Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (4,4′-Di-*tert*-butyl-2,2′-bipyridine-$\kappa^2N,N'$)bis(nitrato-$\kappa^2O,O'$)copper(II)

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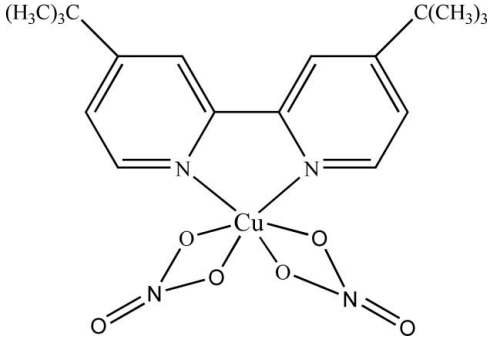
Received 11 January 2009; accepted 12 January 2009

Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.030; $wR$ factor = 0.074; data-to-parameter ratio = 14.1.

In the crystal of the title compound, $[Cu(NO_3)_2(C_{18}H_{24}N_2)]$, the $Cu^{II}$ ion is coordinated by two N atoms of the bipyridine ligand and four O atoms from the two nitrate anions in a distorted octahedral fashion. The dihedral angle between the planes of the two pyridine rings is 11.52 (10)°. In the crystal structure, weak C—H···O interactions may help to establish the packing.

## Related literature

For general background, see: Noro *et al.* (2000); Yaghi *et al.* (1998); Huertas *et al.* (2001); Qin *et al.* (2002).




## Experimental

### Crystal data

$[Cu(NO_3)_2(C_{18}H_{24}N_2)]$
$M_r$ = 455.96
Orthorhombic, $P2_12_12_1$
$a$ = 9.8265 (16) Å
$b$ = 13.247 (2) Å
$c$ = 16.138 (3) Å
$V$ = 2100.7 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.08 mm$^{-1}$
$T$ = 173 (2) K
0.27 × 0.25 × 0.17 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.759, $T_{max}$ = 0.837
11065 measured reflections
3642 independent reflections
3450 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.074
$S$ = 1.05
3642 reflections
258 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.81 e Å$^{-3}$
Absolute structure: Flack (1983), 1522 Friedel pairs
Flack parameter: 0.012 (13)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O4$^{i}$ | 0.93 | 2.46 | 3.124 (3) | 129 |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors gratefully acknowledge the Natural Science Foundation of China (No. 20767001), the International Collaborative Project of Guizhou Province, the Governor Foundation of Guizhou Province and the Natural Science Youth Foundation of Guizhou University (No. 2007–005) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2708).

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# supporting information

*Acta Cryst.* (2009). E**65**, m202 [doi:10.1107/S1600536809001457]

## (4,4′-Di-*tert*-butyl-2,2′-bipyridine-$\kappa^2N,N'$)bis(nitrato-$\kappa^2O,O'$)copper(II)

**Xin Xiao, Zai-Ying Rao, Yun-Qiang Zhang, Sai-Feng Xue and Zhu Tao**

### S1. Comment

Research into transition metal complexes has been rapidly expanding because of their fascinating structural diversity, as well as their potential applications as functional materials and enzymes (Noro *et al.*, 2000; Yaghi *et al.*, 1998). And 4,4′-di-*tert*-butyl-2,2′-bipyridine has been used as a ligand in coordination chemistry (Huertas *et al.*, 2001; Qin *et al.*, 2002). We report here the crystal structure of the title copper(II)complex, (I), containing a bipyridine ligand.

In the crystal of (I), the $Cu^{II}$ ion is coordinated by two N atoms of the 4,4′-di-*tert*-butyl-2,2′-bipyridine ligand and four O atoms from the two nitrate anions. The dihedral angle between the planes of two pyridine rings is 11.52 (10)°. The title compound forms intermolecular H bond whereas the protonated C1 atom act as hydrogen-bond donor and O4 atom act as hydrogen-bond acceptor, the distance of the C1—H1···O4 hydrogen bonds is 3.124 (3) Å (Table 1). Weak C—H···O interactions may help to establish the packing.

### S2. Experimental

A solution of 4,4′-di-*tert*-butyl-2,2′-bipyridine (0.15 g, 0.56 mmol) in ethanol (50 ml) was added to a solution of $Cu(N0_3)_2$, (0.09 g, 0.56 mmol) in $H_2O$ (20 ml), and the resulting blue solution was stirred for 10 min at 313 K. Then, it was left to evaporate slowly at room temperature. After one week, blue crystals of (I) were isolated.

### S3. Refinement

H atoms were placed in calculated positions and refined as riding, with C—H = 0.93- and 0.96 Å, and $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C).

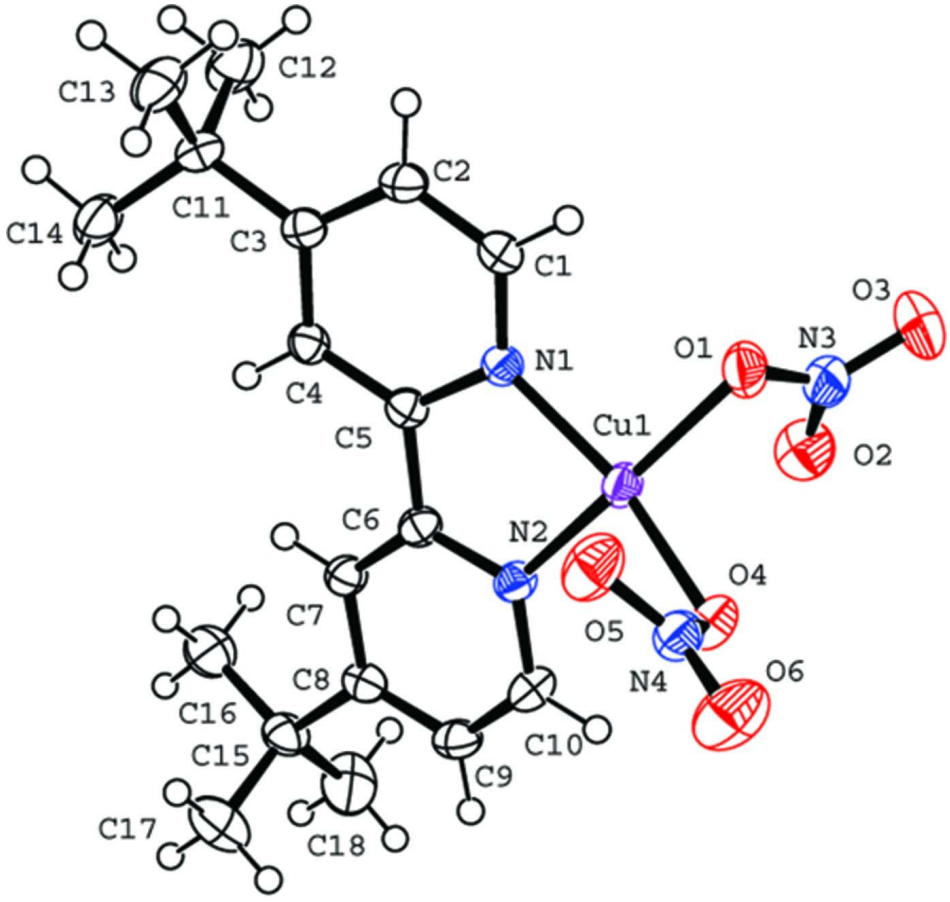


**Figure 1**

The molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**(4,4′-Di-*tert*-butyl-2,2′-bipyridine-$\kappa^2N,N'$)bis(nitrato-$\kappa^2O,O'$)copper(II)**

*Crystal data*

$[Cu(NO_3)_2(C_{18}H_{24}N_2)]$
$M_r$ = 455.96
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a$ = 9.8265 (16) Å
$b$ = 13.247 (2) Å
$c$ = 16.138 (3) Å
$V$ = 2100.7 (6) Å$^3$
$Z$ = 4
$F(000)$ = 948
$D_x$ = 1.442 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2120 reflections
$\theta$ = 2.0–25.0°
$\mu$ = 1.08 mm$^{-1}$
$T$ = 173 K
Block, blue
0.27 × 0.25 × 0.17 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.759, $T_{max}$ = 0.837
11065 measured reflections
3642 independent reflections
3450 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.022
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.0°
$h$ = −11→11
$k$ = −15→15
$l$ = −19→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.074
$S$ = 1.05
3642 reflections
258 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 0.8717P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.64 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.81 e Å$^{-3}$
Absolute structure: Flack (1983), 1522 Freidel pairs
Absolute structure parameter: 0.012 (13)

*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 | 0.58577 (3) | 0.98172 (2) | 0.72968 (2) | 0.02515 (10) |
| O2 | 0.3672 (2) | 1.0193 (2) | 0.66313 (14) | 0.0434 (6) |
| O1 | 0.4195 (2) | 0.89792 (15) | 0.74670 (14) | 0.0387 (5) |
| O4 | 0.5221 (2) | 1.08313 (16) | 0.81065 (13) | 0.0328 (5) |
| N2 | 0.7365 (2) | 1.06673 (17) | 0.68765 (15) | 0.0243 (5) |
| N4 | 0.5626 (2) | 1.05068 (18) | 0.88143 (15) | 0.0300 (6) |
| O5 | 0.6358 (2) | 0.97414 (17) | 0.88213 (13) | 0.035 |
| N1 | 0.6896 (2) | 0.87411 (17) | 0.67467 (15) | 0.0242 (5) |
| N3 | 0.3281 (3) | 0.9442 (2) | 0.70369 (17) | 0.0381 (6) |
| O6 | 0.5273 (3) | 1.0950 (2) | 0.94430 (15) | 0.0558 (7) |
| C15 | 1.0722 (3) | 1.2220 (2) | 0.56813 (19) | 0.0308 (7) |
| C6 | 0.8337 (3) | 1.0146 (2) | 0.64671 (16) | 0.0225 (6) |
| C11 | 0.9809 (3) | 0.6535 (2) | 0.58589 (19) | 0.0279 (6) |
| O3 | 0.2114 (2) | 0.9132 (2) | 0.7046 (2) | 0.0649 (9) |
| C2 | 0.7514 (3) | 0.7040 (2) | 0.64459 (18) | 0.0275 (6) |
| H2 | 0.7265 | 0.6363 | 0.6436 | 0.033* |
| C3 | 0.8801 (3) | 0.7323 (2) | 0.61767 (18) | 0.0233 (6) |
| C8 | 0.9527 (3) | 1.1675 (2) | 0.61021 (18) | 0.0253 (6) |
| C7 | 0.9411 (3) | 1.0624 (2) | 0.60741 (17) | 0.0252 (6) |
| H7 | 1.0057 | 1.0245 | 0.5791 | 0.030* |

| | | | | |
|---|---|---|---|---|
| C5 | 0.8133 (3) | 0.9040 (2) | 0.64572 (17) | 0.0225 (6) |
| C4 | 0.9100 (3) | 0.83539 (19) | 0.61865 (16) | 0.0223 (5) |
| H4 | 0.9948 | 0.8580 | 0.6011 | 0.027* |
| C1 | 0.6602 (3) | 0.7753 (2) | 0.67289 (19) | 0.0281 (6) |
| H1 | 0.5752 | 0.7541 | 0.6914 | 0.034* |
| C10 | 0.7481 (3) | 1.1682 (2) | 0.69174 (19) | 0.0290 (6) |
| H10 | 0.6821 | 1.2047 | 0.7202 | 0.035* |
| C17 | 1.1679 (4) | 1.2577 (3) | 0.6369 (2) | 0.0507 (10) |
| H17A | 1.2445 | 1.2919 | 0.6128 | 0.076* |
| H17B | 1.1993 | 1.2006 | 0.6681 | 0.076* |
| H17C | 1.1202 | 1.3032 | 0.6730 | 0.076* |
| C9 | 0.8536 (3) | 1.2190 (2) | 0.65550 (19) | 0.0302 (7) |
| H9 | 0.8594 | 1.2888 | 0.6611 | 0.036* |
| C14 | 1.1222 (3) | 0.6979 (3) | 0.5698 (2) | 0.0400 (8) |
| H14A | 1.1817 | 0.6459 | 0.5498 | 0.060* |
| H14B | 1.1580 | 0.7251 | 0.6205 | 0.060* |
| H14C | 1.1155 | 0.7507 | 0.5292 | 0.060* |
| C13 | 0.9948 (3) | 0.5689 (2) | 0.6509 (2) | 0.0397 (8) |
| H13A | 1.0577 | 0.5189 | 0.6312 | 0.060* |
| H13B | 0.9076 | 0.5381 | 0.6600 | 0.060* |
| H13C | 1.0276 | 0.5969 | 0.7020 | 0.060* |
| C16 | 1.1495 (3) | 1.1522 (3) | 0.5092 (2) | 0.0410 (8) |
| H16A | 1.2235 | 1.1885 | 0.4844 | 0.062* |
| H16B | 1.0890 | 1.1287 | 0.4667 | 0.062* |
| H16C | 1.1845 | 1.0955 | 0.5396 | 0.062* |
| C12 | 0.9251 (4) | 0.6105 (3) | 0.5041 (2) | 0.0440 (8) |
| H12A | 0.9871 | 0.5607 | 0.4829 | 0.066* |
| H12B | 0.9154 | 0.6641 | 0.4645 | 0.066* |
| H12C | 0.8380 | 0.5798 | 0.5139 | 0.066* |
| C18 | 1.0207 (4) | 1.3135 (3) | 0.5182 (3) | 0.0512 (10) |
| H18A | 1.0965 | 1.3467 | 0.4923 | 0.077* |
| H18B | 0.9755 | 1.3598 | 0.5547 | 0.077* |
| H18C | 0.9581 | 1.2910 | 0.4764 | 0.077* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.02290 (16) | 0.02379 (17) | 0.02875 (18) | 0.00229 (14) | 0.00540 (15) | −0.00019 (15) |
| O2 | 0.021 | 0.0581 (15) | 0.0509 (13) | 0.0047 (11) | −0.0042 (9) | 0.0038 (14) |
| O1 | 0.0287 (10) | 0.0327 (11) | 0.0548 (15) | −0.0013 (9) | 0.0091 (10) | 0.0042 (9) |
| O4 | 0.0379 (11) | 0.0321 (12) | 0.0285 (11) | 0.0100 (9) | 0.0039 (10) | 0.0011 (10) |
| N2 | 0.0264 (12) | 0.0209 (12) | 0.0256 (12) | 0.0016 (10) | 0.0028 (10) | 0.0006 (10) |
| N4 | 0.0287 (13) | 0.0328 (14) | 0.0283 (13) | 0.0002 (11) | 0.0005 (11) | −0.0032 (11) |
| O5 | 0.033 | 0.034 | 0.038 | 0.0127 (10) | −0.0048 (9) | 0.0036 (10) |
| N1 | 0.0248 (11) | 0.0220 (13) | 0.0260 (13) | −0.0020 (10) | 0.0038 (10) | 0.0000 (10) |
| N3 | 0.0263 (13) | 0.0424 (16) | 0.0455 (17) | 0.0029 (11) | 0.0057 (10) | −0.0132 (13) |
| O6 | 0.0737 (18) | 0.0623 (17) | 0.0313 (14) | 0.0154 (14) | 0.0022 (13) | −0.0100 (12) |
| C15 | 0.0309 (16) | 0.0254 (15) | 0.0361 (17) | −0.0065 (14) | −0.0001 (15) | 0.0046 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0253 (13) | 0.0220 (14) | 0.0201 (13) | 0.0005 (12) | 0.0013 (11) | 0.0000 (12) |
| C11 | 0.0330 (15) | 0.0207 (15) | 0.0299 (16) | 0.0024 (13) | 0.0008 (13) | −0.0045 (12) |
| O3 | 0.0275 (13) | 0.0736 (19) | 0.094 (2) | −0.0068 (12) | −0.0036 (13) | −0.0171 (17) |
| C2 | 0.0291 (14) | 0.0201 (14) | 0.0332 (17) | −0.0039 (12) | 0.0012 (13) | −0.0010 (12) |
| C3 | 0.0286 (16) | 0.0214 (14) | 0.0200 (14) | 0.0008 (11) | −0.0055 (12) | 0.0007 (11) |
| C8 | 0.0287 (15) | 0.0230 (15) | 0.0242 (16) | −0.0037 (11) | −0.0047 (12) | 0.0036 (12) |
| C7 | 0.0239 (15) | 0.0255 (14) | 0.0262 (15) | −0.0011 (11) | 0.0027 (12) | −0.0024 (12) |
| C5 | 0.0246 (13) | 0.0227 (15) | 0.0202 (14) | −0.0013 (11) | 0.0003 (12) | −0.0016 (12) |
| C4 | 0.0206 (12) | 0.0243 (14) | 0.0218 (13) | −0.0023 (12) | 0.0018 (13) | −0.0016 (11) |
| C1 | 0.0258 (15) | 0.0240 (15) | 0.0344 (17) | −0.0039 (12) | 0.0010 (13) | −0.0002 (13) |
| C10 | 0.0345 (15) | 0.0232 (15) | 0.0295 (16) | 0.0059 (13) | 0.0041 (13) | −0.0012 (12) |
| C17 | 0.045 (2) | 0.056 (2) | 0.051 (2) | −0.0223 (18) | −0.0037 (18) | −0.0033 (19) |
| C9 | 0.0381 (16) | 0.0187 (15) | 0.0339 (17) | −0.0004 (12) | −0.0017 (14) | −0.0016 (13) |
| C14 | 0.0333 (18) | 0.0337 (18) | 0.053 (2) | 0.0072 (14) | 0.0107 (15) | −0.0022 (16) |
| C13 | 0.0459 (19) | 0.0285 (17) | 0.045 (2) | 0.0100 (15) | −0.0019 (16) | 0.0064 (15) |
| C16 | 0.0365 (17) | 0.0393 (19) | 0.047 (2) | −0.0091 (15) | 0.0115 (16) | 0.0047 (16) |
| C12 | 0.051 (2) | 0.043 (2) | 0.0384 (18) | 0.0096 (18) | −0.0011 (17) | −0.0151 (14) |
| C18 | 0.047 (2) | 0.040 (2) | 0.067 (3) | −0.0033 (17) | 0.0112 (19) | 0.0231 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.965 (2) | C8—C9 | 1.396 (4) |
| Cu1—O4 | 1.976 (2) | C8—C7 | 1.398 (4) |
| Cu1—N2 | 1.980 (2) | C7—H7 | 0.9300 |
| Cu1—O1 | 1.994 (2) | C5—C4 | 1.385 (4) |
| O2—N3 | 1.251 (4) | C4—H4 | 0.9300 |
| O1—N3 | 1.290 (3) | C1—H1 | 0.9300 |
| O4—N4 | 1.284 (3) | C10—C9 | 1.368 (4) |
| N2—C6 | 1.351 (3) | C10—H10 | 0.9300 |
| N2—C10 | 1.350 (4) | C17—H17A | 0.9600 |
| N4—O6 | 1.223 (3) | C17—H17B | 0.9600 |
| N4—O5 | 1.243 (3) | C17—H17C | 0.9600 |
| N1—C1 | 1.340 (4) | C9—H9 | 0.9300 |
| N1—C5 | 1.360 (4) | C14—H14A | 0.9600 |
| N3—O3 | 1.218 (3) | C14—H14B | 0.9600 |
| C15—C16 | 1.528 (4) | C14—H14C | 0.9600 |
| C15—C17 | 1.531 (5) | C13—H13A | 0.9600 |
| C15—C8 | 1.536 (4) | C13—H13B | 0.9600 |
| C15—C18 | 1.541 (4) | C13—H13C | 0.9600 |
| C6—C7 | 1.385 (4) | C16—H16A | 0.9600 |
| C6—C5 | 1.479 (4) | C16—H16B | 0.9600 |
| C11—C3 | 1.528 (4) | C16—H16C | 0.9600 |
| C11—C14 | 1.530 (4) | C12—H12A | 0.9600 |
| C11—C12 | 1.539 (4) | C12—H12B | 0.9600 |
| C11—C13 | 1.541 (4) | C12—H12C | 0.9600 |
| C2—C1 | 1.380 (4) | C18—H18A | 0.9600 |
| C2—C3 | 1.389 (4) | C18—H18B | 0.9600 |
| C2—H2 | 0.9300 | C18—H18C | 0.9600 |

| | | | |
|---|---|---|---|
| C3—C4 | 1.396 (4) | | |
| | | | |
| N1—Cu1—O4 | 163.03 (9) | C4—C5—C6 | 124.1 (2) |
| N1—Cu1—N2 | 82.49 (9) | C5—C4—C3 | 120.0 (3) |
| O4—Cu1—N2 | 94.41 (9) | C5—C4—H4 | 120.0 |
| N1—Cu1—O1 | 94.82 (9) | C3—C4—H4 | 120.0 |
| O4—Cu1—O1 | 91.59 (9) | N1—C1—C2 | 122.4 (3) |
| N2—Cu1—O1 | 167.53 (10) | N1—C1—H1 | 118.8 |
| N3—O1—Cu1 | 103.37 (17) | C2—C1—H1 | 118.8 |
| N4—O4—Cu1 | 105.23 (16) | N2—C10—C9 | 122.2 (3) |
| C6—N2—C10 | 118.2 (2) | N2—C10—H10 | 118.9 |
| C6—N2—Cu1 | 113.90 (18) | C9—C10—H10 | 118.9 |
| C10—N2—Cu1 | 127.8 (2) | C15—C17—H17A | 109.5 |
| O6—N4—O5 | 123.3 (3) | C15—C17—H17B | 109.5 |
| O6—N4—O4 | 119.3 (2) | H17A—C17—H17B | 109.5 |
| O5—N4—O4 | 117.4 (2) | C15—C17—H17C | 109.5 |
| C1—N1—C5 | 118.0 (2) | H17A—C17—H17C | 109.5 |
| C1—N1—Cu1 | 127.3 (2) | H17B—C17—H17C | 109.5 |
| C5—N1—Cu1 | 114.09 (18) | C10—C9—C8 | 120.8 (3) |
| O3—N3—O2 | 124.3 (3) | C10—C9—H9 | 119.6 |
| O3—N3—O1 | 119.2 (3) | C8—C9—H9 | 119.6 |
| O2—N3—O1 | 116.5 (2) | C11—C14—H14A | 109.5 |
| C16—C15—C17 | 109.4 (3) | C11—C14—H14B | 109.5 |
| C16—C15—C8 | 111.8 (2) | H14A—C14—H14B | 109.5 |
| C17—C15—C8 | 107.1 (3) | C11—C14—H14C | 109.5 |
| C16—C15—C18 | 108.3 (3) | H14A—C14—H14C | 109.5 |
| C17—C15—C18 | 109.7 (3) | H14B—C14—H14C | 109.5 |
| C8—C15—C18 | 110.5 (3) | C11—C13—H13A | 109.5 |
| N2—C6—C7 | 121.9 (3) | C11—C13—H13B | 109.5 |
| N2—C6—C5 | 114.6 (2) | H13A—C13—H13B | 109.5 |
| C7—C6—C5 | 123.5 (3) | C11—C13—H13C | 109.5 |
| C3—C11—C14 | 112.4 (2) | H13A—C13—H13C | 109.5 |
| C3—C11—C12 | 108.1 (3) | H13B—C13—H13C | 109.5 |
| C14—C11—C12 | 108.7 (3) | C15—C16—H16A | 109.5 |
| C3—C11—C13 | 109.0 (2) | C15—C16—H16B | 109.5 |
| C14—C11—C13 | 108.4 (3) | H16A—C16—H16B | 109.5 |
| C12—C11—C13 | 110.3 (3) | C15—C16—H16C | 109.5 |
| C1—C2—C3 | 120.6 (3) | H16A—C16—H16C | 109.5 |
| C1—C2—H2 | 119.7 | H16B—C16—H16C | 109.5 |
| C3—C2—H2 | 119.7 | C11—C12—H12A | 109.5 |
| C2—C3—C4 | 116.9 (3) | C11—C12—H12B | 109.5 |
| C2—C3—C11 | 120.7 (2) | H12A—C12—H12B | 109.5 |
| C4—C3—C11 | 122.4 (3) | C11—C12—H12C | 109.5 |
| C9—C8—C7 | 116.5 (3) | H12A—C12—H12C | 109.5 |
| C9—C8—C15 | 122.4 (3) | H12B—C12—H12C | 109.5 |
| C7—C8—C15 | 121.0 (3) | C15—C18—H18A | 109.5 |
| C6—C7—C8 | 120.2 (3) | C15—C18—H18B | 109.5 |
| C6—C7—H7 | 119.9 | H18A—C18—H18B | 109.5 |

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|---|---|---|---|
| C8—C7—H7 | 119.9 | C15—C18—H18C | 109.5 |
| N1—C5—C4 | 122.0 (3) | H18A—C18—H18C | 109.5 |
| N1—C5—C6 | 113.9 (2) | H18B—C18—H18C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O4$^{i}$ | 0.93 | 2.46 | 3.124 (3) | 129 |

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+3/2.