

Nitrato(1,10-phenanthroline)(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

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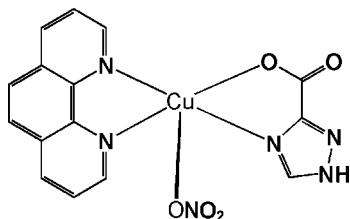
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.030; wR factor = 0.087; data-to-parameter ratio = 10.7.

In the title complex, $[\text{Cu}(\text{C}_3\text{H}_2\text{N}_3\text{O}_2)(\text{NO}_3)(\text{C}_{12}\text{H}_8\text{N}_2)]$, the Cu^{II} ion is coordinated by an N and an O atom from a bidentate 1*H*-1,2,4-triazole-3-carboxylate (TRIA) ligand, two N atoms from a 1,10-phenanthroline (phen) ligand, and an O atom from a nitrate ligand in a slightly distorted square-pyramidal environment. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link molecules into one-dimensional chains propagating along the b axis direction.

Related literature

For related literature, see: Guo & Wang (2005); Zhu *et al.* (2007); Zhu, Yin, Feng, Zhang *et al.* (2008); Zhu, Yin, Feng, Hu *et al.* (2008).



Experimental

Crystal data

$[\text{Cu}(\text{C}_3\text{H}_2\text{N}_3\text{O}_2)(\text{NO}_3)(\text{C}_{12}\text{H}_8\text{N}_2)]$
 $M_r = 417.83$

Monoclinic, $P2_1/c$
 $a = 12.3779$ (14) Å
 $b = 12.6444$ (15) Å
 $c = 10.0196$ (10) Å
 $\beta = 107.416$ (2)°

$V = 1496.3$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.51$ mm⁻¹
 $T = 298$ (2) K
 $0.34 \times 0.30 \times 0.25$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.628$, $T_{\text{max}} = 0.704$

7489 measured reflections
 2601 independent reflections
 2102 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.086$
 $S = 1.06$
 2601 reflections

244 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|--------|-------------|--------|-----------|
| Cu1—O1 | 1.9540 (19) | Cu1—N5 | 2.015 (2) |
| Cu1—N4 | 1.988 (2) | Cu1—O3 | 2.315 (2) |
| Cu1—N3 | 2.005 (2) | | |

Table 2

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1}\cdots\text{O2}^i$ | 0.86 | 1.92 | 2.775 (3) | 172 |

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2590).

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supplementary materials

Acta Cryst. (2008). E64, m392 [doi:10.1107/S1600536808001803]

Nitrato(1,10-phenanthroline)(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

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Comment

In connection with our on-going studies in coordination chemistry (Zhu *et al.*, 2007; Zhu, Yin, Feng, Hu *et al.*, 2008; Zhu, Yin, Feng, Zhang *et al.*, 2008) and the biological importance of triazole molecules (Guo *et al.*, 2005), the crystal structure of a new ternary Cu(II) complex with 1*H*-1,2,4-triazole-3-carboxylate (TRIA), 1,10-phenanthroline (phen) and NO₃ ligands is described. The molecular structure of the title compound is shown in Fig. 1. The Cu^{II} ion is bis-chelated by an N and an O atom, from a TRIA ligand, two N atoms from the chelating phen ligand, and the coordination geometry is completed by a O atom from an NO₃ ligand. The atom O3 from the NO₃ ligand occupies the apical site in a slightly distorted square-pyramidal ON₃O coordination environment. The primary intermolecular contacts in the crystal structure are of the type N—H···O and involve the non-coordinating O atom of the carbonyl group and the N—H group of the TRIA ligand.

Experimental

CuNO₃·3H₂O (0.5 mmol, 120.8 mg) dissolved in distilled water (5 ml) was added with stirring at 323 K to 1*H*-1,2,4-triazole-3-carboxylic acid (0.5 mmol, 56.5 mg) also dissolved in distilled water (15 ml). The resulting blue solution was allowed to react for 30 min and 1,10-phenanthroline (0.5 mmol, 99.1 mg) dissolved in ethanol (5 ml) was added. Dark-blue crystals suitable for X-ray analysis were obtained by slow evaporation over a period of one month (yield 55%). Analysis. Found: C 43.28, H 2.22, N 20.33, O 19.01%. C₁₅H₁₀CuN₆O₅ requires: C 43.12, H 2.41, N 20.11, O 19.15%.

Refinement

H atoms were placed in calculated positions and included in the refinement in the riding-model approximation with N—H = 0.86 Å and C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Figures

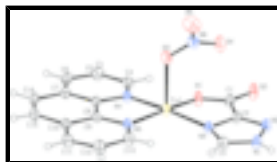


Fig. 1. The molecular structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

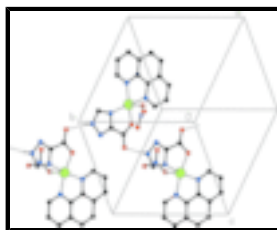


Fig. 2. Part of the crystal structure of the title compound showing hydrogen bonds as dashed lines.

Nitrato(1,10-phenanthroline)(1*H*-1,2,4-triazole-3-carboxylato)copper(II)

Crystal data

| | |
|--|---|
| [Cu(C ₃ H ₂ N ₃ O ₂)(NO ₃)(C ₁₂ H ₈ N ₂)] | $F_{000} = 844$ |
| $M_r = 417.83$ | $D_x = 1.855 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| Hall symbol: -P 2ybc | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 12.3779 (14) \text{ \AA}$ | Cell parameters from 3888 reflections |
| $b = 12.6444 (15) \text{ \AA}$ | $\theta = 2.7\text{--}27.7^\circ$ |
| $c = 10.0196 (10) \text{ \AA}$ | $\mu = 1.51 \text{ mm}^{-1}$ |
| $\beta = 107.416 (2)^\circ$ | $T = 298 (2) \text{ K}$ |
| $V = 1496.3 (3) \text{ \AA}^3$ | Block, dark-blue |
| $Z = 4$ | $0.34 \times 0.30 \times 0.25 \text{ mm}$ |

Data collection

| | |
|---|--|
| Bruker SMART CCD diffractometer | 2601 independent reflections |
| Radiation source: fine-focus sealed tube | 2102 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.033$ |
| $T = 298(2) \text{ K}$ | $\theta_{\text{max}} = 25.0^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 1.7^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -14 \rightarrow 8$ |
| $T_{\text{min}} = 0.628$, $T_{\text{max}} = 0.704$ | $k = -14 \rightarrow 15$ |
| 7489 measured reflections | $l = -11 \rightarrow 11$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | H-atom parameters constrained |
| $wR(F^2) = 0.086$ | $w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.8762P]$ |
| $S = 1.06$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2601 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 244 parameters | $\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$ |
| | 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 $F^2 > 2\sigma(F^2)$ 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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|-------------|----------------------------------|
| Cu1 | 0.67882 (3) | 1.02713 (2) | 0.58353 (3) | 0.02944 (14) |
| N1 | 0.57639 (19) | 1.32426 (17) | 0.6760 (2) | 0.0321 (5) |
| H1 | 0.5704 | 1.3918 | 0.6815 | 0.039* |
| N2 | 0.52709 (19) | 1.25284 (17) | 0.7412 (2) | 0.0309 (5) |
| N3 | 0.62666 (18) | 1.17198 (17) | 0.6177 (2) | 0.0279 (5) |
| N4 | 0.69970 (18) | 0.87706 (17) | 0.5374 (2) | 0.0277 (5) |
| N5 | 0.78098 (19) | 1.05325 (17) | 0.4636 (2) | 0.0298 (5) |
| N6 | 0.8485 (2) | 1.07924 (19) | 0.8885 (2) | 0.0360 (6) |
| O1 | 0.56644 (17) | 0.98205 (14) | 0.6733 (2) | 0.0369 (5) |
| O2 | 0.46508 (19) | 1.03880 (15) | 0.8074 (2) | 0.0449 (6) |
| O3 | 0.83942 (18) | 1.03049 (17) | 0.7753 (2) | 0.0451 (5) |
| O4 | 0.76459 (19) | 1.08825 (19) | 0.9301 (2) | 0.0512 (6) |
| O5 | 0.9405 (2) | 1.1152 (2) | 0.9554 (3) | 0.0639 (7) |
| C1 | 0.5273 (2) | 1.0534 (2) | 0.7344 (3) | 0.0304 (6) |
| C2 | 0.5598 (2) | 1.1626 (2) | 0.7031 (3) | 0.0268 (6) |
| C3 | 0.6344 (2) | 1.2759 (2) | 0.6036 (3) | 0.0315 (6) |
| H3 | 0.6746 | 1.3093 | 0.5507 | 0.038* |
| C4 | 0.6555 (2) | 0.7905 (2) | 0.5753 (3) | 0.0312 (6) |
| H4A | 0.6063 | 0.7972 | 0.6290 | 0.037* |
| C5 | 0.6811 (2) | 0.6898 (2) | 0.5364 (3) | 0.0355 (7) |
| H5A | 0.6479 | 0.6306 | 0.5629 | 0.043* |
| C6 | 0.7544 (2) | 0.6778 (2) | 0.4597 (3) | 0.0367 (7) |
| H6 | 0.7714 | 0.6107 | 0.4336 | 0.044* |
| C7 | 0.8041 (2) | 0.7676 (2) | 0.4206 (3) | 0.0300 (6) |
| C8 | 0.7725 (2) | 0.8658 (2) | 0.4602 (3) | 0.0255 (6) |
| C9 | 0.8155 (2) | 0.9609 (2) | 0.4195 (2) | 0.0261 (6) |
| C10 | 0.8887 (2) | 0.9563 (2) | 0.3374 (3) | 0.0314 (6) |
| C11 | 0.9255 (3) | 1.0523 (3) | 0.2966 (3) | 0.0403 (7) |
| H11 | 0.9718 | 1.0534 | 0.2387 | 0.048* |
| C12 | 0.8919 (3) | 1.1448 (2) | 0.3435 (3) | 0.0427 (8) |
| H12 | 0.9169 | 1.2092 | 0.3190 | 0.051* |
| C13 | 0.8209 (2) | 1.1429 (2) | 0.4275 (3) | 0.0375 (7) |
| H13 | 0.8005 | 1.2066 | 0.4597 | 0.045* |

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|-----|------------|------------|------------|------------|
| C14 | 0.8817 (2) | 0.7653 (2) | 0.3406 (3) | 0.0371 (7) |
| H14 | 0.9051 | 0.7004 | 0.3153 | 0.044* |
| C15 | 0.9220 (2) | 0.8549 (2) | 0.3007 (3) | 0.0368 (7) |
| H15 | 0.9725 | 0.8508 | 0.2483 | 0.044* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|--------------|-------------|---------------|--------------|---------------|
| Cu1 | 0.0405 (2) | 0.01967 (19) | 0.0373 (2) | -0.00062 (14) | 0.02555 (16) | -0.00268 (14) |
| N1 | 0.0420 (14) | 0.0163 (11) | 0.0440 (13) | 0.0013 (10) | 0.0220 (12) | -0.0007 (10) |
| N2 | 0.0386 (13) | 0.0201 (11) | 0.0407 (13) | 0.0001 (10) | 0.0221 (11) | 0.0015 (10) |
| N3 | 0.0353 (13) | 0.0223 (11) | 0.0327 (12) | -0.0008 (9) | 0.0202 (10) | -0.0008 (9) |
| N4 | 0.0314 (12) | 0.0261 (12) | 0.0292 (11) | -0.0020 (10) | 0.0146 (10) | -0.0007 (10) |
| N5 | 0.0370 (13) | 0.0252 (12) | 0.0329 (12) | -0.0017 (10) | 0.0190 (11) | -0.0019 (10) |
| N6 | 0.0483 (16) | 0.0258 (12) | 0.0368 (14) | -0.0026 (11) | 0.0172 (13) | 0.0039 (11) |
| O1 | 0.0511 (13) | 0.0207 (10) | 0.0525 (12) | -0.0022 (8) | 0.0361 (11) | -0.0036 (9) |
| O2 | 0.0627 (15) | 0.0243 (11) | 0.0683 (14) | 0.0007 (9) | 0.0509 (12) | 0.0013 (10) |
| O3 | 0.0444 (13) | 0.0571 (15) | 0.0368 (11) | 0.0069 (10) | 0.0165 (10) | -0.0106 (10) |
| O4 | 0.0593 (15) | 0.0496 (14) | 0.0559 (14) | 0.0053 (11) | 0.0343 (12) | -0.0101 (11) |
| O5 | 0.0640 (17) | 0.0648 (17) | 0.0596 (15) | -0.0248 (14) | 0.0132 (13) | -0.0089 (13) |
| C1 | 0.0362 (16) | 0.0225 (13) | 0.0379 (15) | 0.0015 (11) | 0.0194 (13) | 0.0012 (12) |
| C2 | 0.0298 (14) | 0.0226 (14) | 0.0310 (14) | 0.0013 (11) | 0.0140 (12) | -0.0009 (11) |
| C3 | 0.0387 (16) | 0.0241 (14) | 0.0367 (15) | -0.0015 (12) | 0.0189 (13) | 0.0011 (12) |
| C4 | 0.0370 (16) | 0.0276 (14) | 0.0306 (14) | -0.0006 (12) | 0.0129 (13) | 0.0009 (11) |
| C5 | 0.0420 (17) | 0.0244 (14) | 0.0406 (16) | -0.0032 (12) | 0.0134 (14) | 0.0017 (12) |
| C6 | 0.0425 (18) | 0.0239 (14) | 0.0427 (16) | 0.0052 (12) | 0.0109 (14) | -0.0039 (12) |
| C7 | 0.0340 (15) | 0.0281 (15) | 0.0292 (14) | 0.0029 (12) | 0.0112 (12) | -0.0035 (11) |
| C8 | 0.0267 (14) | 0.0271 (14) | 0.0237 (13) | 0.0011 (11) | 0.0090 (11) | -0.0028 (11) |
| C9 | 0.0290 (14) | 0.0270 (14) | 0.0243 (13) | 0.0001 (11) | 0.0109 (11) | -0.0019 (11) |
| C10 | 0.0284 (15) | 0.0396 (17) | 0.0291 (14) | -0.0008 (12) | 0.0130 (12) | -0.0023 (12) |
| C11 | 0.0413 (18) | 0.0448 (19) | 0.0421 (17) | -0.0041 (14) | 0.0237 (15) | 0.0021 (14) |
| C12 | 0.0499 (19) | 0.0366 (17) | 0.0524 (19) | -0.0053 (14) | 0.0319 (16) | 0.0055 (14) |
| C13 | 0.0464 (18) | 0.0246 (15) | 0.0483 (18) | -0.0022 (12) | 0.0245 (15) | -0.0018 (13) |
| C14 | 0.0417 (17) | 0.0338 (16) | 0.0390 (16) | 0.0071 (13) | 0.0169 (14) | -0.0092 (13) |
| C15 | 0.0340 (16) | 0.0440 (18) | 0.0389 (16) | 0.0040 (13) | 0.0207 (13) | -0.0072 (13) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-------------|--------|-----------|
| Cu1—O1 | 1.9540 (19) | C3—H3 | 0.9300 |
| Cu1—N4 | 1.988 (2) | C4—C5 | 1.396 (4) |
| Cu1—N3 | 2.005 (2) | C4—H4A | 0.9300 |
| Cu1—N5 | 2.015 (2) | C5—C6 | 1.362 (4) |
| Cu1—O3 | 2.315 (2) | C5—H5A | 0.9300 |
| N1—C3 | 1.314 (3) | C6—C7 | 1.402 (4) |
| N1—N2 | 1.361 (3) | C6—H6 | 0.9300 |
| N1—H1 | 0.8600 | C7—C8 | 1.395 (4) |
| N2—C2 | 1.305 (3) | C7—C14 | 1.424 (4) |
| N3—C3 | 1.329 (3) | C8—C9 | 1.423 (4) |
| N3—C2 | 1.363 (3) | C9—C10 | 1.396 (4) |

| | | | |
|-------------|-------------|-------------|-----------|
| N4—C4 | 1.329 (3) | C10—C11 | 1.401 (4) |
| N4—C8 | 1.359 (3) | C10—C15 | 1.427 (4) |
| N5—C13 | 1.329 (4) | C11—C12 | 1.371 (4) |
| N5—C9 | 1.362 (3) | C11—H11 | 0.9300 |
| N6—O5 | 1.223 (3) | C12—C13 | 1.387 (4) |
| N6—O4 | 1.234 (3) | C12—H12 | 0.9300 |
| N6—O3 | 1.267 (3) | C13—H13 | 0.9300 |
| O1—C1 | 1.266 (3) | C14—C15 | 1.347 (4) |
| O2—C1 | 1.225 (3) | C14—H14 | 0.9300 |
| C1—C2 | 1.497 (4) | C15—H15 | 0.9300 |
| O1—Cu1—N4 | 89.34 (8) | N4—C4—C5 | 121.7 (3) |
| O1—Cu1—N3 | 82.99 (8) | N4—C4—H4A | 119.2 |
| N4—Cu1—N3 | 169.22 (9) | C5—C4—H4A | 119.2 |
| O1—Cu1—N5 | 169.26 (8) | C6—C5—C4 | 120.3 (3) |
| N4—Cu1—N5 | 82.50 (9) | C6—C5—H5A | 119.9 |
| N3—Cu1—N5 | 104.10 (9) | C4—C5—H5A | 119.9 |
| O1—Cu1—O3 | 100.15 (8) | C5—C6—C7 | 119.3 (3) |
| N4—Cu1—O3 | 94.09 (8) | C5—C6—H6 | 120.3 |
| N3—Cu1—O3 | 94.71 (8) | C7—C6—H6 | 120.3 |
| N5—Cu1—O3 | 87.45 (8) | C8—C7—C6 | 117.2 (2) |
| C3—N1—N2 | 110.7 (2) | C8—C7—C14 | 118.2 (3) |
| C3—N1—H1 | 124.6 | C6—C7—C14 | 124.5 (3) |
| N2—N1—H1 | 124.6 | N4—C8—C7 | 123.0 (2) |
| C2—N2—N1 | 102.5 (2) | N4—C8—C9 | 116.3 (2) |
| C3—N3—C2 | 103.2 (2) | C7—C8—C9 | 120.6 (2) |
| C3—N3—Cu1 | 148.06 (19) | N5—C9—C10 | 123.3 (2) |
| C2—N3—Cu1 | 108.37 (16) | N5—C9—C8 | 116.8 (2) |
| C4—N4—C8 | 118.4 (2) | C10—C9—C8 | 119.9 (2) |
| C4—N4—Cu1 | 128.81 (18) | C9—C10—C11 | 117.4 (3) |
| C8—N4—Cu1 | 112.74 (17) | C9—C10—C15 | 118.6 (3) |
| C13—N5—C9 | 117.7 (2) | C11—C10—C15 | 124.0 (3) |
| C13—N5—Cu1 | 130.77 (19) | C12—C11—C10 | 118.8 (3) |
| C9—N5—Cu1 | 111.51 (17) | C12—C11—H11 | 120.6 |
| O5—N6—O4 | 121.3 (3) | C10—C11—H11 | 120.6 |
| O5—N6—O3 | 119.4 (3) | C11—C12—C13 | 120.3 (3) |
| O4—N6—O3 | 119.3 (2) | C11—C12—H12 | 119.8 |
| C1—O1—Cu1 | 116.28 (17) | C13—C12—H12 | 119.8 |
| N6—O3—Cu1 | 125.19 (17) | N5—C13—C12 | 122.4 (3) |
| O2—C1—O1 | 125.5 (2) | N5—C13—H13 | 118.8 |
| O2—C1—C2 | 121.4 (2) | C12—C13—H13 | 118.8 |
| O1—C1—C2 | 113.0 (2) | C15—C14—C7 | 121.5 (3) |
| N2—C2—N3 | 114.1 (2) | C15—C14—H14 | 119.3 |
| N2—C2—C1 | 128.3 (2) | C7—C14—H14 | 119.3 |
| N3—C2—C1 | 117.6 (2) | C14—C15—C10 | 121.2 (3) |
| N1—C3—N3 | 109.4 (2) | C14—C15—H15 | 119.4 |
| N1—C3—H3 | 125.3 | C10—C15—H15 | 119.4 |
| N3—C3—H3 | 125.3 | | |
| C3—N1—N2—C2 | 0.2 (3) | O1—C1—C2—N2 | 174.8 (3) |

supplementary materials

| | | | |
|---------------|--------------|-----------------|-------------|
| O1—Cu1—N3—C3 | -178.1 (4) | O2—C1—C2—N3 | -178.1 (3) |
| N4—Cu1—N3—C3 | -133.1 (5) | O1—C1—C2—N3 | -1.0 (4) |
| N5—Cu1—N3—C3 | -6.3 (4) | N2—N1—C3—N3 | -0.2 (3) |
| O3—Cu1—N3—C3 | 82.3 (4) | C2—N3—C3—N1 | 0.2 (3) |
| O1—Cu1—N3—C2 | 10.49 (17) | Cu1—N3—C3—N1 | -171.5 (3) |
| N4—Cu1—N3—C2 | 55.4 (5) | C8—N4—C4—C5 | -0.7 (4) |
| N5—Cu1—N3—C2 | -177.73 (17) | Cu1—N4—C4—C5 | -178.4 (2) |
| O3—Cu1—N3—C2 | -89.18 (18) | N4—C4—C5—C6 | 1.1 (4) |
| O1—Cu1—N4—C4 | -5.8 (2) | C4—C5—C6—C7 | 0.1 (4) |
| N3—Cu1—N4—C4 | -50.4 (6) | C5—C6—C7—C8 | -1.7 (4) |
| N5—Cu1—N4—C4 | -178.8 (2) | C5—C6—C7—C14 | -179.9 (3) |
| O3—Cu1—N4—C4 | 94.3 (2) | C4—N4—C8—C7 | -0.9 (4) |
| O1—Cu1—N4—C8 | 176.37 (18) | Cu1—N4—C8—C7 | 177.13 (19) |
| N3—Cu1—N4—C8 | 131.8 (4) | C4—N4—C8—C9 | 178.6 (2) |
| N5—Cu1—N4—C8 | 3.38 (17) | Cu1—N4—C8—C9 | -3.4 (3) |
| O3—Cu1—N4—C8 | -83.50 (18) | C6—C7—C8—N4 | 2.1 (4) |
| O1—Cu1—N5—C13 | 139.0 (4) | C14—C7—C8—N4 | -179.5 (2) |
| N4—Cu1—N5—C13 | 179.9 (3) | C6—C7—C8—C9 | -177.4 (2) |
| N3—Cu1—N5—C13 | 8.6 (3) | C14—C7—C8—C9 | 1.0 (4) |
| O3—Cu1—N5—C13 | -85.6 (3) | C13—N5—C9—C10 | -0.9 (4) |
| O1—Cu1—N5—C9 | -43.7 (5) | Cu1—N5—C9—C10 | -178.6 (2) |
| N4—Cu1—N5—C9 | -2.82 (17) | C13—N5—C9—C8 | 179.5 (2) |
| N3—Cu1—N5—C9 | -174.14 (17) | Cu1—N5—C9—C8 | 1.8 (3) |
| O3—Cu1—N5—C9 | 91.65 (18) | N4—C8—C9—N5 | 1.0 (3) |
| N4—Cu1—O1—C1 | 175.3 (2) | C7—C8—C9—N5 | -179.5 (2) |
| N3—Cu1—O1—C1 | -12.3 (2) | N4—C8—C9—C10 | -178.6 (2) |
| N5—Cu1—O1—C1 | -144.3 (4) | C7—C8—C9—C10 | 0.9 (4) |
| O3—Cu1—O1—C1 | 81.2 (2) | N5—C9—C10—C11 | -1.6 (4) |
| O5—N6—O3—Cu1 | -148.4 (2) | C8—C9—C10—C11 | 178.0 (2) |
| O4—N6—O3—Cu1 | 32.6 (3) | N5—C9—C10—C15 | 178.1 (2) |
| O1—Cu1—O3—N6 | -52.7 (2) | C8—C9—C10—C15 | -2.3 (4) |
| N4—Cu1—O3—N6 | -142.7 (2) | C9—C10—C11—C12 | 2.6 (4) |
| N3—Cu1—O3—N6 | 31.0 (2) | C15—C10—C11—C12 | -177.0 (3) |
| N5—Cu1—O3—N6 | 135.0 (2) | C10—C11—C12—C13 | -1.3 (5) |
| Cu1—O1—C1—O2 | -172.5 (2) | C9—N5—C13—C12 | 2.4 (4) |
| Cu1—O1—C1—C2 | 10.6 (3) | Cu1—N5—C13—C12 | 179.5 (2) |
| N1—N2—C2—N3 | -0.1 (3) | C11—C12—C13—N5 | -1.3 (5) |
| N1—N2—C2—C1 | -176.0 (3) | C8—C7—C14—C15 | -1.6 (4) |
| C3—N3—C2—N2 | 0.0 (3) | C6—C7—C14—C15 | 176.7 (3) |
| Cu1—N3—C2—N2 | 175.33 (18) | C7—C14—C15—C10 | 0.2 (4) |
| C3—N3—C2—C1 | 176.3 (2) | C9—C10—C15—C14 | 1.8 (4) |
| Cu1—N3—C2—C1 | -8.3 (3) | C11—C10—C15—C14 | -178.5 (3) |
| O2—C1—C2—N2 | -2.3 (5) | | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------|-------|-------------|-------------|---------------|
| N1—H1 \cdots O2 ⁱ | 0.86 | 1.92 | 2.775 (3) | 172 |

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

Fig. 1

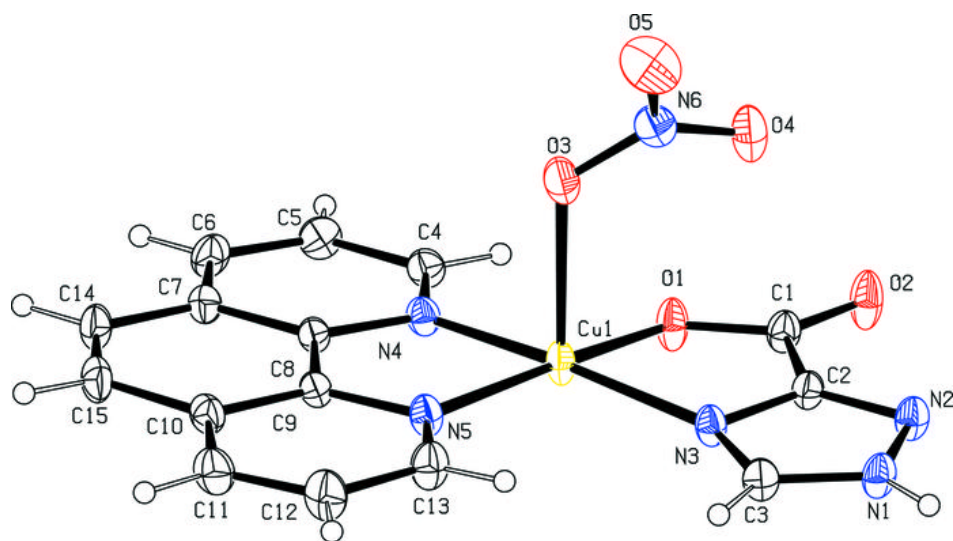


Fig. 2

