002 (2) |
| C5 | 0.043 (3) | 0.041 (3) | 0.031 (2) | 0.005 (2) | 0.011 (2) | −0.005 (2) |
| C6 | 0.036 (2) | 0.040 (3) | 0.033 (2) | 0.014 (2) | 0.005 (2) | −0.006 (2) |
| C7 | 0.033 (2) | 0.035 (3) | 0.023 (2) | 0.0064 (19) | 0.0021 (19) | −0.0029 (18) |
| C8 | 0.022 (2) | 0.031 (2) | 0.027 (2) | 0.0049 (17) | 0.0033 (17) | 0.0016 (18) |
| C9 | 0.040 (3) | 0.041 (3) | 0.034 (2) | 0.015 (2) | 0.005 (2) | −0.007 (2) |
| C10 | 0.040 (3) | 0.047 (3) | 0.028 (2) | 0.011 (2) | −0.001 (2) | −0.005 (2) |
| C11 | 0.035 (2) | 0.045 (3) | 0.034 (2) | 0.002 (2) | 0.006 (2) | −0.010 (2) |
| C12 | 0.026 (2) | 0.042 (3) | 0.035 (2) | 0.006 (2) | 0.0054 (19) | −0.002 (2) |
| C13 | 0.026 (2) | 0.027 (2) | 0.028 (2) | 0.0003 (17) | 0.0086 (18) | 0.0022 (18) |
| C14 | 0.029 (2) | 0.032 (3) | 0.029 (2) | 0.0042 (19) | 0.0052 (18) | −0.0044 (19) |
| C15 | 0.029 (2) | 0.043 (3) | 0.032 (2) | 0.003 (2) | 0.001 (2) | −0.001 (2) |
| C16 | 0.027 (2) | 0.029 (2) | 0.026 (2) | 0.0028 (18) | 0.0038 (18) | 0.0024 (18) |
| C17 | 0.026 (2) | 0.028 (2) | 0.027 (2) | −0.0003 (18) | 0.0060 (18) | 0.0015 (18) |
| C18 | 0.024 (2) | 0.028 (2) | 0.029 (2) | 0.0002 (17) | 0.0048 (18) | 0.0023 (18) |
| Cu1 | 0.0337 (3) | 0.0470 (4) | 0.0281 (3) | −0.0141 (3) | 0.0034 (2) | −0.0025 (3) |
| N1 | 0.037 (2) | 0.044 (2) | 0.0250 (18) | −0.0085 (17) | 0.0054 (16) | 0.0013 (16) |
| N2 | 0.0297 (19) | 0.035 (2) | 0.0277 (18) | 0.0108 (16) | 0.0024 (16) | 0.0016 (16) |
| N3 | 0.0270 (19) | 0.037 (2) | 0.034 (2) | 0.0079 (16) | 0.0077 (16) | −0.0036 (17) |
| N4 | 0.0312 (19) | 0.032 (2) | 0.0281 (18) | 0.0071 (15) | 0.0048 (16) | 0.0006 (15) |
| N5 | 0.0273 (18) | 0.032 (2) | 0.0249 (18) | 0.0054 (15) | 0.0038 (15) | −0.0011 (15) |
| N6 | 0.0275 (17) | 0.032 (2) | 0.0303 (18) | 0.0049 (17) | 0.0052 (15) | −0.0014 (17) |
| N7 | 0.044 (3) | 0.080 (4) | 0.058 (3) | 0.017 (3) | 0.010 (2) | 0.012 (3) |
| O1 | 0.054 (2) | 0.097 (3) | 0.097 (3) | −0.008 (2) | 0.032 (2) | 0.008 (3) |
| O2 | 0.064 (3) | 0.190 (5) | 0.060 (3) | −0.006 (3) | 0.025 (2) | 0.000 (3) |
| O3 | 0.068 (3) | 0.131 (4) | 0.071 (3) | 0.022 (3) | −0.002 (2) | −0.021 (3) |
| O4W | 0.088 (3) | 0.100 (4) | 0.130 (4) | 0.007 (3) | −0.005 (3) | −0.021 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.332 (5) | C12—C13 | 1.384 (5) |
| C1—C2 | 1.367 (5) | C12—H12 | 0.9300 |
| C1—H1 | 0.9300 | C13—C14 | 1.381 (5) |
| C2—C3 | 1.386 (5) | C13—C18 | 1.473 (5) |
| C2—H2 | 0.9300 | C14—C15 | 1.366 (5) |
| C3—C4 | 1.380 (5) | C14—H14 | 0.9300 |

| | | | |
|---|---|---|---|
| C3—C16 | 1.479 (5) | C15—N3 | 1.342 (5) |
| C4—C5 | 1.367 (5) | C15—H15 | 0.9300 |
| C4—H4 | 0.9300 | C16—N4 | 1.329 (5) |
| C5—N1 | 1.338 (5) | C16—N5 | 1.334 (5) |
| C5—H5 | 0.9300 | C17—N6 | 1.332 (5) |
| C6—N2 | 1.340 (5) | C17—N5 | 1.334 (5) |
| C6—C7 | 1.368 (5) | C18—N6 | 1.331 (5) |
| C6—H6 | 0.9300 | C18—N4 | 1.336 (5) |
| C7—C8 | 1.383 (5) | Cu1—N2$^{i}$ | 1.962 (3) |
| C7—H7 | 0.9300 | Cu1—N1 | 1.978 (3) |
| C8—C9 | 1.382 (5) | Cu1—N3$^{ii}$ | 2.019 (3) |
| C8—C17 | 1.474 (5) | N2—Cu1$^{iii}$ | 1.962 (3) |
| C9—C10 | 1.376 (5) | N3—Cu1$^{iv}$ | 2.019 (3) |
| C9—H9 | 0.9300 | N7—O3 | 1.218 (5) |
| C10—N2 | 1.326 (5) | N7—O1 | 1.226 (5) |
| C10—H10 | 0.9300 | N7—O2 | 1.243 (5) |
| C11—N3 | 1.335 (5) | O4W—H4WA | 0.9125 |
| C11—C12 | 1.374 (6) | O4W—H4WB | 0.9175 |
| C11—H11 | 0.9300 | | |
| N1—C1—C2 | 123.3 (4) | C14—C13—C18 | 120.0 (3) |
| N1—C1—H1 | 118.4 | C12—C13—C18 | 122.0 (3) |
| C2—C1—H1 | 118.4 | C15—C14—C13 | 119.4 (4) |
| C1—C2—C3 | 119.3 (4) | C15—C14—H14 | 120.3 |
| C1—C2—H2 | 120.4 | C13—C14—H14 | 120.3 |
| C3—C2—H2 | 120.4 | N3—C15—C14 | 123.3 (4) |
| C4—C3—C2 | 118.0 (4) | N3—C15—H15 | 118.3 |
| C4—C3—C16 | 120.8 (3) | C14—C15—H15 | 118.3 |
| C2—C3—C16 | 121.2 (4) | N4—C16—N5 | 124.8 (3) |
| C5—C4—C3 | 118.8 (4) | N4—C16—C3 | 118.4 (3) |
| C5—C4—H4 | 120.6 | N5—C16—C3 | 116.7 (4) |
| C3—C4—H4 | 120.6 | N6—C17—N5 | 125.1 (3) |
| N1—C5—C4 | 123.7 (4) | N6—C17—C8 | 118.8 (3) |
| N1—C5—H5 | 118.1 | N5—C17—C8 | 116.0 (4) |
| C4—C5—H5 | 118.1 | N6—C18—N4 | 125.1 (4) |
| N2—C6—C7 | 123.3 (4) | N6—C18—C13 | 118.5 (3) |
| N2—C6—H6 | 118.4 | N4—C18—C13 | 116.3 (3) |
| C7—C6—H6 | 118.4 | N2$^{i}$—Cu1—N1 | 128.12 (14) |
| C6—C7—C8 | 119.4 (4) | N2$^{i}$—Cu1—N3$^{ii}$ | 122.55 (14) |
| C6—C7—H7 | 120.3 | N1—Cu1—N3$^{ii}$ | 109.03 (14) |
| C8—C7—H7 | 120.3 | C1—N1—C5 | 116.9 (3) |
| C9—C8—C7 | 118.0 (4) | C1—N1—Cu1 | 120.2 (3) |
| C9—C8—C17 | 122.5 (4) | C5—N1—Cu1 | 122.1 (3) |
| C7—C8—C17 | 119.5 (3) | C10—N2—C6 | 116.7 (3) |
| C10—C9—C8 | 118.5 (4) | C10—N2—Cu1$^{iii}$ | 124.9 (3) |
| C10—C9—H9 | 120.8 | C6—N2—Cu1$^{iii}$ | 118.3 (3) |
| C8—C9—H9 | 120.8 | C11—N3—C15 | 116.6 (4) |
| N2—C10—C9 | 124.2 (4) | C11—N3—Cu1$^{iv}$ | 123.3 (3) |

| | | | |
|---|---|---|---|
| N2—C10—H10 | 117.9 | C15—N3—Cu1$^{iv}$ | 119.1 (3) |
| C9—C10—H10 | 117.9 | C16—N4—C18 | 115.1 (3) |
| N3—C11—C12 | 123.9 (4) | C17—N5—C16 | 115.1 (3) |
| N3—C11—H11 | 118.1 | C18—N6—C17 | 114.7 (3) |
| C12—C11—H11 | 118.1 | O3—N7—O1 | 121.1 (5) |
| C11—C12—C13 | 118.6 (4) | O3—N7—O2 | 119.7 (5) |
| C11—C12—H12 | 120.7 | O1—N7—O2 | 119.1 (5) |
| C13—C12—H12 | 120.7 | H4WA—O4W—H4WB | 110.6 |
| C14—C13—C12 | 118.0 (4) | | |
| N1—C1—C2—C3 | 0.1 (7) | C12—C13—C18—N4 | −169.4 (4) |
| C1—C2—C3—C4 | −0.4 (6) | C2—C1—N1—C5 | 0.2 (7) |
| C1—C2—C3—C16 | −178.4 (4) | C2—C1—N1—Cu1 | −170.1 (3) |
| C2—C3—C4—C5 | 0.4 (6) | C4—C5—N1—C1 | −0.1 (6) |
| C16—C3—C4—C5 | 178.4 (4) | C4—C5—N1—Cu1 | 169.9 (3) |
| C3—C4—C5—N1 | −0.2 (7) | N2$^{i}$—Cu1—N1—C1 | −82.3 (4) |
| N2—C6—C7—C8 | −0.4 (7) | N3$^{ii}$—Cu1—N1—C1 | 103.9 (3) |
| C6—C7—C8—C9 | 0.2 (6) | N2$^{i}$—Cu1—N1—C5 | 107.9 (3) |
| C6—C7—C8—C17 | −178.5 (4) | N3$^{ii}$—Cu1—N1—C5 | −65.8 (4) |
| C7—C8—C9—C10 | 0.0 (6) | C9—C10—N2—C6 | −0.3 (7) |
| C17—C8—C9—C10 | 178.6 (4) | C9—C10—N2—Cu1$^{iii}$ | −176.6 (4) |
| C8—C9—C10—N2 | 0.1 (7) | C7—C6—N2—C10 | 0.5 (7) |
| N3—C11—C12—C13 | 1.8 (7) | C7—C6—N2—Cu1$^{iii}$ | 177.0 (3) |
| C11—C12—C13—C14 | 0.6 (6) | C12—C11—N3—C15 | −2.5 (7) |
| C11—C12—C13—C18 | −177.1 (4) | C12—C11—N3—Cu1$^{iv}$ | 165.7 (3) |
| C12—C13—C14—C15 | −2.2 (6) | C14—C15—N3—C11 | 0.8 (6) |
| C18—C13—C14—C15 | 175.6 (4) | C14—C15—N3—Cu1$^{iv}$ | −167.9 (3) |
| C13—C14—C15—N3 | 1.5 (7) | N5—C16—N4—C18 | 0.7 (6) |
| C4—C3—C16—N4 | 176.4 (4) | C3—C16—N4—C18 | 178.4 (3) |
| C2—C3—C16—N4 | −5.6 (6) | N6—C18—N4—C16 | −2.4 (6) |
| C4—C3—C16—N5 | −5.7 (6) | C13—C18—N4—C16 | −179.3 (3) |
| C2—C3—C16—N5 | 172.2 (4) | N6—C17—N5—C16 | −2.1 (6) |
| C9—C8—C17—N6 | −4.5 (6) | C8—C17—N5—C16 | 175.8 (3) |
| C7—C8—C17—N6 | 174.0 (4) | N4—C16—N5—C17 | 1.3 (6) |
| C9—C8—C17—N5 | 177.5 (4) | C3—C16—N5—C17 | −176.4 (3) |
| C7—C8—C17—N5 | −4.0 (6) | N4—C18—N6—C17 | 1.7 (6) |
| C14—C13—C18—N6 | −164.3 (4) | C13—C18—N6—C17 | 178.6 (3) |
| C12—C13—C18—N6 | 13.4 (6) | N5—C17—N6—C18 | 0.7 (6) |
| C14—C13—C18—N4 | 12.9 (5) | C8—C17—N6—C18 | −177.1 (4) |

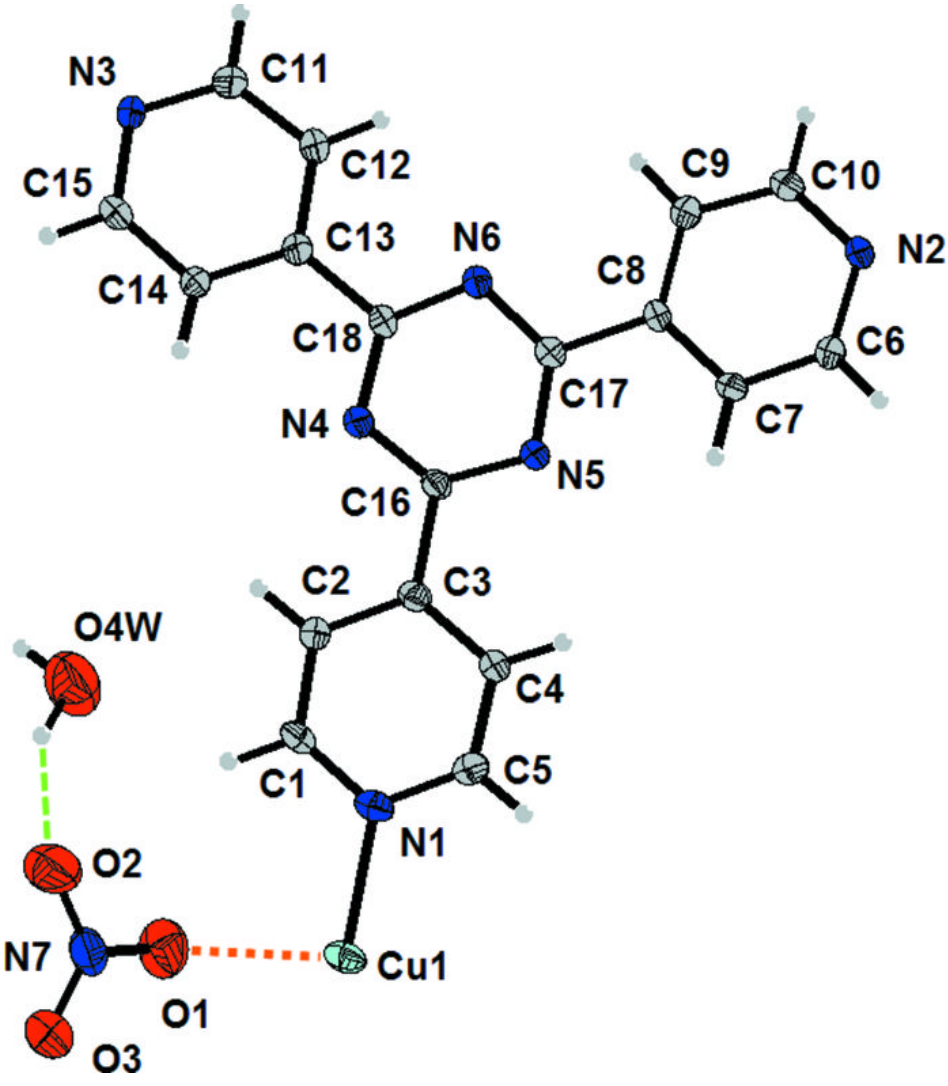
Symmetry codes: (i) *x*−1, −*y*+1/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) *x*+1, −*y*+1/2, *z*+1/2; (iv) *x*, −*y*+3/2, *z*+1/2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4W—H4WA···O2 | 0.91 | 2.23 | 3.057 (7) | 151 |
| O4W—H4WB···O2$^{v}$ | 0.92 | 2.23 | 3.082 (7) | 155 |

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

**Fig. 1**


N3
C11
C12
C15
C13
N6
C9
C10
N2
C14
C8
C18
C6
C17
N4
C7
N5
C16
C2
C3
O4W
C4
C1
C5
N1
O2
N7
Cu1
O1
O3