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# Bis[2-(pyrrolidin-2-yl)-1*H*-benzimidazole-$\kappa^2N^2,N^3$]copper(II) dinitrate dihydrate

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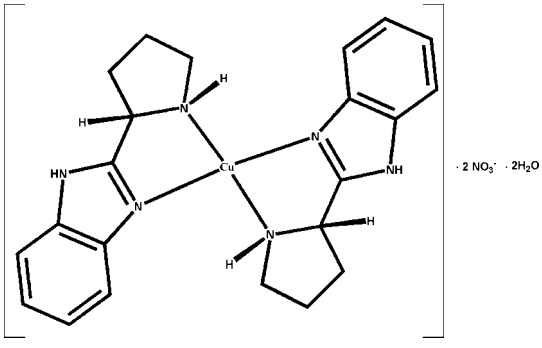
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.043; $wR$ factor = 0.101; data-to-parameter ratio = 15.5.

In the title compound, $[Cu(C_{11}H_{13}N_3)_2](NO_3)_2\cdot 2H_2O$, synthesized by hydrothermal reaction of $Cu(NO_3)_2$ and racemic 2-(pyrrolidin-2-yl)-1*H*-1,3-benzimidazole, the $Cu^{II}$ atom lies on an inversion centre. The distorted octahedral $Cu^{II}$ environment contains two planar *trans*-related *N*,*N*-chelating 2-(pyrrolidin-2-yl)-1*H*-1,3-benzimidazole ligands in the equatorial plane and two monodentate nitrate anions, which are in weak interaction with the Cu atom, in the axial positions. The two benzimidazole ligands have opposite configurations (*R*/*S* and *S*/*R*) and compound is a *meso* complex. In the crystal, N—H···O and O—H···O hydrogen bonds generate an infinite three-dimensional network. One methylene group of the pyrrolidine ring is disordered over two position with a 0.56 (3):0.44 (3) occupancy.

## Related literature

For physical properties such as the ferroelectric and dielectric behavior of metal-organic coordination compounds, see: Fu *et al.* (2007). For the synthesis, see: Aminabhavi *et al.* (1986). For related structures, see: Dai & Fu (2008*a*,*b*); Fu & Ye (2007).




## Experimental

### Crystal data

$[Cu(C_{11}H_{13}N_3)_2](NO_3)_2\cdot 2H_2O$
$M_r$ = 598.08
Triclinic, $P\overline{1}$
$a$ = 8.2790 (17) Å
$b$ = 8.4446 (17) Å
$c$ = 9.759 (2) Å
$\alpha$ = 100.37 (3)°
$\beta$ = 107.15 (3)°
$\gamma$ = 91.37 (3)°
$V$ = 639.1 (2) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.92 mm$^{-1}$
$T$ = 298 K
0.35 × 0.30 × 0.15 mm

### Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.732, $T_{max}$ = 0.871
6713 measured reflections
2914 independent reflections
2566 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.101
$S$ = 1.11
2914 reflections
188 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$B$···O1$^{i}$ | 0.91 | 2.25 | 2.986 (3) | 137 |
| O1$W$—H1$WA$···O2$^{ii}$ | 0.93 | 1.92 | 2.836 (4) | 169 |
| O1$W$—H1$WB$···O2$^{iii}$ | 0.98 | 1.94 | 2.861 (3) | 155 |
| N2—H2$B$···O1$W$ | 0.86 | 1.86 | 2.706 (3) | 168 |

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

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: *SHELXTL*.

This work was supported by a Start-up Grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2443).

## References

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# supporting information

*Acta Cryst.* (2009). E**65**, m661 [doi:10.1107/S160053680901808X]

## Bis[2-(pyrrolidin-2-yl)-1*H*-benzimidazole-$\kappa^2N^2,N^3$]copper(II) dinitrate dihydrate

**Jing Dai**

### S1. Comment

Amino acid derivatives have found wide range of applications in material science, such as ferroelectric, fluorescence and dielectric behaviors. And there has been an increased interest in the preparation of amino acid coordination compound (Aminabhavi *et al.,* 1986; Dai & Fu 2008*a*; Fu & Ye 2007; Dai & Fu 2008*b*; Fu, *et al.* 2007). We report here the crystal structure of the title compound, [Nitrate-[2-(pyrrolidin-2-yl)-1*H*-benzimidazole] Copper(II)] dihydrate.

In the title compound, the $Cu^{II}$ atom lies on an inversion centre. The distorted octahedral $Cu^{II}$ environment contains two planar *trans*-related *N*,*N*-chelating 2-(pyrrolidin-2-yl)-1*H*-1,3-benzimidazole ligands in the equatorial plane and two monodentate nitrate anion ligands which are in weak interaction with the Cu atom in the axial position. The two benzimidazole ligands have opposite configuration *R*,*S* and S,*R* and the complex is *meso*(Fig. 1).

In the crystal structure, molecules are linked into a three-dimension network by N—H···O and O—H···O hydrogen bonds.(Fig.2, Table 1).

### S2. Experimental

The racemic ligand 2-(pyrrolidin-2-yl)-1*H*-benzo[*d*]imidazole was synthesized by reaction of *S*-pyrrolidine-2-carboxylic acid and benzene-1,2-diamine according to the procedure described in the literature(Aminabhavi, *et al.*(1986)). A mixture of 2-(pyrrolidin-2-yl)-1*H*-benzo[*d*]imidazole (0.1 mmol) and $Cu(NO_3)_2$ (0.1 mmol) and water (1 ml) sealed in a glass tube were maintained at 70 °C. Crystals suitable for X-ray analysis were obtained after 5 days.

### S3. Refinement

All H atoms attached to C and N atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic), 0.97 Å (methylene) or 0.98 Å (methine) and N—H = 0.91 Å (N3), 0.86 Å (N2) with $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*). H atoms of water molecule located in difference Fouriermaps and in the last stage of refinement they were treated as riding on the O atom with $U_{iso}$(H) = 1.5$U_{eq}$(O).

One of the pyrrolidine rings is disordered with the C10 atom statistically distributed over two positions. These disorders were treated using the tools (SAME and PART) available in *SHELXL97* (Sheldrick, 2008).

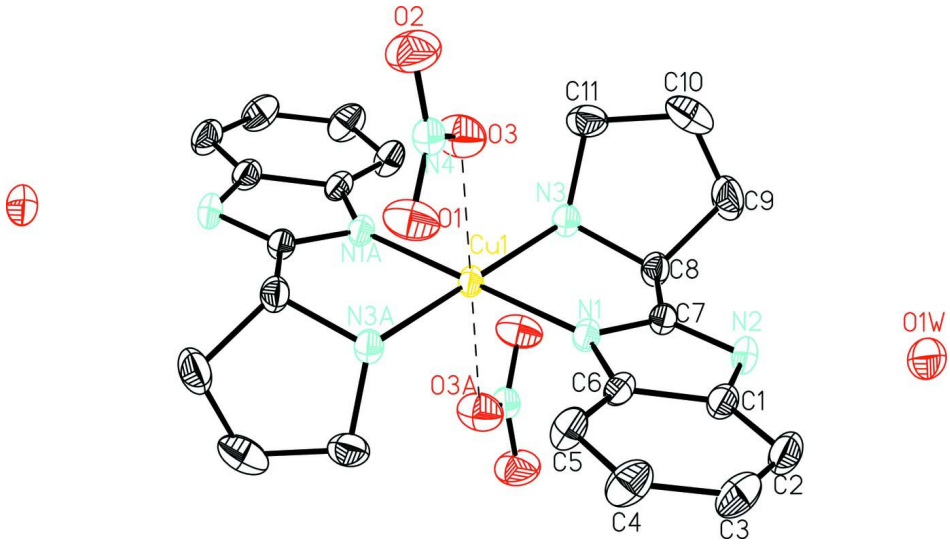


**Figure 1**

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level. H atoms have been omitted. The weak interaction of $Cu^{II}$ with nitrate is shown.

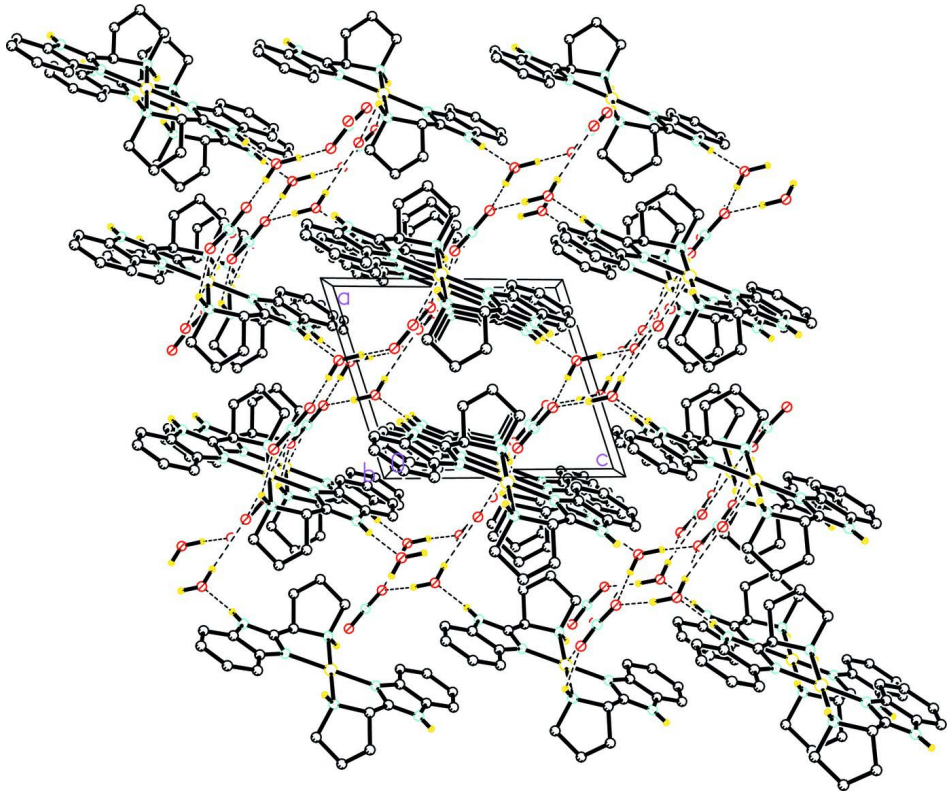

**Figure 2**

The crystal packing of the title compound viewed along the *a* axis and all hydrogen atoms not involved in hydrogen bonding (dashed lines) were omitted for clarity.

**Bis[2-(pyrrolidin-2-yl)-1*H*-benzimidazole-$\kappa^2N^2,N^3$]copper(II) dinitrate dihydrate**

*Crystal data*

$[Cu(C_{11}H_{13}N_3)_2](NO_3)_2\cdot 2H_2O$
$M_r = 598.08$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2790$ (17) Å
$b = 8.4446$ (17) Å
$c = 9.759$ (2) Å
$\alpha = 100.37$ (3)°
$\beta = 107.15$ (3)°
$\gamma = 91.37$ (3)°
$V = 639.1$ (2) Å$^3$
$Z = 1$
$F(000) = 311$
$D_x = 1.554$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2913 reflections
$\theta = 3.4$–27.5°
$\mu = 0.92$ mm$^{-1}$
$T = 298$ K
Block, blue
0.35 × 0.30 × 0.15 mm

*Data collection*

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm$^{-1}$
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.732$, $T_{max} = 0.871$
6713 measured reflections
2914 independent reflections
2566 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -10\rightarrow 10$
$k = -10\rightarrow 10$
$l = -12\rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.101$
$S = 1.11$
2914 reflections
188 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 0.444P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$

*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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cu1 | 1.0000 | 0.5000 | 0.5000 | 0.03289 (14) | |
| O1 | 0.8537 (3) | 0.0645 (3) | 0.4119 (3) | 0.0643 (6) | |
| O2 | 0.6487 (3) | 0.0360 (3) | 0.2118 (3) | 0.0745 (7) | |

| | | | | | |
|---|---|---|---|---|---|
| O3 | 0.7605 (3) | 0.2727 (3) | 0.3222 (3) | 0.0647 (6) | |
| N1 | 0.9102 (2) | 0.4814 (2) | 0.6652 (2) | 0.0329 (4) | |
| N2 | 0.7676 (3) | 0.5950 (3) | 0.8117 (2) | 0.0406 (5) | |
| H2B | 0.7115 | 0.6647 | 0.8502 | 0.049* | |
| N3 | 0.8509 (3) | 0.6877 (2) | 0.4834 (2) | 0.0345 (4) | |
| H3B | 0.9103 | 0.7701 | 0.4663 | 0.041* | |
| N4 | 0.7551 (3) | 0.1246 (3) | 0.3161 (2) | 0.0425 (5) | |
| C1 | 0.8109 (3) | 0.4496 (3) | 0.8525 (3) | 0.0383 (6) | |
| C2 | 0.7753 (4) | 0.3760 (4) | 0.9580 (3) | 0.0507 (7) | |
| H2A | 0.7151 | 0.4256 | 1.0184 | 0.061* | |
| C3 | 0.8337 (4) | 0.2263 (4) | 0.9686 (3) | 0.0552 (8) | |
| H3A | 0.8115 | 0.1721 | 1.0369 | 0.066* | |
| C4 | 0.9250 (4) | 0.1551 (4) | 0.8794 (3) | 0.0564 (8) | |
| H4A | 0.9643 | 0.0545 | 0.8909 | 0.068* | |
| C5 | 0.9603 (4) | 0.2272 (3) | 0.7737 (3) | 0.0467 (6) | |
| H5A | 1.0208 | 0.1769 | 0.7139 | 0.056* | |
| C6 | 0.9014 (3) | 0.3778 (3) | 0.7609 (2) | 0.0348 (5) | |
| C7 | 0.8291 (3) | 0.6078 (3) | 0.7009 (3) | 0.0338 (5) | |
| C8 | 0.8131 (3) | 0.7461 (3) | 0.6234 (3) | 0.0380 (6) | |
| H8A | 0.8966 | 0.8350 | 0.6830 | 0.046* | |
| C9 | 0.6378 (4) | 0.8083 (5) | 0.5821 (4) | 0.0658 (9) | |
| H9A | 0.5789 | 0.7940 | 0.6520 | 0.079* | |
| H9B | 0.6446 | 0.9216 | 0.5764 | 0.079* | |
| C11 | 0.6832 (4) | 0.6571 (4) | 0.3660 (3) | 0.0542 (8) | |
| H11A | 0.6811 | 0.7192 | 0.2911 | 0.065* | |
| H11B | 0.6610 | 0.5435 | 0.3209 | 0.065* | |
| O1W | 0.5901 (3) | 0.7856 (3) | 0.9583 (3) | 0.0757 (7) | |
| H1WA | 0.5045 | 0.8317 | 0.8968 | 0.113* | |
| H1WB | 0.6169 | 0.8451 | 1.0596 | 0.113* | |
| C10 | 0.5552 (12) | 0.709 (2) | 0.4410 (13) | 0.066 (3) | 0.56 (3) |
| H10A | 0.4736 | 0.7698 | 0.3822 | 0.079* | 0.56 (3) |
| H10B | 0.4948 | 0.6151 | 0.4524 | 0.079* | 0.56 (3) |
| C10′ | 0.5655 (18) | 0.773 (2) | 0.4195 (16) | 0.055 (3) | 0.44 (3) |
| H10C | 0.5642 | 0.8711 | 0.3809 | 0.066* | 0.44 (3) |
| H10D | 0.4507 | 0.7226 | 0.3896 | 0.066* | 0.44 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0347 (2) | 0.0409 (3) | 0.0285 (2) | 0.01231 (17) | 0.01597 (17) | 0.00874 (17) |
| O1 | 0.0575 (13) | 0.0570 (13) | 0.0686 (14) | 0.0016 (10) | −0.0016 (11) | 0.0231 (11) |
| O2 | 0.0782 (16) | 0.0615 (14) | 0.0594 (14) | 0.0032 (12) | −0.0028 (13) | −0.0098 (11) |
| O3 | 0.0681 (15) | 0.0449 (12) | 0.0709 (15) | 0.0090 (10) | 0.0053 (12) | 0.0119 (11) |
| N1 | 0.0356 (10) | 0.0360 (10) | 0.0300 (10) | 0.0063 (8) | 0.0148 (8) | 0.0052 (8) |
| N2 | 0.0427 (12) | 0.0473 (12) | 0.0368 (11) | 0.0108 (10) | 0.0227 (10) | 0.0027 (9) |
| N3 | 0.0368 (11) | 0.0351 (10) | 0.0355 (11) | 0.0066 (8) | 0.0161 (9) | 0.0077 (8) |
| N4 | 0.0372 (12) | 0.0490 (13) | 0.0411 (12) | 0.0057 (10) | 0.0151 (10) | 0.0025 (10) |
| C1 | 0.0386 (13) | 0.0454 (14) | 0.0311 (12) | −0.0013 (11) | 0.0142 (10) | 0.0025 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0549 (17) | 0.0651 (19) | 0.0374 (14) | −0.0001 (14) | 0.0250 (13) | 0.0056 (13) |
| C3 | 0.075 (2) | 0.0581 (18) | 0.0381 (15) | −0.0063 (16) | 0.0241 (14) | 0.0133 (13) |
| C4 | 0.085 (2) | 0.0457 (16) | 0.0441 (16) | 0.0056 (15) | 0.0246 (16) | 0.0150 (13) |
| C5 | 0.0660 (18) | 0.0421 (15) | 0.0378 (14) | 0.0090 (13) | 0.0244 (13) | 0.0076 (11) |
| C6 | 0.0401 (13) | 0.0387 (13) | 0.0257 (11) | 0.0003 (10) | 0.0127 (10) | 0.0024 (10) |
| C7 | 0.0313 (12) | 0.0393 (13) | 0.0306 (12) | 0.0026 (10) | 0.0120 (10) | 0.0016 (10) |
| C8 | 0.0420 (14) | 0.0362 (13) | 0.0383 (13) | 0.0094 (11) | 0.0177 (11) | 0.0033 (10) |
| C9 | 0.064 (2) | 0.081 (2) | 0.071 (2) | 0.0437 (18) | 0.0356 (18) | 0.0315 (19) |
| C11 | 0.0545 (18) | 0.0480 (16) | 0.0471 (16) | 0.0155 (13) | −0.0014 (14) | 0.0035 (13) |
| O1W | 0.0743 (16) | 0.0971 (18) | 0.0527 (13) | 0.0449 (14) | 0.0207 (12) | 0.0000 (12) |
| C10 | 0.036 (3) | 0.071 (7) | 0.086 (5) | 0.000 (4) | 0.003 (3) | 0.032 (5) |
| C10′ | 0.041 (5) | 0.049 (7) | 0.071 (6) | 0.018 (5) | 0.012 (4) | 0.009 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1$^{i}$ | 1.9922 (19) | C4—C5 | 1.384 (4) |
| Cu1—N1 | 1.9922 (19) | C4—H4A | 0.9300 |
| Cu1—N3 | 2.032 (2) | C5—C6 | 1.386 (4) |
| Cu1—N3$^{i}$ | 2.032 (2) | C5—H5A | 0.9300 |
| O1—N4 | 1.241 (3) | C7—C8 | 1.490 (3) |
| O2—N4 | 1.240 (3) | C8—C9 | 1.520 (4) |
| O3—N4 | 1.241 (3) | C8—H8A | 0.9800 |
| N1—C7 | 1.324 (3) | C9—C10 | 1.438 (13) |
| N1—C6 | 1.405 (3) | C9—C10′ | 1.492 (15) |
| N2—C7 | 1.343 (3) | C9—H9A | 0.9700 |
| N2—C1 | 1.382 (3) | C9—H9B | 0.9700 |
| N2—H2B | 0.8600 | C11—C10 | 1.488 (12) |
| N3—C8 | 1.491 (3) | C11—C10′ | 1.529 (11) |
| N3—C11 | 1.499 (3) | C11—H11A | 0.9700 |
| N3—H3B | 0.9100 | C11—H11B | 0.9700 |
| C1—C2 | 1.391 (4) | O1W—H1WA | 0.9281 |
| C1—C6 | 1.397 (3) | O1W—H1WB | 0.9827 |
| C2—C3 | 1.375 (4) | C10—H10A | 0.9700 |
| C2—H2A | 0.9300 | C10—H10B | 0.9700 |
| C3—C4 | 1.383 (4) | C10′—H10C | 0.9700 |
| C3—H3A | 0.9300 | C10′—H10D | 0.9700 |
| | | | |
| N1$^{i}$—Cu1—N1 | 180.000 (1) | N1—C7—C8 | 121.5 (2) |
| N1$^{i}$—Cu1—N3 | 97.34 (8) | N2—C7—C8 | 126.0 (2) |
| N1—Cu1—N3 | 82.66 (8) | C7—C8—N3 | 106.82 (19) |
| N1$^{i}$—Cu1—N3$^{i}$ | 82.66 (8) | C7—C8—C9 | 115.3 (2) |
| N1—Cu1—N3$^{i}$ | 97.34 (8) | N3—C8—C9 | 106.4 (2) |
| N3—Cu1—N3$^{i}$ | 180.00 (12) | C7—C8—H8A | 109.4 |
| C7—N1—C6 | 105.71 (19) | N3—C8—H8A | 109.4 |
| C7—N1—Cu1 | 112.43 (16) | C9—C8—H8A | 109.4 |
| C6—N1—Cu1 | 141.85 (16) | C10—C9—C8 | 102.8 (6) |
| C7—N2—C1 | 107.5 (2) | C10′—C9—C8 | 108.6 (5) |
| C7—N2—H2B | 126.2 | C10—C9—H9A | 111.2 |

| | | | |
|---|---|---|---|
| C1—N2—H2B | 126.2 | C10′—C9—H9A | 126.7 |
| C8—N3—C11 | 106.2 (2) | C8—C9—H9A | 111.2 |
| C8—N3—Cu1 | 110.88 (15) | C10—C9—H9B | 111.2 |
| C11—N3—Cu1 | 116.78 (16) | C10′—C9—H9B | 87.2 |
| C8—N3—H3B | 107.5 | C8—C9—H9B | 111.2 |
| C11—N3—H3B | 107.5 | H9A—C9—H9B | 109.1 |
| Cu1—N3—H3B | 107.5 | C10—C11—N3 | 105.4 (5) |
| O2—N4—O3 | 118.9 (2) | N3—C11—C10′ | 106.2 (5) |
| O2—N4—O1 | 119.9 (2) | C10—C11—H11A | 110.7 |
| O3—N4—O1 | 121.2 (2) | N3—C11—H11A | 110.7 |
| N2—C1—C2 | 131.1 (2) | C10′—C11—H11A | 88.8 |
| N2—C1—C6 | 106.1 (2) | C10—C11—H11B | 110.7 |
| C2—C1—C6 | 122.8 (3) | N3—C11—H11B | 110.7 |
| C3—C2—C1 | 116.6 (3) | C10′—C11—H11B | 129.2 |
| C3—C2—H2A | 121.7 | H11A—C11—H11B | 108.8 |
| C1—C2—H2A | 121.7 | H1WA—O1W—H1WB | 110.4 |
| C2—C3—C4 | 121.0 (3) | C9—C10—C11 | 109.9 (6) |
| C2—C3—H3A | 119.5 | C9—C10—H10A | 109.7 |
| C4—C3—H3A | 119.5 | C11—C10—H10A | 109.7 |
| C3—C4—C5 | 122.7 (3) | C9—C10—H10B | 109.7 |
| C3—C4—H4A | 118.7 | C11—C10—H10B | 109.7 |
| C5—C4—H4A | 118.7 | H10A—C10—H10B | 108.2 |
| C4—C5—C6 | 117.1 (3) | C9—C10′—C11 | 104.9 (8) |
| C4—C5—H5A | 121.5 | C9—C10′—H10C | 110.8 |
| C6—C5—H5A | 121.5 | C11—C10′—H10C | 110.8 |
| C5—C6—C1 | 119.8 (2) | C9—C10′—H10D | 110.8 |
| C5—C6—N1 | 132.0 (2) | C11—C10′—H10D | 110.8 |
| C1—C6—N1 | 108.1 (2) | H10C—C10′—H10D | 108.8 |
| N1—C7—N2 | 112.5 (2) | | |

| | | | |
|---|---|---|---|
| N3—Cu1—N1—C7 | −11.34 (17) | Cu1—N1—C7—C8 | −0.8 (3) |
| N3$^{i}$—Cu1—N1—C7 | 168.66 (17) | C1—N2—C7—N1 | −0.1 (3) |
| N3—Cu1—N1—C6 | 168.4 (3) | C1—N2—C7—C8 | −179.6 (2) |
| N3$^{i}$—Cu1—N1—C6 | −11.6 (3) | N1—C7—C8—N3 | 17.5 (3) |
| N1$^{i}$—Cu1—N3—C8 | −159.18 (16) | N2—C7—C8—N3 | −163.0 (2) |
| N1—Cu1—N3—C8 | 20.82 (16) | N1—C7—C8—C9 | 135.5 (3) |
| N1$^{i}$—Cu1—N3—C11 | 79.0 (2) | N2—C7—C8—C9 | −45.1 (4) |
| N1—Cu1—N3—C11 | −101.0 (2) | C11—N3—C8—C7 | 102.9 (2) |
| C7—N2—C1—C2 | −178.2 (3) | Cu1—N3—C8—C7 | −24.9 (2) |
| C7—N2—C1—C6 | 0.3 (3) | C11—N3—C8—C9 | −20.7 (3) |
| N2—C1—C2—C3 | 178.1 (3) | Cu1—N3—C8—C9 | −148.6 (2) |
| C6—C1—C2—C3 | −0.2 (4) | C7—C8—C9—C10 | −88.1 (7) |
| C1—C2—C3—C4 | 0.8 (5) | N3—C8—C9—C10 | 30.0 (7) |
| C2—C3—C4—C5 | −1.2 (5) | C7—C8—C9—C10′ | −112.9 (9) |
| C3—C4—C5—C6 | 0.7 (5) | N3—C8—C9—C10′ | 5.3 (10) |
| C4—C5—C6—C1 | −0.1 (4) | C8—N3—C11—C10 | 3.6 (8) |
| C4—C5—C6—N1 | −178.1 (3) | Cu1—N3—C11—C10 | 127.8 (7) |
| N2—C1—C6—C5 | −178.9 (2) | C8—N3—C11—C10′ | 28.3 (10) |

| | | | |
|---|---|---|---|
| C2—C1—C6—C5 | −0.2 (4) | Cu1—N3—C11—C10′ | 152.6 (9) |
| N2—C1—C6—N1 | −0.4 (3) | C10′—C9—C10—C11 | 78.5 (18) |
| C2—C1—C6—N1 | 178.3 (2) | C8—C9—C10—C11 | −28.4 (12) |
| C7—N1—C6—C5 | 178.6 (3) | N3—C11—C10—C9 | 16.2 (12) |
| Cu1—N1—C6—C5 | −1.1 (5) | C10′—C11—C10—C9 | −79 (2) |
| C7—N1—C6—C1 | 0.4 (3) | C10—C9—C10′—C11 | −68.1 (16) |
| Cu1—N1—C6—C1 | −179.4 (2) | C8—C9—C10′—C11 | 11.8 (14) |
| C6—N1—C7—N2 | −0.2 (3) | C10—C11—C10′—C9 | 67 (2) |
| Cu1—N1—C7—N2 | 179.63 (16) | N3—C11—C10′—C9 | −24.6 (14) |
| C6—N1—C7—C8 | 179.4 (2) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*B*···O1$^{i}$ | 0.91 | 2.25 | 2.986 (3) | 137 |
| O1*W*—H1*WA*···O2$^{ii}$ | 0.93 | 1.92 | 2.836 (4) | 169 |
| O1*W*—H1*WB*···O2$^{iii}$ | 0.98 | 1.94 | 2.861 (3) | 155 |
| N2—H2*B*···O1*W* | 0.86 | 1.86 | 2.706 (3) | 168 |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*+1, *z*+1.