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# Di-$\mu$-nitrito-$\kappa^4O$:$O$-bis[bis(1-ethyl-1*H*-imidazole-$\kappa N^3$)(nitrito-$\kappa O$)copper(II)]

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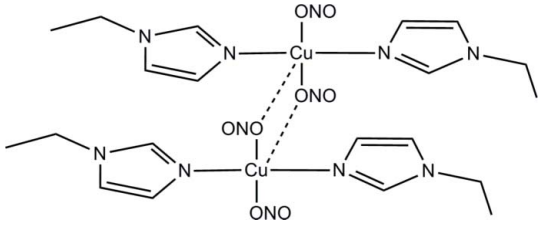
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.127; data-to-parameter ratio = 18.1.

In the structure of the title compound, $[Cu_2(NO_2)_4(C_5H_8N_2)_4]$, the asymmetric unit consists of two moieties containing one Cu ion, two nitrite ions and two 1-ethyl-1*H*-imidazole molecules associated *via* weak Cu—O interactions. Each $Cu^{II}$ atom displays an elongted square-pyramidal $CuN_2O_3$ coordination geometry with a slight tetrahedral distortion in the basal plane. The dimeric units are linked into a three-dimensional network by C—H···O hydrogen bonds.

## Related literature

For general background on ferroelectric metal–organic compounds with framework structures, see: Fu *et al.* (2009); Ye *et al.* (2006); Zhang *et al.* (2008, 2010). For a related structure, see: Costes *et al.* (1995).




## Experimental

### Crystal data

$[Cu_2(NO_2)_4(C_5H_8N_2)_4]$
$M_r$ = 695.64
Tetragonal, $I4_1/a$
$a$ = 28.136 (7) Å
$c$ = 7.669 (2) Å
$V$ = 6071 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.46 mm$^{-1}$
$T$ = 293 K
0.30 × 0.25 × 0.20 mm

### Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.651, $T_{max}$ = 0.746
31845 measured reflections
3462 independent reflections
3188 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.127
$S$ = 1.15
3462 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2004).

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# supporting information

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## Di-$\mu$-nitrito-$\kappa^4O$:$O$-bis[bis(1-ethyl-1*H*-imidazole-$\kappa N^3$)(nitrito-$\kappa O$)copper(II)]

**Run-Qiang Zhu**

### S1. Comment

As part of our ongoing study of potential ferroelectric phase change materials we have determined the structures of several copper complexes and examined the changes in their dielectric constants with temperature. This is the usual method for detecting such behavior. (Fu *et al.*, 2009; Ye *et al.*, 2006; Zhang *et al.*, 2008; Zhang *et al.*, 2010). Unfortunately, the dielectric constant for (I) does not show any behavior indicating the onset of a ferroelectric phase change over the range 80 K to 298 K (m.p.219–229).

As shown in Fig. 1, the Cu ion adopts an elongated square pyramidal geometry with a slight tetrahedral distortion in the basal plane which is primarily associated with the coordination of the nitrite ions (O1—Cu1—O3 = 164.12 (11)°). This displaces O3 from the ideal coordination plane towards the centrosymmetrically-related copper atom (Cu1′) resulting in an O3—Cu1′ distance of 2.637 (2) Å. While this distance is considerably longer than the in-plane Cu1—O1 and Cu—O3 bond lengths of 2.025 (3) Å and 2.058 (5) Å, respectively, the direction of displacement of O3 and the orientations of the two nitrite ligands which place both O1 and O4 on the opposite side of the coordination plane from Cu1′, suggests that there is a weak association of one $Cu(NO_2)_2(C_5H_8N_2)_2$unit with its centrosymmetrically-related counterpart. A similar weak association has been postulated to occur between two similar centrosymmetrically related $Cu(NO_2)(OC(CH_3)CHC(CH_3)N(CH_2)_2NH_2)$ units (Cu—O = 2.014 (4) Å, Cu′—O = 2.634 (3) Å) (Costes, *et al.* 1995).

### S2. Experimental

An aqueous solution of 1-ethyl imidazole (2.4 g, 25 mmol) and $H_2SO_4$(12.5 mmol) was treated with $CuSO_4$ (250 g, 12.5 mmol). After the mixture was stirred for a few minutes, $Ba(NO_2)_2$ (6.18 g, 25 mmol) was added to give a blue solution. Slow evaporation of the solution following removal of the precipitated $BaSO_4$ yielded blue crystals after a few days.

### S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93–0.96 Å, and with $U_{iso}$(H) = 1.2 $U_{iso}$(C) or 1.5 $U_{iso}$(C) for ethy H atoms.

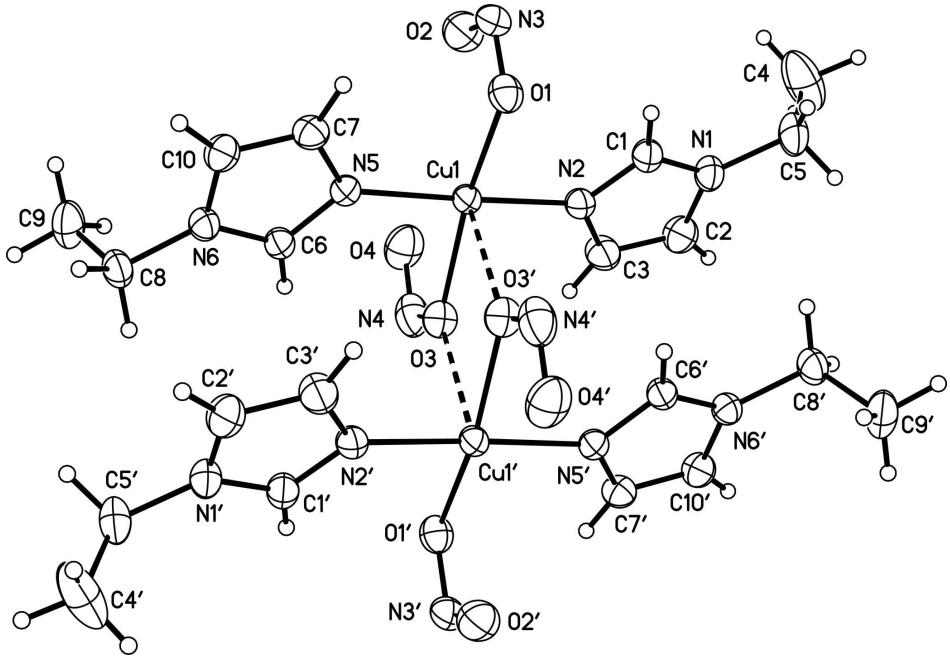


**Figure 1**

A view of the title compound with the displacement ellipsoids drawn at the 30% probability level.

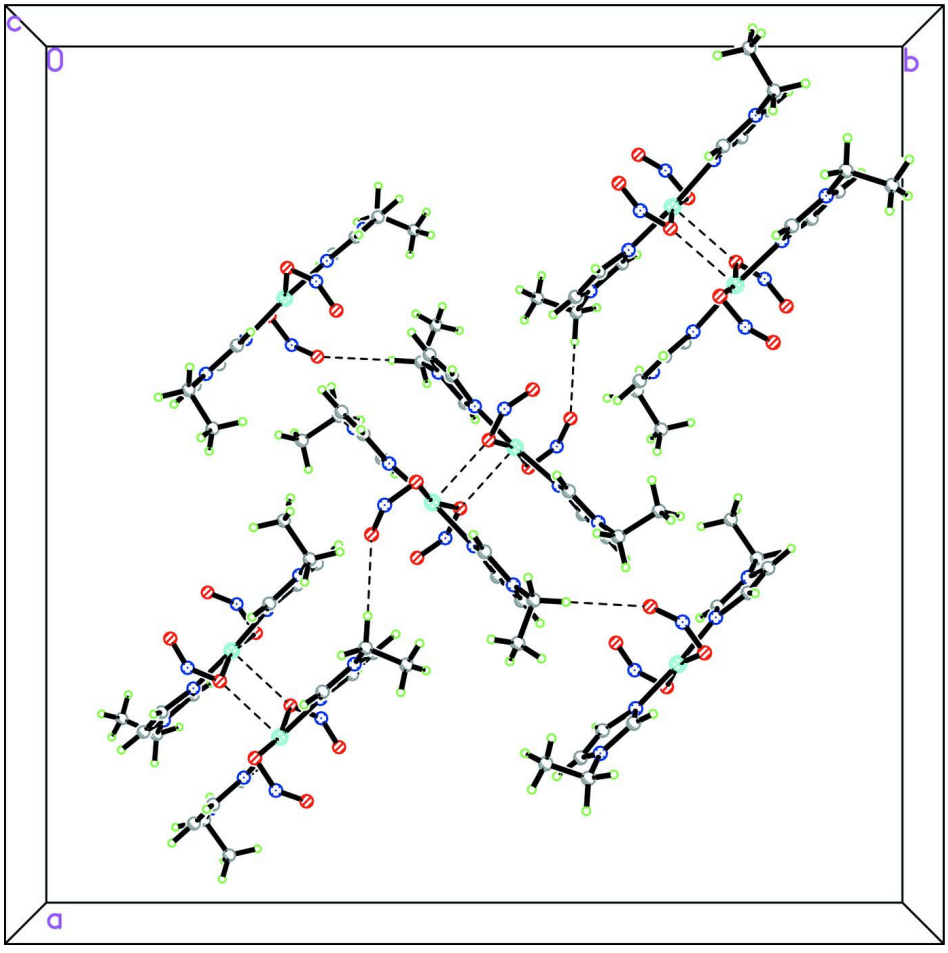


**Figure 2**

Packing diagram of the title compound. The weak Cu—O interactions and the hydrogen bonds are shown as dashed lines.

**Di-$\mu$-nitrito-$\kappa^4O$:$O$-bis[bis(1-ethyl-1*H*- imidazole-$\kappa N^3$)(nitrito-$\kappa O$)copper(II)]**

*Crystal data*

$[Cu_2(NO_2)_4(C_5H_8N_2)_4]$
$M_r$ = 695.64
Tetragonal, $I4_1/a$
Hall symbol: -I 4ad
$a$ = 28.136 (7) Å
$c$ = 7.669 (2) Å
$V$ = 6071 (3) Å$^3$
$Z$ = 8
$F$(000) = 2864
$D_x$ = 1.522 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 7423 reflections
$\theta$ = 2.3–27.5°
$\mu$ = 1.46 mm$^{-1}$
$T$ = 293 K
Prism, blue
0.30 × 0.25 × 0.20 mm

*Data collection*

Rigaku SCXmini CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.651, $T_{max}$ = 0.746
31845 measured reflections
3462 independent reflections
3188 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.049
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.8°
$h$ = −36→35
$k$ = −36→36
$l$ = −9→9

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.127
$S$ = 1.15
3462 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 9.3008P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.82 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.296007 (12) | 0.280780 (13) | 0.10562 (4) | 0.03905 (14) |
| O1 | 0.31265 (8) | 0.25812 (8) | −0.1376 (3) | 0.0515 (5) |
| O2 | 0.36079 (10) | 0.31480 (11) | −0.1169 (4) | 0.0703 (7) |
| O3 | 0.26607 (9) | 0.28842 (10) | 0.3494 (4) | 0.0622 (6) |
| O4 | 0.31466 (11) | 0.34387 (11) | 0.3593 (4) | 0.0786 (9) |
| N1 | 0.20821 (9) | 0.36827 (10) | −0.1798 (4) | 0.0506 (6) |
| N2 | 0.25052 (8) | 0.32796 (9) | 0.0093 (3) | 0.0429 (5) |
| N3 | 0.34610 (10) | 0.28278 (12) | −0.2076 (4) | 0.0567 (7) |
| N4 | 0.28338 (14) | 0.32269 (14) | 0.4337 (4) | 0.0726 (10) |
| N5 | 0.34476 (8) | 0.23769 (8) | 0.2053 (3) | 0.0385 (5) |
| N6 | 0.38648 (9) | 0.19735 (9) | 0.3968 (3) | 0.0423 (5) |
| C1 | 0.23921 (11) | 0.33283 (11) | −0.1568 (4) | 0.0463 (7) |
| H1 | 0.2512 | 0.3140 | −0.2462 | 0.056* |
| C2 | 0.19876 (13) | 0.38696 (13) | −0.0200 (5) | 0.0615 (9) |
| H2 | 0.1782 | 0.4120 | 0.0043 | 0.074* |
| C3 | 0.22491 (13) | 0.36229 (13) | 0.0964 (5) | 0.0597 (9) |
| H3 | 0.2255 | 0.3676 | 0.2161 | 0.072* |
| C4 | 0.2044 (3) | 0.4277 (2) | −0.4124 (8) | 0.122 (2) |
| H4A | 0.1894 | 0.4348 | −0.5217 | 0.182* |
| H4B | 0.2382 | 0.4260 | −0.4286 | 0.182* |
| H4C | 0.1971 | 0.4522 | −0.3295 | 0.182* |
| C5 | 0.18697 (14) | 0.38208 (15) | −0.3476 (5) | 0.0690 (11) |

| | | | | |
|---|---|---|---|---|
| H5A | 0.1901 | 0.3558 | −0.4286 | 0.083* |
| H5B | 0.1533 | 0.3878 | −0.3305 | 0.083* |
| C6 | 0.35428 (10) | 0.23166 (10) | 0.3735 (4) | 0.0405 (6) |
| H6 | 0.3404 | 0.2490 | 0.4632 | 0.049* |
| C7 | 0.37254 (11) | 0.20505 (11) | 0.1186 (4) | 0.0461 (7) |
| H7 | 0.3735 | 0.2009 | −0.0016 | 0.055* |
| C8 | 0.40610 (12) | 0.18264 (12) | 0.5666 (4) | 0.0511 (7) |
| H8A | 0.4144 | 0.1492 | 0.5617 | 0.061* |
| H8B | 0.3820 | 0.1866 | 0.6558 | 0.061* |
| C9 | 0.44914 (14) | 0.21084 (15) | 0.6157 (6) | 0.0697 (11) |
| H9A | 0.4734 | 0.2065 | 0.5291 | 0.105* |
| H9B | 0.4607 | 0.2002 | 0.7268 | 0.105* |
| H9C | 0.4409 | 0.2439 | 0.6228 | 0.105* |
| C10 | 0.39807 (11) | 0.18017 (11) | 0.2355 (4) | 0.0492 (7) |
| H10 | 0.4195 | 0.1559 | 0.2113 | 0.059* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0390 (2) | 0.0460 (2) | 0.0321 (2) | 0.00571 (13) | 0.00052 (13) | 0.00114 (13) |
| O1 | 0.0565 (13) | 0.0524 (12) | 0.0458 (12) | 0.0022 (10) | −0.0071 (10) | −0.0053 (10) |
| O2 | 0.0689 (17) | 0.0750 (18) | 0.0670 (17) | −0.0149 (14) | −0.0035 (13) | 0.0023 (14) |
| O3 | 0.0548 (14) | 0.0698 (16) | 0.0622 (16) | 0.0070 (12) | −0.0010 (12) | 0.0094 (13) |
| O4 | 0.0654 (17) | 0.0681 (17) | 0.102 (2) | −0.0119 (14) | −0.0124 (16) | 0.0019 (16) |
| N1 | 0.0453 (14) | 0.0531 (15) | 0.0533 (16) | 0.0069 (11) | −0.0072 (12) | 0.0064 (12) |
| N2 | 0.0424 (13) | 0.0464 (13) | 0.0400 (13) | 0.0058 (10) | 0.0016 (10) | 0.0036 (10) |
| N3 | 0.0550 (16) | 0.077 (2) | 0.0380 (14) | 0.0110 (14) | 0.0067 (12) | 0.0059 (14) |
| N4 | 0.078 (2) | 0.086 (2) | 0.0532 (18) | 0.031 (2) | −0.0105 (17) | −0.0114 (17) |
| N5 | 0.0373 (11) | 0.0406 (12) | 0.0377 (12) | 0.0023 (9) | 0.0004 (9) | 0.0001 (10) |
| N6 | 0.0419 (13) | 0.0409 (12) | 0.0441 (13) | 0.0018 (10) | −0.0018 (10) | 0.0061 (10) |
| C1 | 0.0435 (15) | 0.0509 (17) | 0.0446 (16) | 0.0051 (13) | −0.0030 (12) | 0.0010 (13) |
| C2 | 0.058 (2) | 0.058 (2) | 0.068 (2) | 0.0182 (16) | 0.0029 (17) | 0.0028 (17) |
| C3 | 0.065 (2) | 0.067 (2) | 0.0463 (18) | 0.0236 (17) | 0.0062 (15) | −0.0030 (16) |
| C4 | 0.178 (6) | 0.091 (4) | 0.096 (4) | −0.014 (4) | −0.050 (4) | 0.042 (3) |
| C5 | 0.062 (2) | 0.079 (3) | 0.067 (2) | 0.0125 (19) | −0.0202 (18) | 0.014 (2) |
| C6 | 0.0411 (14) | 0.0434 (15) | 0.0370 (14) | 0.0035 (11) | −0.0009 (11) | 0.0003 (11) |
| C7 | 0.0506 (17) | 0.0440 (15) | 0.0437 (16) | 0.0043 (13) | 0.0045 (13) | −0.0041 (12) |
| C8 | 0.0530 (17) | 0.0497 (17) | 0.0505 (18) | 0.0039 (13) | −0.0085 (14) | 0.0125 (14) |
| C9 | 0.060 (2) | 0.067 (2) | 0.082 (3) | −0.0045 (17) | −0.028 (2) | 0.011 (2) |
| C10 | 0.0492 (16) | 0.0441 (16) | 0.0543 (18) | 0.0097 (12) | 0.0024 (14) | −0.0011 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N5 | 1.984 (2) | C2—C3 | 1.350 (5) |
| Cu1—N2 | 1.987 (2) | C2—H2 | 0.9300 |
| Cu1—O1 | 2.026 (2) | C3—H3 | 0.9300 |
| Cu1—O3 | 2.062 (3) | C4—C5 | 1.460 (7) |
| O1—N3 | 1.287 (4) | C4—H4A | 0.9600 |

| | | | |
|---|---|---|---|
| O2—N3 | 1.211 (4) | C4—H4B | 0.9600 |
| O3—N4 | 1.259 (4) | C4—H4C | 0.9600 |
| O4—N4 | 1.206 (5) | C5—H5A | 0.9705 |
| N1—C1 | 1.337 (4) | C5—H5B | 0.9686 |
| N1—C2 | 1.360 (5) | C6—H6 | 0.9300 |
| N1—C5 | 1.471 (4) | C7—C10 | 1.345 (4) |
| N2—C1 | 1.319 (4) | C7—H7 | 0.9300 |
| N2—C3 | 1.378 (4) | C8—C9 | 1.496 (5) |
| N5—C6 | 1.329 (4) | C8—H8A | 0.9700 |
| N5—C7 | 1.377 (4) | C8—H8B | 0.9700 |
| N6—C6 | 1.336 (4) | C9—H9A | 0.9600 |
| N6—C10 | 1.368 (4) | C9—H9B | 0.9600 |
| N6—C8 | 1.474 (4) | C9—H9C | 0.9600 |
| C1—H1 | 0.9300 | C10—H10 | 0.9300 |

| | | | |
|---|---|---|---|
| N5—Cu1—N2 | 175.68 (10) | C5—C4—H4B | 109.5 |
| N5—Cu1—O1 | 90.14 (10) | H4A—C4—H4B | 109.5 |
| N2—Cu1—O1 | 90.96 (10) | C5—C4—H4C | 109.5 |
| N5—Cu1—O3 | 89.82 (10) | H4A—C4—H4C | 109.5 |
| N2—Cu1—O3 | 90.25 (10) | H4B—C4—H4C | 109.5 |
| O1—Cu1—O3 | 164.17 (11) | C4—C5—N1 | 113.2 (4) |
| N3—O1—Cu1 | 112.57 (19) | C4—C5—H5A | 114.9 |
| N4—O3—Cu1 | 112.8 (2) | N1—C5—H5A | 108.7 |
| C1—N1—C2 | 107.3 (3) | C4—C5—H5B | 103.2 |
| C1—N1—C5 | 125.3 (3) | N1—C5—H5B | 108.8 |
| C2—N1—C5 | 127.4 (3) | H5A—C5—H5B | 107.6 |
| C1—N2—C3 | 105.6 (3) | N5—C6—N6 | 111.0 (3) |
| C1—N2—Cu1 | 125.7 (2) | N5—C6—H6 | 124.5 |
| C3—N2—Cu1 | 128.7 (2) | N6—C6—H6 | 124.5 |
| O2—N3—O1 | 114.3 (3) | C10—C7—N5 | 109.2 (3) |
| O4—N4—O3 | 114.7 (3) | C10—C7—H7 | 125.4 |
| C6—N5—C7 | 105.6 (2) | N5—C7—H7 | 125.4 |
| C6—N5—Cu1 | 126.3 (2) | N6—C8—C9 | 112.1 (3) |
| C7—N5—Cu1 | 127.9 (2) | N6—C8—H8A | 109.2 |
| C6—N6—C10 | 107.2 (2) | C9—C8—H8A | 109.2 |
| C6—N6—C8 | 125.1 (3) | N6—C8—H8B | 109.2 |
| C10—N6—C8 | 127.6 (3) | C9—C8—H8B | 109.2 |
| N2—C1—N1 | 111.3 (3) | H8A—C8—H8B | 107.9 |
| N2—C1—H1 | 124.4 | C8—C9—H9A | 109.5 |
| N1—C1—H1 | 124.4 | C8—C9—H9B | 109.5 |
| C3—C2—N1 | 106.9 (3) | H9A—C9—H9B | 109.5 |
| C3—C2—H2 | 126.5 | C8—C9—H9C | 109.5 |
| N1—C2—H2 | 126.5 | H9A—C9—H9C | 109.5 |
| C2—C3—N2 | 108.9 (3) | H9B—C9—H9C | 109.5 |
| C2—C3—H3 | 125.5 | C7—C10—N6 | 107.0 (3) |
| N2—C3—H3 | 125.5 | C7—C10—H10 | 126.5 |
| C5—C4—H4A | 109.5 | N6—C10—H10 | 126.5 |

| | | | |
|---|---|---|---|
| N5—Cu1—O1—N3 | −89.0 (2) | Cu1—N2—C1—N1 | −179.0 (2) |
| N2—Cu1—O1—N3 | 86.8 (2) | C2—N1—C1—N2 | −0.5 (4) |
| O3—Cu1—O1—N3 | −178.8 (3) | C5—N1—C1—N2 | −177.7 (3) |
| N5—Cu1—O3—N4 | 90.2 (2) | C1—N1—C2—C3 | 0.5 (4) |
| N2—Cu1—O3—N4 | −85.4 (2) | C5—N1—C2—C3 | 177.6 (4) |
| O1—Cu1—O3—N4 | −179.9 (3) | N1—C2—C3—N2 | −0.3 (4) |
| N5—Cu1—N2—C1 | 109.0 (13) | C1—N2—C3—C2 | 0.0 (4) |
| O1—Cu1—N2—C1 | 4.2 (3) | Cu1—N2—C3—C2 | 179.3 (2) |
| O3—Cu1—N2—C1 | −160.0 (3) | C1—N1—C5—C4 | −109.8 (5) |
| N5—Cu1—N2—C3 | −70.1 (14) | C2—N1—C5—C4 | 73.6 (6) |
| O1—Cu1—N2—C3 | −174.9 (3) | C7—N5—C6—N6 | 0.3 (3) |
| O3—Cu1—N2—C3 | 20.9 (3) | Cu1—N5—C6—N6 | 175.07 (18) |
| Cu1—O1—N3—O2 | −0.8 (3) | C10—N6—C6—N5 | −0.4 (3) |
| Cu1—O3—N4—O4 | −1.6 (4) | C8—N6—C6—N5 | 178.0 (3) |
| N2—Cu1—N5—C6 | 77.2 (14) | C6—N5—C7—C10 | 0.0 (3) |
| O1—Cu1—N5—C6 | −178.0 (2) | Cu1—N5—C7—C10 | −174.7 (2) |
| O3—Cu1—N5—C6 | −13.8 (3) | C6—N6—C8—C9 | −88.7 (4) |
| N2—Cu1—N5—C7 | −109.1 (13) | C10—N6—C8—C9 | 89.4 (4) |
| O1—Cu1—N5—C7 | −4.3 (2) | N5—C7—C10—N6 | −0.3 (4) |
| O3—Cu1—N5—C7 | 159.9 (3) | C6—N6—C10—C7 | 0.4 (3) |
| C3—N2—C1—N1 | 0.3 (4) | C8—N6—C10—C7 | −178.0 (3) |