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(2-Acetylphenolato)(2,2'-bipyridine)-nitratocopper(II)

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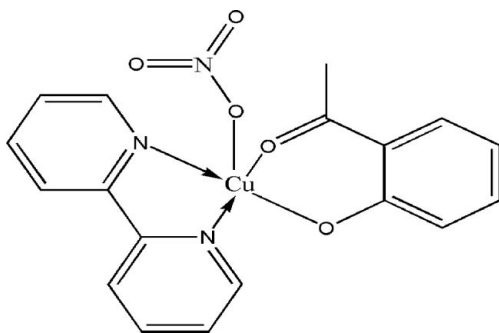
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.029; wR factor = 0.074; data-to-parameter ratio = 11.9.

In the title compound, $[\text{Cu}(\text{C}_8\text{H}_7\text{O}_2)(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)]$, the Cu^{II} ion is five-coordinate in a distorted square-pyramidal geometry. The basal positions are occupied by two N atoms from a 2,2'-bipyridine ligand and two O atoms from the 2-acetylphenolate anion. The axial position is occupied by one O atom of a nitrate anion. In the bipyridine ligand, the two pyridine rings are slightly twisted by an angle of 3.5 (1°). The crystal structure is stabilized by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds

Related literature

For related structures, see: Bevan *et al.* (1963); Falguni *et al.* (1998); Garland *et al.* (1986); Gasque *et al.* (1999); Ming *et al.* (1995); Reki *et al.* (1998); Solans *et al.* (1987). For the synthesis, see: Plesch *et al.* (1997).



Experimental

Crystal data

 $[\text{Cu}(\text{C}_8\text{H}_7\text{O}_2)(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)]$
 $M_r = 416.87$

 Monoclinic, $P2_1/n$
 $a = 13.4683$ (12) Å

 $b = 8.3101$ (8) Å

 $c = 15.5924$ (15) Å

 $\beta = 108.583$ (1°)

 $V = 1654.2$ (3) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 1.36$ mm⁻¹
 $T = 296$ K

 $0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.686$, $T_{\text{max}} = 0.773$

8261 measured reflections

2917 independent reflections

 2370 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.074$
 $S = 1.03$

2917 reflections

245 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³
Table 1

Selected bond lengths (Å).

| | | | |
|--------|-------------|--------|-----------|
| Cu1—O1 | 1.8832 (17) | Cu1—N1 | 1.998 (2) |
| Cu1—O2 | 1.9307 (17) | Cu1—O3 | 2.434 (2) |
| Cu1—N2 | 1.9941 (19) | | |

Table 2

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C2}-\text{H2}\cdots\text{O3}^{\text{i}}$ | 0.93 | 2.59 | 3.401 (4) | 146 |
| $\text{C7}-\text{H7}\cdots\text{O3}^{\text{ii}}$ | 0.93 | 2.51 | 3.343 (3) | 150 |

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); 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); 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: CI2918).

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supplementary materials

Acta Cryst. (2009). E65, m1427 [doi:10.1107/S1600536809042718]

(2-Acetylphenolato)(2,2'-bipyridine)nitratocopper(II)

L.-H. Chen, G.-Q. Zhao, X. Wang, Q.-L. Peng and Z.-H. Pan

Comment

Crystal structures of bis(salicylaldehydato)copper(II) (Bevan *et al.*, 1963), (1,10-phenanthroline)(salicylaldehydato)copper(II) (Solans *et al.*, 1987), Aqua(4,7-diphenyl-1,10-phenanthroline)(salicylaldehydato)copper(II) nitrate monohydrate (Gasque *et al.*, 1999), (2,2'-bipyridine)(salicylaldehydato)copper(II) (Garland *et al.*, 1986), [Cu(5-carboxysalicylaldehyde)(2,2'-bipyridine)(ClO₄)] and [Cu(5-carboxysalicylaldehyde)(2,2'-bipyridine)(2H₂O)] (Reki *et al.*, 1998), [Cu(salicylaldehyde)(1,10-phenanthroline)(ClO₄)₂] (Ming *et al.*, 1995). We report here the crystal structure of the title Cu^{II} complex.

In the title compound, the Cu^{II} ion is in a distorted square-pyramidal geometry (Fig. 1 and Table 1). The four basal positions are occupied by two N donor atoms from a 2,2'-bipyridine ligand and two O atoms from the 2-acetylphenolate anion. The axial position is occupied by one O atom of a nitrate anion. The Cu1 atom is displaced from the O1/O2/N1/N2 basal plane toward the O3 atom by 0.1472 (3) Å. In the bipyridine ligand, the two pyridine rings are twisted slightly by an angle of 3.5 (1)°. The N1- and N2-pyridine rings form dihedral angles of 16.2 (1) and 15.6 (1)°, respectively, with the benzene ring.

The crystal structure is stabilized by C—H···O hydrogen bonds (Table 2).

Experimental

The crystal used in this structure determination was obtained adventitiously from an attempted preparation of a copper(II)-Schiff base complex. It was synthesized as described in the literature (Plesch *et al.*, 1997). 2-Hydroxyacetophenone (1.00 mmol) in methanol (10 ml) was added dropwise to a solution of beta-alanine (1.00 mmol) and potassium hydroxide (1.00 mmol) in methanol (10 ml). The yellow solution was stirred for 2 h at 333 K. The resultant mixture was added dropwise to copper(II) nitrate trihydrate (1.00 mmol) and 2,2'-bipyridine (1.00 mmol) in an aqueous methanolic solution (20 ml, 1:1 v/v), and heated with stirring for 2 h at 333 K. The dark blue solution obtained was filtered and left for several days; dark blue crystals were formed which were filtered off, washed with water, and dried under vacuum.

Refinement

H atoms were positioned geometrically and refined as riding, with C-H = 0.93 (CH) or 0.96 Å (CH₃) and $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N})$, where $x = 1.5$ for methyl H atoms and 1.2 for other H atoms.

Figures

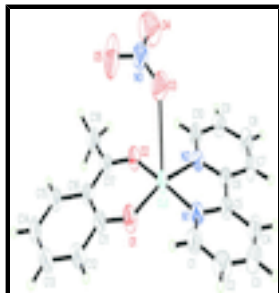


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

(2-Acetylphenolato)(2,2'-bipyridine)nitratocopper(II)

Crystal data

[Cu(C₈H₇O₂)(NO₃)(C₁₀H₈N₂)]

$M_r = 416.87$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 13.4683$ (12) Å

$b = 8.3101$ (8) Å

$c = 15.5924$ (15) Å

$\beta = 108.583$ (1)°

$V = 1654.2$ (3) Å³

$Z = 4$

$F_{000} = 852$

$D_x = 1.674$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3127 reflections

$\theta = 2.4$ – 27.0 °

$\mu = 1.36$ mm⁻¹

$T = 296$ K

Block, dark green

$0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.686$, $T_{\max} = 0.773$

8261 measured reflections

2917 independent reflections

2370 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 25.1$ °

$\theta_{\min} = 2.4$ °

$h = -15 \rightarrow 15$

$k = -9 \rightarrow 7$

$l = -18 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.074$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.9795P]$

| | |
|--|--|
| $S = 1.03$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2917 reflections | $(\Delta/\sigma)_{\max} = 0.001$ |
| 245 parameters | $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$ |
| | Extinction correction: none |

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|---------------|----------------------------------|
| Cu1 | 0.77943 (2) | 0.96237 (4) | 0.03090 (2) | 0.03038 (11) |
| C1 | 0.7404 (2) | 1.1660 (3) | 0.17445 (18) | 0.0395 (7) |
| H1 | 0.8040 | 1.1268 | 0.2122 | 0.047* |
| C2 | 0.6852 (2) | 1.2727 (4) | 0.20915 (19) | 0.0453 (7) |
| H2 | 0.7101 | 1.3038 | 0.2696 | 0.054* |
| C3 | 0.5919 (2) | 1.3328 (4) | 0.1521 (2) | 0.0473 (7) |
| H3 | 0.5538 | 1.4070 | 0.1735 | 0.057* |
| C4 | 0.5554 (2) | 1.2825 (3) | 0.06330 (19) | 0.0400 (7) |
| H4 | 0.4924 | 1.3216 | 0.0245 | 0.048* |
| C5 | 0.61386 (18) | 1.1732 (3) | 0.03286 (16) | 0.0300 (6) |
| C6 | 0.58213 (18) | 1.1050 (3) | -0.05922 (16) | 0.0292 (6) |
| C7 | 0.4907 (2) | 1.1450 (3) | -0.12742 (17) | 0.0377 (6) |
| H7 | 0.4449 | 1.2210 | -0.1174 | 0.045* |
| C8 | 0.4688 (2) | 1.0699 (3) | -0.21052 (18) | 0.0418 (7) |
| H8 | 0.4079 | 1.0951 | -0.2572 | 0.050* |
| C9 | 0.5378 (2) | 0.9575 (3) | -0.22366 (17) | 0.0376 (6) |
| H9 | 0.5242 | 0.9058 | -0.2791 | 0.045* |
| C10 | 0.6270 (2) | 0.9231 (3) | -0.15362 (17) | 0.0352 (6) |
| H10 | 0.6733 | 0.8467 | -0.1623 | 0.042* |
| C11 | 0.99646 (19) | 0.9179 (3) | 0.13299 (17) | 0.0324 (6) |
| C12 | 1.08113 (19) | 0.9544 (3) | 0.21194 (18) | 0.0378 (6) |

supplementary materials

| | | | | |
|------|--------------|------------|---------------|------------|
| H12 | 1.0700 | 1.0212 | 0.2559 | 0.045* |
| C13 | 1.1790 (2) | 0.8929 (4) | 0.2243 (2) | 0.0441 (7) |
| H13 | 1.2334 | 0.9192 | 0.2764 | 0.053* |
| C14 | 1.1984 (2) | 0.7920 (3) | 0.1607 (2) | 0.0443 (7) |
| H14 | 1.2647 | 0.7482 | 0.1711 | 0.053* |
| C15 | 1.11933 (19) | 0.7571 (3) | 0.08252 (19) | 0.0384 (6) |
| H15 | 1.1331 | 0.6919 | 0.0392 | 0.046* |
| C16 | 1.01667 (18) | 0.8190 (3) | 0.06647 (17) | 0.0306 (6) |
| C17 | 0.93694 (19) | 0.7830 (3) | -0.01883 (17) | 0.0309 (6) |
| C18 | 0.9599 (2) | 0.6816 (3) | -0.08916 (19) | 0.0445 (7) |
| H18A | 0.8996 | 0.6788 | -0.1425 | 0.067* |
| H18B | 0.9769 | 0.5743 | -0.0664 | 0.067* |
| H18C | 1.0182 | 0.7265 | -0.1039 | 0.067* |
| N1 | 0.70583 (15) | 1.1164 (2) | 0.08838 (13) | 0.0309 (5) |
| N2 | 0.64940 (15) | 0.9956 (2) | -0.07351 (13) | 0.0285 (5) |
| N3 | 0.73727 (19) | 0.5847 (3) | 0.03372 (17) | 0.0450 (6) |
| O1 | 0.90495 (13) | 0.9788 (2) | 0.12828 (12) | 0.0381 (4) |
| O2 | 0.84484 (12) | 0.8358 (2) | -0.04004 (11) | 0.0332 (4) |
| O3 | 0.70722 (15) | 0.7105 (2) | 0.06448 (14) | 0.0491 (5) |
| O4 | 0.6824 (2) | 0.5290 (3) | -0.03905 (18) | 0.0818 (8) |
| O5 | 0.8215 (2) | 0.5239 (3) | 0.07571 (19) | 0.0848 (9) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|-------------|--------------|--------------|--------------|---------------|
| Cu1 | 0.02264 (17) | 0.0360 (2) | 0.03004 (18) | 0.00320 (14) | 0.00488 (12) | -0.00188 (14) |
| C1 | 0.0357 (15) | 0.0422 (16) | 0.0360 (15) | -0.0034 (12) | 0.0049 (12) | -0.0056 (12) |
| C2 | 0.0476 (18) | 0.0519 (18) | 0.0375 (16) | -0.0052 (15) | 0.0152 (14) | -0.0125 (14) |
| C3 | 0.0493 (18) | 0.0474 (18) | 0.0527 (19) | 0.0033 (14) | 0.0266 (15) | -0.0135 (14) |
| C4 | 0.0335 (15) | 0.0429 (16) | 0.0458 (17) | 0.0060 (13) | 0.0156 (13) | 0.0001 (13) |
| C5 | 0.0266 (13) | 0.0314 (14) | 0.0328 (14) | 0.0008 (11) | 0.0106 (11) | 0.0004 (11) |
| C6 | 0.0250 (13) | 0.0294 (13) | 0.0342 (14) | 0.0003 (11) | 0.0107 (11) | 0.0023 (11) |
| C7 | 0.0310 (14) | 0.0416 (16) | 0.0384 (15) | 0.0110 (12) | 0.0078 (12) | 0.0040 (12) |
| C8 | 0.0319 (15) | 0.0528 (19) | 0.0341 (15) | 0.0050 (13) | 0.0010 (12) | 0.0070 (13) |
| C9 | 0.0374 (15) | 0.0428 (16) | 0.0290 (14) | 0.0006 (13) | 0.0056 (11) | -0.0032 (12) |
| C10 | 0.0315 (14) | 0.0380 (15) | 0.0350 (15) | 0.0028 (12) | 0.0093 (11) | -0.0061 (11) |
| C11 | 0.0268 (14) | 0.0333 (14) | 0.0343 (14) | -0.0015 (11) | 0.0058 (11) | 0.0095 (11) |
| C12 | 0.0303 (14) | 0.0448 (17) | 0.0347 (15) | -0.0050 (13) | 0.0052 (11) | 0.0065 (12) |
| C13 | 0.0304 (15) | 0.0487 (17) | 0.0450 (17) | -0.0069 (13) | 0.0006 (12) | 0.0133 (14) |
| C14 | 0.0233 (14) | 0.0453 (17) | 0.0602 (19) | 0.0046 (12) | 0.0076 (13) | 0.0179 (15) |
| C15 | 0.0283 (14) | 0.0352 (15) | 0.0513 (17) | 0.0021 (12) | 0.0122 (13) | 0.0079 (13) |
| C16 | 0.0254 (13) | 0.0304 (14) | 0.0345 (14) | 0.0004 (11) | 0.0073 (11) | 0.0066 (11) |
| C17 | 0.0285 (14) | 0.0269 (13) | 0.0382 (14) | 0.0010 (11) | 0.0120 (11) | 0.0064 (11) |
| C18 | 0.0360 (15) | 0.0458 (17) | 0.0486 (17) | 0.0083 (13) | 0.0094 (13) | -0.0072 (14) |
| N1 | 0.0260 (11) | 0.0327 (12) | 0.0322 (12) | -0.0015 (9) | 0.0068 (9) | -0.0027 (9) |
| N2 | 0.0228 (11) | 0.0312 (12) | 0.0303 (12) | -0.0001 (9) | 0.0066 (9) | -0.0001 (9) |
| N3 | 0.0406 (14) | 0.0425 (15) | 0.0541 (16) | 0.0045 (12) | 0.0183 (12) | 0.0111 (12) |
| O1 | 0.0268 (10) | 0.0503 (12) | 0.0340 (10) | 0.0036 (8) | 0.0052 (8) | -0.0058 (8) |

| | | | | | | |
|----|-------------|-------------|-------------|--------------|-------------|--------------|
| O2 | 0.0252 (9) | 0.0395 (10) | 0.0334 (10) | 0.0030 (8) | 0.0070 (7) | -0.0010 (8) |
| O3 | 0.0493 (12) | 0.0463 (12) | 0.0590 (13) | 0.0069 (10) | 0.0275 (10) | 0.0012 (10) |
| O4 | 0.0774 (18) | 0.088 (2) | 0.0722 (18) | -0.0149 (15) | 0.0133 (15) | -0.0282 (15) |
| O5 | 0.0627 (16) | 0.094 (2) | 0.091 (2) | 0.0436 (15) | 0.0165 (15) | 0.0261 (16) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-------------|-----------|
| Cu1—O1 | 1.8832 (17) | C9—H9 | 0.93 |
| Cu1—O2 | 1.9307 (17) | C10—N2 | 1.332 (3) |
| Cu1—N2 | 1.9941 (19) | C10—H10 | 0.93 |
| Cu1—N1 | 1.998 (2) | C11—O1 | 1.313 (3) |
| Cu1—O3 | 2.434 (2) | C11—C16 | 1.416 (4) |
| C1—N1 | 1.338 (3) | C11—C12 | 1.419 (3) |
| C1—C2 | 1.374 (4) | C12—C13 | 1.369 (4) |
| C1—H1 | 0.93 | C12—H12 | 0.93 |
| C2—C3 | 1.381 (4) | C13—C14 | 1.386 (4) |
| C2—H2 | 0.93 | C13—H13 | 0.93 |
| C3—C4 | 1.378 (4) | C14—C15 | 1.370 (4) |
| C3—H3 | 0.93 | C14—H14 | 0.93 |
| C4—C5 | 1.381 (4) | C15—C16 | 1.421 (3) |
| C4—H4 | 0.93 | C15—H15 | 0.93 |
| C5—N1 | 1.350 (3) | C16—C17 | 1.450 (3) |
| C5—C6 | 1.474 (3) | C17—O2 | 1.256 (3) |
| C6—N2 | 1.351 (3) | C17—C18 | 1.492 (4) |
| C6—C7 | 1.387 (3) | C18—H18A | 0.96 |
| C7—C8 | 1.383 (4) | C18—H18B | 0.96 |
| C7—H7 | 0.93 | C18—H18C | 0.96 |
| C8—C9 | 1.379 (4) | N3—O5 | 1.224 (3) |
| C8—H8 | 0.93 | N3—O4 | 1.230 (3) |
| C9—C10 | 1.371 (3) | N3—O3 | 1.269 (3) |
| O1—Cu1—O2 | 92.60 (7) | O1—C11—C16 | 125.4 (2) |
| O1—Cu1—N2 | 167.80 (8) | O1—C11—C12 | 116.5 (2) |
| O2—Cu1—N2 | 92.87 (8) | C16—C11—C12 | 118.1 (2) |
| O1—Cu1—N1 | 92.18 (8) | C13—C12—C11 | 120.9 (3) |
| O2—Cu1—N1 | 171.30 (8) | C13—C12—H12 | 119.5 |
| N2—Cu1—N1 | 81.10 (8) | C11—C12—H12 | 119.5 |
| O1—Cu1—O3 | 101.92 (8) | C12—C13—C14 | 121.2 (3) |
| O2—Cu1—O3 | 86.63 (7) | C12—C13—H13 | 119.4 |
| N2—Cu1—O3 | 89.28 (7) | C14—C13—H13 | 119.4 |
| N1—Cu1—O3 | 99.49 (7) | C15—C14—C13 | 119.6 (3) |
| N1—C1—C2 | 122.4 (3) | C15—C14—H14 | 120.2 |
| N1—C1—H1 | 118.8 | C13—C14—H14 | 120.2 |
| C2—C1—H1 | 118.8 | C14—C15—C16 | 121.1 (3) |
| C1—C2—C3 | 118.3 (3) | C14—C15—H15 | 119.4 |
| C1—C2—H2 | 120.8 | C16—C15—H15 | 119.4 |
| C3—C2—H2 | 120.8 | C11—C16—C15 | 119.0 (2) |
| C4—C3—C2 | 119.8 (3) | C11—C16—C17 | 122.2 (2) |
| C4—C3—H3 | 120.1 | C15—C16—C17 | 118.8 (2) |
| C2—C3—H3 | 120.1 | O2—C17—C16 | 123.4 (2) |

supplementary materials

| | | | |
|------------|-----------|---------------|-------------|
| C3—C4—C5 | 119.0 (3) | O2—C17—C18 | 115.0 (2) |
| C3—C4—H4 | 120.5 | C16—C17—C18 | 121.6 (2) |
| C5—C4—H4 | 120.5 | C17—C18—H18A | 109.5 |
| N1—C5—C4 | 121.1 (2) | C17—C18—H18B | 109.5 |
| N1—C5—C6 | 114.3 (2) | H18A—C18—H18B | 109.5 |
| C4—C5—C6 | 124.6 (2) | C17—C18—H18C | 109.5 |
| N2—C6—C7 | 120.9 (2) | H18A—C18—H18C | 109.5 |
| N2—C6—C5 | 114.7 (2) | H18B—C18—H18C | 109.5 |
| C7—C6—C5 | 124.4 (2) | C1—N1—C5 | 119.3 (2) |
| C8—C7—C6 | 118.8 (2) | C1—N1—Cu1 | 125.73 (18) |
| C8—C7—H7 | 120.6 | C5—N1—Cu1 | 114.92 (16) |
| C6—C7—H7 | 120.6 | C10—N2—C6 | 119.7 (2) |
| C9—C8—C7 | 119.5 (2) | C10—N2—Cu1 | 125.48 (17) |
| C9—C8—H8 | 120.2 | C6—N2—Cu1 | 114.78 (16) |
| C7—C8—H8 | 120.2 | O5—N3—O4 | 121.3 (3) |
| C10—C9—C8 | 118.9 (3) | O5—N3—O3 | 119.4 (3) |
| C10—C9—H9 | 120.5 | O4—N3—O3 | 119.2 (3) |
| C8—C9—H9 | 120.5 | C11—O1—Cu1 | 127.05 (16) |
| N2—C10—C9 | 122.1 (2) | C17—O2—Cu1 | 129.18 (16) |
| N2—C10—H10 | 118.9 | N3—O3—Cu1 | 115.43 (16) |
| C9—C10—H10 | 118.9 | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------|-------|-------------|-------------|---------------|
| C2—H2 \cdots O3 ⁱ | 0.93 | 2.59 | 3.401 (4) | 146 |
| C7—H7 \cdots O3 ⁱⁱ | 0.93 | 2.51 | 3.343 (3) | 150 |

Symmetry codes: (i) $-x+3/2, y+1/2, -z+1/2$; (ii) $-x+1, -y+2, -z$.

