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# Bis(nitrato-$\kappa O$)tetrakis[1-phenyl-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one]-copper(II)

**Hua Cai,* Ying Guo, Jian-Gang Li and Yao Wu**

College of Science, Civil Aviation University of China, Tianjin 300300, People's Republic of China
Correspondence e-mail: caihua-1109@163.com

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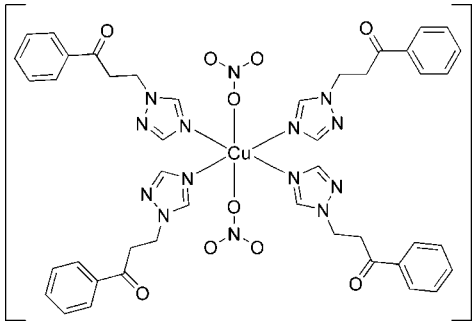
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.040; $wR$ factor = 0.105; data-to-parameter ratio = 12.5.

In the title complex, $[Cu(NO_3)_2(C_{11}H_{11}N_3O)_4]$, the $Cu^{II}$ atom is situated on a centre of inversion and is coordinated by two O atoms from two nitrate anions and four N atoms from four monodentate 1-phenyl-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one ligands in a distorted octahedral geometry. Weak intermolecular C—H···O and C—H···N hydrogen bonds result in a supramolecular layer parallel to (101). These layers are connected by $\pi$–$\pi$ interactions between the benzene rings [centroid–centroid distance = 3.891 (2) Å].

## Related literature

For background to complexes with neutral N-containing ligands, see: Barnett & Champness (2003); Roesky & Andruh (2003); Zaworotko (2001). For a related structure, see: Cai *et al.* (2010).



## Experimental

### Crystal data

$[Cu(NO_3)_2(C_{11}H_{11}N_3O)_4]$ $M_r$ = 992.47
Triclinic, $P\overline{1}$
$a$ = 7.7742 (14) Å
$b$ = 12.472 (2) Å
$c$ = 12.498 (2) Å
$\alpha$ = 102.232 (3)°
$\beta$ = 100.737 (3)°
$\gamma$ = 104.394 (3)°
$V$ = 1110.0 (3) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.57 mm$^{-1}$
$T$ = 296 K
0.24 × 0.20 × 0.14 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.876, $T_{max}$ = 0.925
5737 measured reflections
3905 independent reflections
3295 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
$S$ = 1.03
3905 reflections
313 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14$A$···N2$^{i}$ | 0.97 | 2.50 | 3.368 (4) | 148 |
| C19—H19···O5$^{ii}$ | 0.93 | 2.56 | 3.291 (4) | 136 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg & Berndt, 1999); 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: HY2463).

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# supporting information

*Acta Cryst.* (2011). E**67**, m1385 [https://doi.org/10.1107/S160053681103529X]

## Bis(nitrato-$\kappa O$)tetrakis[1-phenyl-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one]copper(II)

**Hua Cai, Ying Guo, Jian-Gang Li and Yao Wu**

### S1. Comment

Neutral organic ligands containing rigid or flexible spacers, such as 4,4′-bipyridine, 1,2-bis(4-pyridyl)ethane, 1,2-bis(4-pyridyl)propane and many others, have been used to generate a rich variety of metal-organic architectures with different metal ions by various reaction procedures (Barnett & Champness, 2003; Roesky & Andruh, 2003; Zaworotko, 2001). Recently, we have initiated a research program of synthesizing supermolecules based on pseudohalides and a flexible ligand, which consists of a propanone unit substituted with a triazole and a phenyl group (Cai *et al.*, 2010). To further explore this series, we synthesized the title compound, a new Cu(II) complex based on the ligand 1-phenyl-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one (*L*).

In the neutral mononuclear title complex (Fig. 1), the $Cu^{II}$ atom is six-coordinated by four monodentate *L* ligands in the equatorial plane and two O atoms from two $NO_3^-$ anions in the axial positions, displaying a $CuN_4O_2$ octahedral geometry. The triazol and phenyl rings in the ligands are not coplanar. The dihedral angels formed by the least-squares planes of the phenyl and triazole rings are 43.8 (2) and 65.9 (2)°. Weak intermolecular C—H···O and C—H···N hydrogen bonds (Table 1) extend the monomeric units into a two-dimensional supramolecular layer parallel to (1 0 1), as shown in Fig. 2.

### S2. Experimental

$Cu(NO_3)_2.3H_2O$ (24.2 mg, 0.1 mmol) and *L* (22.3 mg, 0.1 mmol) were mixed in a $CH_3CN/H_2O$ (20 ml, v/v 1:1) solution with vigorous stirring for *ca* 30 min. The resulting solution was filtered and left to stand at room temperature. Colourless block crystals of the title compound suitable for X-ray analysis were obtained in 65% yield by slow evaporation of the solvent over a period of 1 week. Analysis, calculated for $C_{46}H_{44}MnN_{14}O_4S_2$: C 53.25, H 4.47, N 19.76%; found: C 53.45, H 4.43, N 19.62%.

### S3. Refinement

Although all H atoms were visible in difference Fourier maps, they were finally placed in geometrically calculated positions and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.97 (methylene) Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

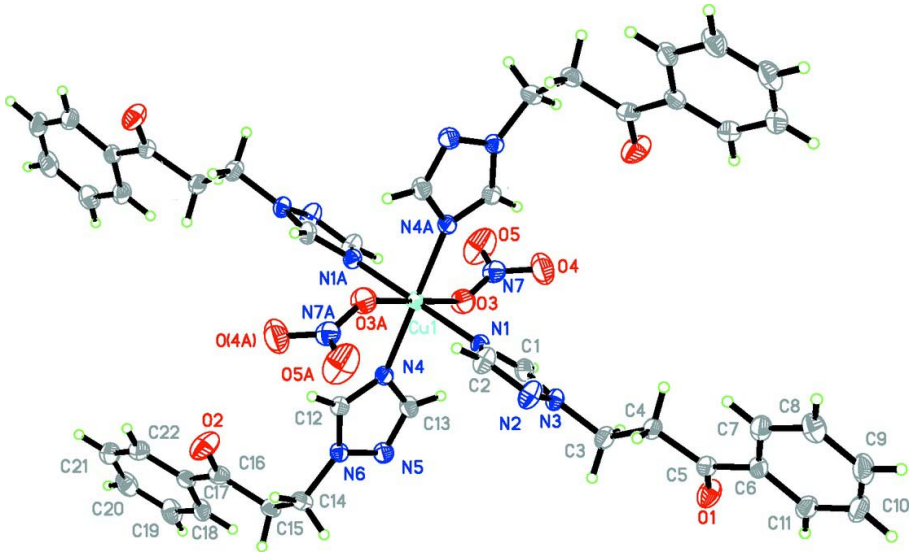


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) -x, 1-y, -z.]

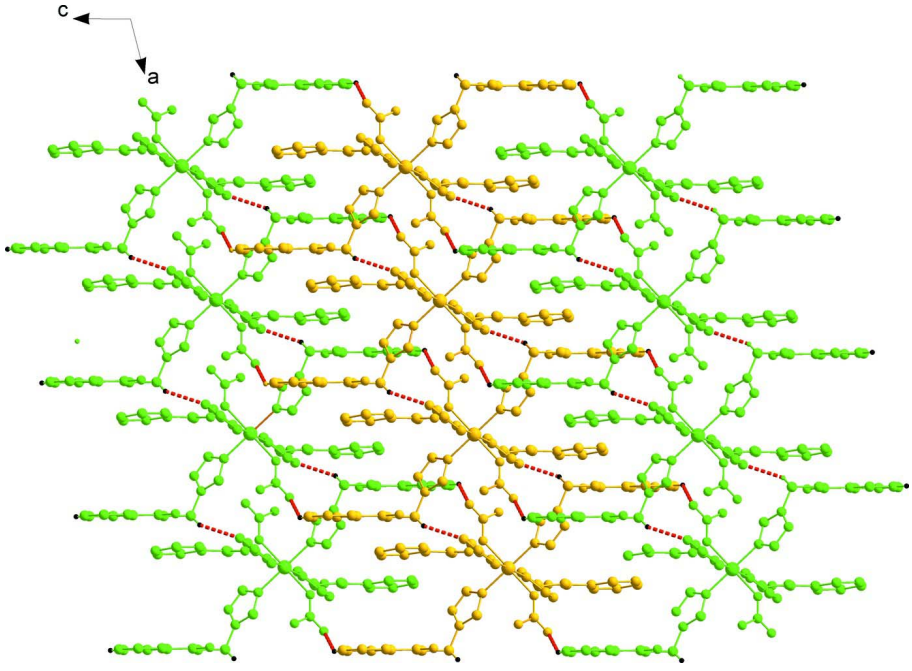


**Figure 2**

The two-dimensional layer structure of the title compound, showing C—H···O and C—H···N hydrogen bonds as red dashed lines.

**Bis(nitrato-*κO*)tetrakis[1-phenyl-3-(1*H*-1,2,4-triazol- 1-yl)propan-1-one]copper(II)**

*Crystal data*

$[Cu(NO_3)_2(C_{11}H_{11}N_3O)_4]$
$M_r$ = 992.47

Triclinic, $P\overline{1}$
Hall symbol: -P 1

$a$ = 7.7742 (14) Å
$b$ = 12.472 (2) Å
$c$ = 12.498 (2) Å
$\alpha$ = 102.232 (3)°
$\beta$ = 100.737 (3)°
$\gamma$ = 104.394 (3)°
$V$ = 1110.0 (3) Å$^3$
$Z$ = 1
$F$(000) = 515

$D_x$ = 1.485 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2167 reflections
$\theta$ = 2.8–25.5°
$\mu$ = 0.57 mm$^{-1}$
$T$ = 296 K
Block, blue
0.24 × 0.20 × 0.14 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.876, $T_{max}$ = 0.925

5737 measured reflections
3905 independent reflections
3295 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.8°
$h$ = −9→9
$k$ = −14→10
$l$ = −13→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
$S$ = 1.03
3905 reflections
313 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.6085P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.0000 | 0.5000 | 0.0000 | 0.03192 (15) |
| O1 | 0.1209 (3) | −0.14388 (17) | −0.15924 (18) | 0.0600 (6) |
| O2 | 0.6023 (4) | 0.8407 (2) | 0.42668 (19) | 0.0725 (7) |
| O3 | −0.2044 (3) | 0.38551 (18) | 0.0827 (2) | 0.0617 (6) |
| O4 | −0.4197 (4) | 0.2377 (2) | −0.0202 (2) | 0.0874 (8) |
| O5 | −0.4769 (4) | 0.3628 (3) | 0.1018 (3) | 0.1086 (11) |
| N1 | 0.0657 (3) | 0.36119 (17) | −0.06904 (17) | 0.0338 (5) |
| N2 | 0.2167 (4) | 0.26287 (19) | −0.1668 (2) | 0.0493 (6) |
| N3 | 0.1188 (3) | 0.19722 (17) | −0.11162 (17) | 0.0351 (5) |
| N4 | 0.1884 (3) | 0.51953 (16) | 0.14694 (16) | 0.0335 (5) |
| N5 | 0.3189 (3) | 0.47333 (18) | 0.29969 (18) | 0.0414 (5) |
| N6 | 0.4316 (3) | 0.56936 (17) | 0.28594 (17) | 0.0330 (5) |
| N7 | −0.3682 (3) | 0.3303 (2) | 0.0570 (2) | 0.0495 (6) |
| C1 | 0.0307 (4) | 0.2570 (2) | −0.0540 (2) | 0.0374 (6) |
| H1 | −0.0444 | 0.2297 | −0.0097 | 0.045* |
| C2 | 0.1795 (4) | 0.3605 (2) | −0.1381 (2) | 0.0468 (7) |
| H2 | 0.2276 | 0.4237 | −0.1633 | 0.056* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.1336 (4) | 0.0823 (2) | −0.1151 (2) | 0.0426 (6) |
| H3A | 0.0389 | 0.0418 | −0.0848 | 0.051* |
| H3B | 0.2518 | 0.0884 | −0.0681 | 0.051* |
| C4 | 0.1139 (4) | 0.0150 (2) | −0.2340 (2) | 0.0397 (6) |
| H4A | 0.2116 | 0.0543 | −0.2630 | 0.048* |
| H4B | −0.0020 | 0.0122 | −0.2815 | 0.048* |
| C5 | 0.1208 (3) | −0.1061 (2) | −0.2409 (2) | 0.0382 (6) |
| C6 | 0.1233 (3) | −0.1786 (2) | −0.3521 (2) | 0.0376 (6) |
| C7 | 0.0983 (4) | −0.1428 (2) | −0.4503 (2) | 0.0486 (7) |
| H7 | 0.0843 | −0.0704 | −0.4472 | 0.058* |
| C8 | 0.0941 (4) | −0.2141 (3) | −0.5531 (3) | 0.0581 (8) |
| H8 | 0.0746 | −0.1901 | −0.6187 | 0.070* |
| C9 | 0.1190 (4) | −0.3198 (3) | −0.5576 (3) | 0.0610 (9) |
| H9 | 0.1160 | −0.3677 | −0.6264 | 0.073* |
| C10 | 0.1481 (4) | −0.3550 (2) | −0.4609 (3) | 0.0581 (9) |
| H10 | 0.1668 | −0.4264 | −0.4644 | 0.070* |
| C11 | 0.1500 (4) | −0.2856 (2) | −0.3582 (3) | 0.0461 (7) |
| H11 | 0.1692 | −0.3105 | −0.2932 | 0.055* |
| C12 | 0.3529 (3) | 0.5953 (2) | 0.1955 (2) | 0.0332 (6) |
| H12 | 0.4050 | 0.6574 | 0.1698 | 0.040* |
| C13 | 0.1750 (4) | 0.4467 (2) | 0.2141 (2) | 0.0412 (6) |
| H13 | 0.0727 | 0.3835 | 0.2006 | 0.049* |
| C14 | 0.6175 (3) | 0.6206 (2) | 0.3603 (2) | 0.0400 (6) |
| H14A | 0.6857 | 0.6797 | 0.3316 | 0.048* |
| H14B | 0.6794 | 0.5618 | 0.3585 | 0.048* |
| C15 | 0.6195 (4) | 0.6732 (2) | 0.4821 (2) | 0.0383 (6) |
| H15A | 0.5158 | 0.6264 | 0.5009 | 0.046* |
| H15B | 0.7306 | 0.6721 | 0.5317 | 0.046* |
| C16 | 0.6107 (4) | 0.7953 (2) | 0.5032 (2) | 0.0409 (6) |
| C17 | 0.6149 (3) | 0.8587 (2) | 0.6201 (2) | 0.0382 (6) |
| C18 | 0.6220 (4) | 0.8080 (2) | 0.7086 (2) | 0.0445 (7) |
| H18 | 0.6255 | 0.7325 | 0.6964 | 0.053* |
| C19 | 0.6238 (4) | 0.8694 (3) | 0.8155 (3) | 0.0580 (8) |
| H19 | 0.6280 | 0.8348 | 0.8745 | 0.070* |
| C20 | 0.6193 (4) | 0.9811 (3) | 0.8344 (3) | 0.0600 (9) |
| H20 | 0.6210 | 1.0220 | 0.9062 | 0.072* |
| C21 | 0.6123 (4) | 1.0324 (3) | 0.7475 (3) | 0.0601 (9) |
| H21 | 0.6091 | 1.1081 | 0.7605 | 0.072* |
| C22 | 0.6099 (4) | 0.9717 (2) | 0.6406 (3) | 0.0504 (7) |
| H22 | 0.6049 | 1.0069 | 0.5819 | 0.060* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0358 (3) | 0.0315 (2) | 0.0255 (2) | 0.01221 (18) | 0.00439 (18) | 0.00191 (17) |
| O1 | 0.0937 (17) | 0.0467 (12) | 0.0502 (13) | 0.0292 (12) | 0.0234 (12) | 0.0209 (10) |
| O2 | 0.126 (2) | 0.0701 (15) | 0.0463 (13) | 0.0520 (15) | 0.0302 (14) | 0.0325 (12) |
| O3 | 0.0424 (12) | 0.0555 (13) | 0.0895 (17) | 0.0057 (10) | 0.0197 (11) | 0.0325 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.095 (2) | 0.0634 (16) | 0.0724 (18) | −0.0020 (14) | −0.0014 (15) | 0.0032 (14) |
| O5 | 0.102 (2) | 0.094 (2) | 0.170 (3) | 0.0450 (18) | 0.096 (2) | 0.048 (2) |
| N1 | 0.0401 (12) | 0.0319 (11) | 0.0282 (11) | 0.0125 (9) | 0.0091 (9) | 0.0031 (9) |
| N2 | 0.0711 (17) | 0.0410 (13) | 0.0495 (15) | 0.0233 (12) | 0.0348 (13) | 0.0159 (11) |
| N3 | 0.0445 (12) | 0.0296 (11) | 0.0316 (11) | 0.0116 (9) | 0.0123 (10) | 0.0063 (9) |
| N4 | 0.0382 (12) | 0.0321 (11) | 0.0281 (11) | 0.0103 (9) | 0.0050 (9) | 0.0070 (9) |
| N5 | 0.0489 (13) | 0.0389 (12) | 0.0352 (13) | 0.0097 (10) | 0.0065 (11) | 0.0155 (10) |
| N6 | 0.0361 (11) | 0.0338 (11) | 0.0277 (11) | 0.0090 (9) | 0.0071 (9) | 0.0079 (9) |
| N7 | 0.0480 (15) | 0.0492 (15) | 0.0577 (16) | 0.0122 (12) | 0.0174 (13) | 0.0272 (13) |
| C1 | 0.0429 (15) | 0.0340 (14) | 0.0332 (14) | 0.0084 (11) | 0.0137 (12) | 0.0050 (11) |
| C2 | 0.069 (2) | 0.0383 (15) | 0.0432 (16) | 0.0201 (14) | 0.0271 (15) | 0.0153 (12) |
| C3 | 0.0554 (17) | 0.0328 (14) | 0.0414 (16) | 0.0169 (12) | 0.0116 (13) | 0.0100 (12) |
| C4 | 0.0471 (15) | 0.0319 (13) | 0.0381 (15) | 0.0149 (12) | 0.0068 (12) | 0.0054 (11) |
| C5 | 0.0360 (14) | 0.0334 (13) | 0.0428 (16) | 0.0097 (11) | 0.0065 (12) | 0.0096 (12) |
| C6 | 0.0321 (13) | 0.0309 (13) | 0.0446 (16) | 0.0066 (10) | 0.0067 (12) | 0.0055 (11) |
| C7 | 0.0565 (18) | 0.0384 (15) | 0.0459 (17) | 0.0142 (13) | 0.0092 (14) | 0.0044 (13) |
| C8 | 0.061 (2) | 0.0571 (19) | 0.0442 (18) | 0.0099 (16) | 0.0091 (15) | 0.0020 (15) |
| C9 | 0.0533 (19) | 0.0520 (19) | 0.061 (2) | 0.0097 (15) | 0.0167 (16) | −0.0149 (16) |
| C10 | 0.0476 (17) | 0.0343 (15) | 0.086 (3) | 0.0137 (13) | 0.0185 (17) | −0.0007 (16) |
| C11 | 0.0393 (15) | 0.0345 (14) | 0.064 (2) | 0.0112 (12) | 0.0145 (14) | 0.0115 (13) |
| C12 | 0.0392 (14) | 0.0333 (13) | 0.0278 (13) | 0.0104 (11) | 0.0094 (11) | 0.0097 (10) |
| C13 | 0.0470 (16) | 0.0364 (14) | 0.0347 (15) | 0.0060 (12) | 0.0066 (12) | 0.0090 (11) |
| C14 | 0.0334 (14) | 0.0492 (16) | 0.0356 (15) | 0.0142 (12) | 0.0054 (11) | 0.0087 (12) |
| C15 | 0.0376 (14) | 0.0430 (15) | 0.0302 (14) | 0.0095 (12) | 0.0012 (11) | 0.0110 (11) |
| C16 | 0.0413 (15) | 0.0482 (16) | 0.0348 (15) | 0.0152 (12) | 0.0050 (12) | 0.0166 (12) |
| C17 | 0.0333 (13) | 0.0407 (14) | 0.0349 (15) | 0.0078 (11) | 0.0016 (11) | 0.0089 (11) |
| C18 | 0.0502 (16) | 0.0390 (15) | 0.0350 (15) | 0.0042 (12) | 0.0039 (12) | 0.0076 (12) |
| C19 | 0.066 (2) | 0.0575 (19) | 0.0357 (17) | 0.0012 (16) | 0.0055 (15) | 0.0091 (14) |
| C20 | 0.057 (2) | 0.066 (2) | 0.0393 (18) | 0.0092 (16) | 0.0051 (15) | −0.0056 (15) |
| C21 | 0.060 (2) | 0.0468 (17) | 0.061 (2) | 0.0198 (15) | −0.0002 (16) | −0.0022 (15) |
| C22 | 0.0531 (18) | 0.0471 (17) | 0.0475 (18) | 0.0177 (14) | −0.0001 (14) | 0.0138 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.9931 (19) | C6—C11 | 1.389 (4) |
| Cu1—N4 | 2.0515 (19) | C7—C8 | 1.388 (4) |
| Cu1—O3 | 2.396 (2) | C7—H7 | 0.9300 |
| O1—C5 | 1.211 (3) | C8—C9 | 1.370 (4) |
| O2—C16 | 1.210 (3) | C8—H8 | 0.9300 |
| O3—N7 | 1.232 (3) | C9—C10 | 1.370 (5) |
| O4—N7 | 1.257 (3) | C9—H9 | 0.9300 |
| O5—N7 | 1.201 (3) | C10—C11 | 1.384 (4) |
| N1—C1 | 1.321 (3) | C10—H10 | 0.9300 |
| N1—C2 | 1.346 (3) | C11—H11 | 0.9300 |
| N2—C2 | 1.313 (3) | C12—H12 | 0.9300 |
| N2—N3 | 1.360 (3) | C13—H13 | 0.9300 |
| N3—C1 | 1.325 (3) | C14—C15 | 1.520 (4) |
| N3—C3 | 1.459 (3) | C14—H14A | 0.9700 |

| | | | |
|---|---|---|---|
| N4—C12 | 1.328 (3) | C14—H14B | 0.9700 |
| N4—C13 | 1.360 (3) | C15—C16 | 1.512 (4) |
| N5—C13 | 1.313 (3) | C15—H15A | 0.9700 |
| N5—N6 | 1.361 (3) | C15—H15B | 0.9700 |
| N6—C12 | 1.324 (3) | C16—C17 | 1.496 (4) |
| N6—C14 | 1.467 (3) | C17—C18 | 1.385 (4) |
| C1—H1 | 0.9300 | C17—C22 | 1.391 (4) |
| C2—H2 | 0.9300 | C18—C19 | 1.387 (4) |
| C3—C4 | 1.503 (4) | C18—H18 | 0.9300 |
| C3—H3A | 0.9700 | C19—C20 | 1.373 (5) |
| C3—H3B | 0.9700 | C19—H19 | 0.9300 |
| C4—C5 | 1.510 (3) | C20—C21 | 1.371 (5) |
| C4—H4A | 0.9700 | C20—H20 | 0.9300 |
| C4—H4B | 0.9700 | C21—C22 | 1.384 (4) |
| C5—C6 | 1.495 (4) | C21—H21 | 0.9300 |
| C6—C7 | 1.389 (4) | C22—H22 | 0.9300 |

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| N1—Cu1—N1$^{i}$ | 180.00 (11) | C11—C6—C5 | 119.3 (3) |
| N1—Cu1—N4$^{i}$ | 91.68 (8) | C8—C7—C6 | 120.7 (3) |
| N1$^{i}$—Cu1—N4$^{i}$ | 88.32 (8) | C8—C7—H7 | 119.7 |
| N1—Cu1—N4 | 88.32 (8) | C6—C7—H7 | 119.7 |
| N1$^{i}$—Cu1—N4 | 91.68 (8) | C9—C8—C7 | 119.8 (3) |
| N4$^{i}$—Cu1—N4 | 180.00 (11) | C9—C8—H8 | 120.1 |
| N1—Cu1—O3$^{i}$ | 90.37 (8) | C7—C8—H8 | 120.1 |
| N1$^{i}$—Cu1—O3$^{i}$ | 89.63 (8) | C10—C9—C8 | 120.1 (3) |
| N4$^{i}$—Cu1—O3$^{i}$ | 82.97 (8) | C10—C9—H9 | 119.9 |
| N4—Cu1—O3$^{i}$ | 97.03 (8) | C8—C9—H9 | 119.9 |
| N1—Cu1—O3 | 89.63 (8) | C9—C10—C11 | 120.6 (3) |
| N1$^{i}$—Cu1—O3 | 90.37 (8) | C9—C10—H10 | 119.7 |
| N4$^{i}$—Cu1—O3 | 97.03 (8) | C11—C10—H10 | 119.7 |
| N4—Cu1—O3 | 82.97 (8) | C10—C11—C6 | 120.1 (3) |
| O3$^{i}$—Cu1—O3 | 180.0 | C10—C11—H11 | 120.0 |
| N7—O3—Cu1 | 136.91 (19) | C6—C11—H11 | 120.0 |
| C1—N1—C2 | 103.6 (2) | N6—C12—N4 | 109.9 (2) |
| C1—N1—Cu1 | 132.14 (18) | N6—C12—H12 | 125.1 |
| C2—N1—Cu1 | 123.99 (17) | N4—C12—H12 | 125.1 |
| C2—N2—N3 | 102.5 (2) | N5—C13—N4 | 114.2 (2) |
| C1—N3—N2 | 110.0 (2) | N5—C13—H13 | 122.9 |
| C1—N3—C3 | 129.9 (2) | N4—C13—H13 | 122.9 |
| N2—N3—C3 | 119.9 (2) | N6—C14—C15 | 113.0 (2) |
| C12—N4—C13 | 103.1 (2) | N6—C14—H14A | 109.0 |
| C12—N4—Cu1 | 131.17 (17) | C15—C14—H14A | 109.0 |
| C13—N4—Cu1 | 125.54 (17) | N6—C14—H14B | 109.0 |
| C13—N5—N6 | 102.6 (2) | C15—C14—H14B | 109.0 |
| C12—N6—N5 | 110.2 (2) | H14A—C14—H14B | 107.8 |
| C12—N6—C14 | 130.0 (2) | C16—C15—C14 | 113.0 (2) |
| N5—N6—C14 | 119.5 (2) | C16—C15—H15A | 109.0 |
| O5—N7—O3 | 122.4 (3) | C14—C15—H15A | 109.0 |

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| O5—N7—O4 | 120.4 (3) | C16—C15—H15B | 109.0 |
| O3—N7—O4 | 117.3 (3) | C14—C15—H15B | 109.0 |
| N1—C1—N3 | 109.7 (2) | H15A—C15—H15B | 107.8 |
| N1—C1—H1 | 125.2 | O2—C16—C17 | 121.1 (3) |
| N3—C1—H1 | 125.2 | O2—C16—C15 | 120.1 (3) |
| N2—C2—N1 | 114.3 (2) | C17—C16—C15 | 118.8 (2) |
| N2—C2—H2 | 122.8 | C18—C17—C22 | 118.7 (3) |
| N1—C2—H2 | 122.8 | C18—C17—C16 | 122.1 (2) |
| N3—C3—C4 | 111.1 (2) | C22—C17—C16 | 119.1 (2) |
| N3—C3—H3A | 109.4 | C17—C18—C19 | 120.3 (3) |
| C4—C3—H3A | 109.4 | C17—C18—H18 | 119.8 |
| N3—C3—H3B | 109.4 | C19—C18—H18 | 119.8 |
| C4—C3—H3B | 109.4 | C20—C19—C18 | 120.2 (3) |
| H3A—C3—H3B | 108.0 | C20—C19—H19 | 119.9 |
| C3—C4—C5 | 112.3 (2) | C18—C19—H19 | 119.9 |
| C3—C4—H4A | 109.1 | C21—C20—C19 | 120.1 (3) |
| C5—C4—H4A | 109.1 | C21—C20—H20 | 119.9 |
| C3—C4—H4B | 109.1 | C19—C20—H20 | 119.9 |
| C5—C4—H4B | 109.1 | C20—C21—C22 | 120.0 (3) |
| H4A—C4—H4B | 107.9 | C20—C21—H21 | 120.0 |
| O1—C5—C6 | 121.2 (2) | C22—C21—H21 | 120.0 |
| O1—C5—C4 | 120.9 (2) | C21—C22—C17 | 120.6 (3) |
| C6—C5—C4 | 118.0 (2) | C21—C22—H22 | 119.7 |
| C7—C6—C11 | 118.6 (3) | C17—C22—H22 | 119.7 |
| C7—C6—C5 | 122.1 (2) | | |

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| N1—Cu1—O3—N7 | −92.4 (3) | C3—C4—C5—C6 | −173.5 (2) |
| N1$^{i}$—Cu1—O3—N7 | 87.6 (3) | O1—C5—C6—C7 | 171.1 (3) |
| N4$^{i}$—Cu1—O3—N7 | −0.8 (3) | C4—C5—C6—C7 | −7.5 (4) |
| N4—Cu1—O3—N7 | 179.2 (3) | O1—C5—C6—C11 | −8.4 (4) |
| N4$^{i}$—Cu1—N1—C1 | −107.5 (2) | C4—C5—C6—C11 | 172.9 (2) |
| N4—Cu1—N1—C1 | 72.5 (2) | C11—C6—C7—C8 | 2.1 (4) |
| O3$^{i}$—Cu1—N1—C1 | 169.5 (2) | C5—C6—C7—C8 | −177.5 (3) |
| O3—Cu1—N1—C1 | −10.5 (2) | C6—C7—C8—C9 | −1.5 (5) |
| N4$^{i}$—Cu1—N1—C2 | 79.8 (2) | C7—C8—C9—C10 | −0.1 (5) |
| N4—Cu1—N1—C2 | −100.2 (2) | C8—C9—C10—C11 | 1.0 (5) |
| O3$^{i}$—Cu1—N1—C2 | −3.2 (2) | C9—C10—C11—C6 | −0.4 (4) |
| O3—Cu1—N1—C2 | 176.8 (2) | C7—C6—C11—C10 | −1.2 (4) |
| C2—N2—N3—C1 | −0.2 (3) | C5—C6—C11—C10 | 178.4 (2) |
| C2—N2—N3—C3 | −175.6 (2) | N5—N6—C12—N4 | 0.2 (3) |
| N1—Cu1—N4—C12 | 107.1 (2) | C14—N6—C12—N4 | 173.7 (2) |
| N1$^{i}$—Cu1—N4—C12 | −72.9 (2) | C13—N4—C12—N6 | −0.2 (3) |
| O3$^{i}$—Cu1—N4—C12 | 16.9 (2) | Cu1—N4—C12—N6 | −175.26 (16) |
| O3—Cu1—N4—C12 | −163.1 (2) | N6—N5—C13—N4 | −0.1 (3) |
| N1—Cu1—N4—C13 | −66.9 (2) | C12—N4—C13—N5 | 0.2 (3) |
| N1$^{i}$—Cu1—N4—C13 | 113.1 (2) | Cu1—N4—C13—N5 | 175.61 (17) |
| O3$^{i}$—Cu1—N4—C13 | −157.1 (2) | C12—N6—C14—C15 | 118.9 (3) |
| O3—Cu1—N4—C13 | 22.9 (2) | N5—N6—C14—C15 | −68.1 (3) |

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|---|---|---|---|
| C13—N5—N6—C12 | 0.0 (3) | N6—C14—C15—C16 | −85.4 (3) |
| C13—N5—N6—C14 | −174.4 (2) | C14—C15—C16—O2 | 0.3 (4) |
| Cu1—O3—N7—O5 | −107.0 (4) | C14—C15—C16—C17 | −178.9 (2) |
| Cu1—O3—N7—O4 | 72.1 (4) | O2—C16—C17—C18 | 179.1 (3) |
| C2—N1—C1—N3 | −0.2 (3) | C15—C16—C17—C18 | −1.7 (4) |
| Cu1—N1—C1—N3 | −173.99 (16) | O2—C16—C17—C22 | −0.3 (4) |
| N2—N3—C1—N1 | 0.3 (3) | C15—C16—C17—C22 | 179.0 (2) |
| C3—N3—C1—N1 | 175.1 (2) | C22—C17—C18—C19 | 0.1 (4) |
| N3—N2—C2—N1 | 0.0 (3) | C16—C17—C18—C19 | −179.3 (3) |
| C1—N1—C2—N2 | 0.1 (3) | C17—C18—C19—C20 | −0.2 (5) |
| Cu1—N1—C2—N2 | 174.55 (19) | C18—C19—C20—C21 | 0.2 (5) |
| C1—N3—C3—C4 | 137.6 (3) | C19—C20—C21—C22 | −0.1 (5) |
| N2—N3—C3—C4 | −48.0 (3) | C20—C21—C22—C17 | −0.1 (5) |
| N3—C3—C4—C5 | −177.6 (2) | C18—C17—C22—C21 | 0.1 (4) |
| C3—C4—C5—O1 | 7.8 (4) | C16—C17—C22—C21 | 179.5 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14*A*···N2$^{ii}$ | 0.97 | 2.50 | 3.368 (4) | 148 |
| C19—H19···O5$^{iii}$ | 0.93 | 2.56 | 3.291 (4) | 136 |

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