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# Aqua(2,2′-bipyrimidine-$\kappa^2N,N'$)(succinato-$\kappa^2O^1,O^4$)copper(II) dihydrate

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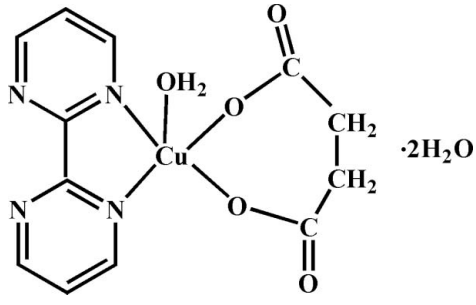
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.043; $wR$ factor = 0.123; data-to-parameter ratio = 11.6.

In the crystal structure of the title compound, $[Cu(C_4H_4O_4)(C_8H_6N_4)(H_2O)]\cdot 2H_2O$, the $Cu^{II}$ atom is chelated by a 2,2′-bipyrimidine (bpm) ligand and a succinate anion in the basal plane; a water molecule in the apical position completes the slightly distorted square-pyramidal coordination geometry. Another carboxylate O atom from an adjacent complex is located in the opposite apical direction, with a Cu···O distance of 2.706 (3) Å, and is not considered as a bridging atom. Extensive O—H···O and O—H···N hydrogen bonding is present in the crystal structure.

## Related literature

For general background, see: McCann *et al.* (1997); Ray *et al.* (2004); Zhang *et al.* (2004).




## Experimental

### Crystal data

$[Cu(C_4H_4O_4)(C_8H_6N_4)(H_2O)]\cdot 2H_2O$
$M_r$ = 391.83
Monoclinic, $P2_1/c$
$a$ = 10.6905 (8) Å
$b$ = 18.9321 (14) Å
$c$ = 7.6105 (6) Å
$\beta$ = 92.2290 (10)°
$V$ = 1539.2 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.46 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.09 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.700, $T_{max}$ = 0.877
7725 measured reflections
2735 independent reflections
2085 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
$S$ = 1.06
2735 reflections
235 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.66 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—O1 | 2.386 (3) | Cu1—N1 | 2.017 (3) |
| Cu1—O2 | 1.918 (3) | Cu1—N2 | 2.012 (3) |
| Cu1—O5 | 1.940 (3) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O1$W$ | 0.85 (4) | 1.89 (4) | 2.703 (5) | 162 (4) |
| O1—H1$B$···O4$^{i}$ | 0.85 (4) | 2.05 (4) | 2.903 (4) | 178 (4) |
| O1$W$—H1$WA$···O2$W^{ii}$ | 0.85 (4) | 1.950 (17) | 2.790 (6) | 169 (5) |
| O1$W$—H1$WB$···N3$^{iii}$ | 0.84 (4) | 2.45 (5) | 3.216 (5) | 152 (4) |
| O1$W$—H1$WB$···N4$^{iii}$ | 0.84 (4) | 2.46 (4) | 3.130 (5) | 137 (5) |
| O2$W$—H2$WA$···O3$^{iii}$ | 0.85 (4) | 2.04 (4) | 2.876 (6) | 167 (5) |
| O2$W$—H2$WB$···O3$^{iv}$ | 0.85 (4) | 1.94 (4) | 2.777 (5) | 168 (4) |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU2509).

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# supporting information

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## Aqua(2,2′-bipyrimidine-$\kappa^2N,N'$)(succinato-$\kappa^2O^1,O^4$)copper(II) dihydrate

**Xi-Jun Ke, Dong-Sheng Li, Jun Zhao, Qiu-Fen He and Cai Li**

### S1. Comment

Recently, the area of metal-organic framework materials has become one of the intense research activities for their fascinating structural diversities and potential applications in catalysis, nonlinear optics and molecular sensing. As an important family of multidentate O-donor ligands, saturated aliphatic carboxylate ligands have been extensively employed in the preparation of metal-organic complexes because of their potential properties and intriguing structural topologies (McCann *et al.*, 1997; Ray *et al.*, 2004; Zhang *et al.* 2004). Herein, we report the structure of the title complex.

The title compound contains one $Cu^{II}$ cation, one suc ligands, one bpm ligands, one coordinated water and two lattice water molecules, as illustrated in Fig. 1. The $Cu^{II}$ atom has a slightly distored square-pyramidal geometry (Table 1), in which the $Cu^{II}$atom is coordinated by two N atoms of bpm ligand, two O atoms from carboxyl groups of succinate anions and one O atom from coordinated water molecule. Each unit is connected by O—H···O hydrogen bonds between carboxyl groups and coordinated water molecules (Table 2) into one-dimensional chain along *c*-axis. The lattice water molecule acts as both hydrogen-bond donor and acceptor. Just through hydrogen bonds (O—H···O) involving lattice water molecules, those one-dimensional chains are further connected to generate a three-dimensional supramolecular framework.

### S2. Experimental

A mixture of $CuCl_2.2H_2O$ (0.017 g, 0.1 mmol), bpm (0.015 g, 0.1 mmol), sodium succinate (0.0139 g, 0.1 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave. The pH value of the mixture was adjusted to 6 by an aqueous solution of NaOH (0.1 mol/*L*), and then heated at 393 K for 3 days; blue crystals were obtained on cooling to room temperature at 5 K/h.

### S3. Refinement

Water H atoms were located in a difference Fourier map and refined with distance restraints O—H = 0.85 (2) Å, $U_{iso}$(H) = 1.5$U_{eq}$(O). Other H atoms were placed in calculated positions and treated using a riding-model approximation with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

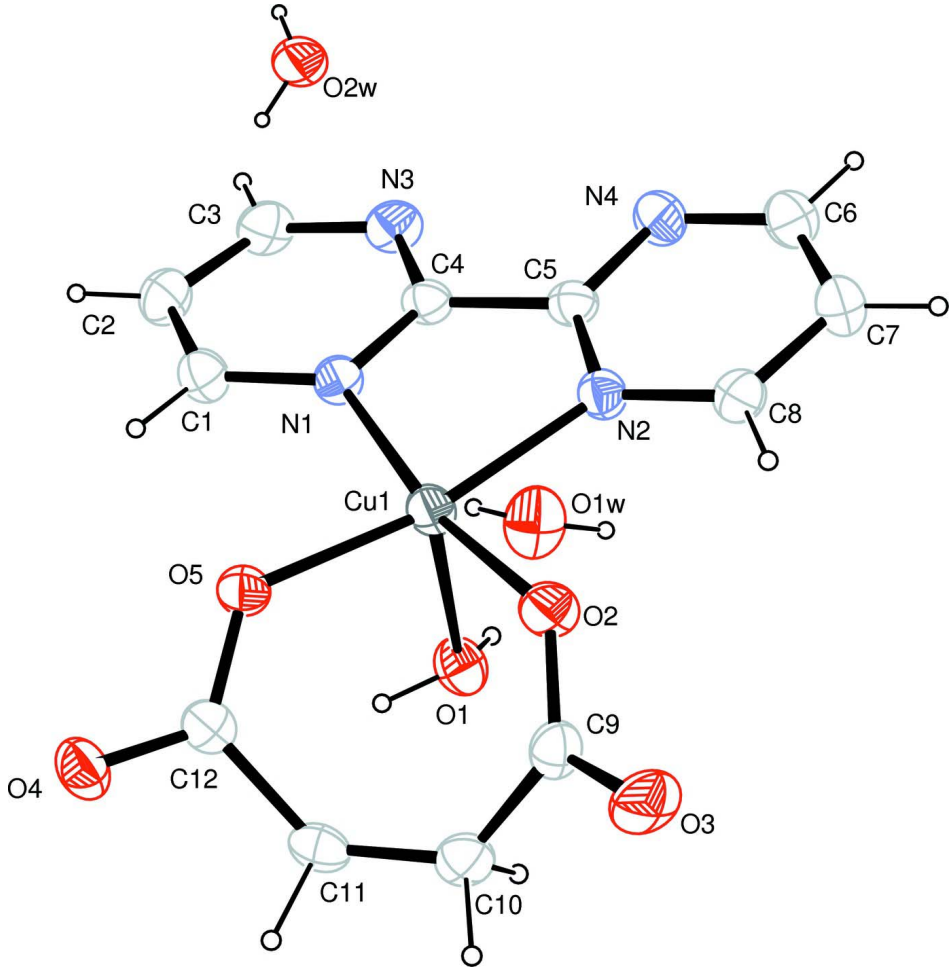


**Figure 1**

View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Aqua(2,2′-bipyrimidine-$\kappa^2N,N'$)(succinato-$\kappa^2O^1,O^4$)copper(II) dihydrate**

*Crystal data*

$[Cu(C_4H_4O_4)(C_8H_6N_4)(H_2O)]\cdot 2H_2O$
$M_r = 391.83$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.6905$ (8) Å
$b = 18.9321$ (14) Å
$c = 7.6105$ (6) Å
$\beta = 92.229$ (1)°
$V = 1539.2$ (2) Å$^3$
$Z = 4$
$F(000) = 804$
$D_x = 1.691$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3225 reflections
$\theta = 1.9$–25.1°
$\mu = 1.46$ mm$^{-1}$
$T = 293$ K
Prism, blue
0.30 × 0.20 × 0.09 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.700$, $T_{max} = 0.877$
7725 measured reflections
2735 independent reflections

2085 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.9°$
$h = -12 \rightarrow 12$
$k = -22 \rightarrow 22$
$l = -9 \rightarrow 4$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.123$
$S = 1.06$
2735 reflections
235 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 1.4777P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.46$ e Å$^{-3}$
$\Delta\rho_{min} = -0.66$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.83883 (5) | 0.98092 (2) | 0.42287 (7) | 0.0376 (2) |
| O1 | 0.7210 (3) | 0.94912 (16) | 0.1622 (4) | 0.0477 (8) |
| H1A | 0.673 (4) | 0.9136 (17) | 0.160 (6) | 0.072* |
| H1B | 0.774 (4) | 0.945 (2) | 0.082 (5) | 0.072* |
| O1W | 0.6018 (4) | 0.82533 (18) | 0.2132 (6) | 0.0724 (11) |
| H1WA | 0.5230 (12) | 0.819 (3) | 0.212 (9) | 0.109* |
| H1WB | 0.637 (4) | 0.790 (2) | 0.170 (9) | 0.109* |
| O2 | 0.7834 (3) | 1.07626 (14) | 0.4543 (4) | 0.0459 (7) |
| O2W | 0.6560 (4) | 0.3145 (2) | 0.2485 (6) | 0.0810 (12) |
| H2WB | 0.674 (7) | 0.2726 (15) | 0.280 (8) | 0.121* |
| H2WA | 0.676 (7) | 0.321 (3) | 0.143 (4) | 0.121* |
| O3 | 0.7344 (3) | 1.18623 (16) | 0.3913 (5) | 0.0606 (9) |
| O4 | 1.1035 (3) | 1.06421 (15) | 0.1176 (4) | 0.0490 (8) |
| O5 | 0.9903 (3) | 1.00736 (14) | 0.3069 (4) | 0.0395 (7) |
| N1 | 0.8883 (3) | 0.87826 (17) | 0.4388 (4) | 0.0362 (8) |
| N2 | 0.7034 (3) | 0.94476 (18) | 0.5757 (4) | 0.0382 (8) |
| N3 | 0.8133 (3) | 0.76731 (17) | 0.5315 (5) | 0.0468 (9) |
| N4 | 0.6295 (3) | 0.8392 (2) | 0.7042 (5) | 0.0494 (10) |
| C1 | 0.9872 (4) | 0.8470 (2) | 0.3680 (6) | 0.0435 (10) |
| H1C | 1.0466 | 0.8745 | 0.3135 | 0.052* |
| C2 | 1.0017 (4) | 0.7748 (2) | 0.3750 (6) | 0.0499 (11) |

| | | | | |
|---|---|---|---|---|
| H2 | 1.0700 | 0.7525 | 0.3272 | 0.060* |
| C3 | 0.9102 (4) | 0.7374 (2) | 0.4561 (6) | 0.0491 (11) |
| H3 | 0.9164 | 0.6884 | 0.4584 | 0.059* |
| C4 | 0.8069 (4) | 0.8370 (2) | 0.5194 (5) | 0.0368 (9) |
| C5 | 0.7056 (4) | 0.8751 (2) | 0.6045 (5) | 0.0376 (9) |
| C6 | 0.5436 (4) | 0.8772 (3) | 0.7835 (7) | 0.0573 (13) |
| H6 | 0.4886 | 0.8539 | 0.8557 | 0.069* |
| C7 | 0.5319 (4) | 0.9492 (3) | 0.7641 (6) | 0.0546 (12) |
| H7 | 0.4704 | 0.9746 | 0.8201 | 0.066* |
| C8 | 0.6163 (4) | 0.9822 (2) | 0.6570 (6) | 0.0459 (11) |
| H8 | 0.6124 | 1.0309 | 0.6414 | 0.055* |
| C9 | 0.7701 (4) | 1.1270 (2) | 0.3460 (6) | 0.0413 (10) |
| C10 | 0.7927 (4) | 1.1167 (2) | 0.1584 (6) | 0.0442 (11) |
| H10A | 0.7179 | 1.0939 | 0.1097 | 0.053* |
| H10B | 0.7932 | 1.1638 | 0.1082 | 0.053* |
| C11 | 0.8904 (4) | 1.0823 (2) | 0.0863 (6) | 0.0409 (10) |
| H11A | 0.9243 | 1.1155 | 0.0036 | 0.049* |
| H11B | 0.8523 | 1.0448 | 0.0156 | 0.049* |
| C12 | 1.0022 (4) | 1.0491 (2) | 0.1772 (5) | 0.0370 (9) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0438 (3) | 0.0255 (3) | 0.0444 (3) | 0.0014 (2) | 0.0122 (2) | 0.0028 (2) |
| O1 | 0.0475 (18) | 0.0452 (17) | 0.0511 (19) | −0.0081 (14) | 0.0088 (15) | −0.0032 (15) |
| O1W | 0.071 (2) | 0.0425 (19) | 0.104 (3) | −0.0055 (18) | 0.012 (2) | −0.008 (2) |
| O2 | 0.0617 (19) | 0.0287 (14) | 0.0479 (18) | 0.0054 (14) | 0.0112 (15) | 0.0025 (13) |
| O2W | 0.100 (3) | 0.063 (2) | 0.081 (3) | 0.028 (2) | 0.022 (3) | 0.024 (2) |
| O3 | 0.083 (2) | 0.0362 (17) | 0.063 (2) | 0.0214 (17) | 0.0051 (19) | −0.0003 (16) |
| O4 | 0.0475 (18) | 0.0434 (17) | 0.057 (2) | −0.0044 (14) | 0.0187 (16) | 0.0048 (15) |
| O5 | 0.0417 (16) | 0.0332 (14) | 0.0439 (17) | −0.0001 (12) | 0.0055 (13) | 0.0063 (13) |
| N1 | 0.0393 (18) | 0.0300 (17) | 0.0395 (19) | 0.0004 (15) | 0.0026 (16) | −0.0003 (15) |
| N2 | 0.0403 (18) | 0.0358 (18) | 0.039 (2) | 0.0019 (15) | 0.0066 (16) | 0.0009 (15) |
| N3 | 0.055 (2) | 0.0281 (18) | 0.057 (2) | −0.0029 (16) | 0.001 (2) | 0.0058 (17) |
| N4 | 0.042 (2) | 0.049 (2) | 0.058 (2) | −0.0074 (17) | 0.0105 (19) | 0.0130 (19) |
| C1 | 0.046 (2) | 0.041 (2) | 0.044 (2) | −0.001 (2) | 0.008 (2) | −0.002 (2) |
| C2 | 0.052 (3) | 0.041 (2) | 0.057 (3) | 0.010 (2) | 0.005 (2) | −0.003 (2) |
| C3 | 0.062 (3) | 0.030 (2) | 0.056 (3) | 0.006 (2) | 0.003 (2) | −0.001 (2) |
| C4 | 0.038 (2) | 0.033 (2) | 0.039 (2) | −0.0051 (17) | 0.0001 (19) | 0.0064 (18) |
| C5 | 0.038 (2) | 0.037 (2) | 0.038 (2) | −0.0028 (18) | −0.0011 (19) | 0.0060 (18) |
| C6 | 0.045 (3) | 0.069 (3) | 0.059 (3) | −0.003 (2) | 0.011 (2) | 0.014 (3) |
| C7 | 0.045 (3) | 0.068 (3) | 0.051 (3) | 0.005 (2) | 0.012 (2) | 0.002 (3) |
| C8 | 0.050 (3) | 0.042 (2) | 0.046 (3) | 0.010 (2) | 0.005 (2) | 0.002 (2) |
| C9 | 0.038 (2) | 0.032 (2) | 0.054 (3) | 0.0007 (18) | 0.006 (2) | 0.001 (2) |
| C10 | 0.044 (2) | 0.033 (2) | 0.056 (3) | −0.0061 (19) | 0.001 (2) | 0.010 (2) |
| C11 | 0.050 (2) | 0.031 (2) | 0.042 (2) | −0.0139 (19) | 0.003 (2) | 0.0073 (19) |
| C12 | 0.048 (2) | 0.0251 (19) | 0.039 (2) | −0.0006 (18) | 0.008 (2) | −0.0044 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 2.386 (3) | N4—C5 | 1.323 (5) |
| Cu1—O2 | 1.918 (3) | N4—C6 | 1.330 (6) |
| Cu1—O5 | 1.940 (3) | C1—C2 | 1.376 (6) |
| Cu1—N1 | 2.017 (3) | C1—H1C | 0.9300 |
| Cu1—N2 | 2.012 (3) | C2—C3 | 1.374 (6) |
| O1—H1A | 0.85 (4) | C2—H2 | 0.9300 |
| O1—H1B | 0.85 (4) | C3—H3 | 0.9300 |
| O1W—H1WA | 0.85 (4) | C4—C5 | 1.472 (6) |
| O1W—H1WB | 0.84 (4) | C6—C7 | 1.377 (7) |
| O2—C9 | 1.270 (5) | C6—H6 | 0.9300 |
| O2W—H2WB | 0.85 (4) | C7—C8 | 1.388 (6) |
| O2W—H2WA | 0.85 (4) | C7—H7 | 0.9300 |
| O3—C9 | 1.239 (5) | C8—H8 | 0.9300 |
| O4—C12 | 1.224 (5) | C9—C10 | 1.469 (6) |
| O5—C12 | 1.275 (5) | C10—C11 | 1.365 (5) |
| N1—C4 | 1.336 (5) | C10—H10A | 0.9700 |
| N1—C1 | 1.343 (5) | C10—H10B | 0.9700 |
| N2—C5 | 1.336 (5) | C11—C12 | 1.495 (6) |
| N2—C8 | 1.341 (5) | C11—H11A | 0.9700 |
| N3—C4 | 1.324 (5) | C11—H11B | 0.9700 |
| N3—C3 | 1.330 (5) | | |
| | | | |
| O2—Cu1—O5 | 94.68 (12) | N3—C4—N1 | 125.6 (4) |
| O2—Cu1—N2 | 90.87 (13) | N3—C4—C5 | 119.7 (3) |
| O5—Cu1—N2 | 169.41 (13) | N1—C4—C5 | 114.7 (3) |
| O2—Cu1—N1 | 168.87 (13) | N4—C5—N2 | 126.5 (4) |
| O5—Cu1—N1 | 93.13 (13) | N4—C5—C4 | 118.6 (4) |
| N2—Cu1—N1 | 80.22 (13) | N2—C5—C4 | 114.9 (3) |
| O2—Cu1—O1 | 100.69 (12) | N4—C6—C7 | 123.2 (4) |
| O5—Cu1—O1 | 96.32 (12) | N4—C6—H6 | 118.4 |
| N2—Cu1—O1 | 91.50 (12) | C7—C6—H6 | 118.4 |
| N1—Cu1—O1 | 86.30 (12) | C6—C7—C8 | 116.8 (4) |
| Cu1—O1—H1A | 121 (4) | C6—C7—H7 | 121.6 |
| Cu1—O1—H1B | 106 (3) | C8—C7—H7 | 121.6 |
| H1A—O1—H1B | 109 (4) | N2—C8—C7 | 120.8 (4) |
| H1WA—O1W—H1WB | 110 (5) | N2—C8—H8 | 119.6 |
| C9—O2—Cu1 | 131.1 (3) | C7—C8—H8 | 119.6 |
| H2WB—O2W—H2WA | 110 (6) | O3—C9—O2 | 122.1 (4) |
| C12—O5—Cu1 | 128.5 (3) | O3—C9—C10 | 117.0 (4) |
| C4—N1—C1 | 117.6 (3) | O2—C9—C10 | 120.9 (4) |
| C4—N1—Cu1 | 114.7 (3) | C11—C10—C9 | 127.7 (4) |
| C1—N1—Cu1 | 127.5 (3) | C11—C10—H10A | 105.4 |
| C5—N2—C8 | 117.0 (4) | C9—C10—H10A | 105.4 |
| C5—N2—Cu1 | 115.0 (3) | C11—C10—H10B | 105.4 |
| C8—N2—Cu1 | 128.0 (3) | C9—C10—H10B | 105.4 |
| C4—N3—C3 | 115.7 (4) | H10A—C10—H10B | 106.0 |

| | | | |
|---|---|---|---|
| C5—N4—C6 | 115.7 (4) | C10—C11—C12 | 128.7 (4) |
| N1—C1—C2 | 120.7 (4) | C10—C11—H11A | 105.1 |
| N1—C1—H1C | 119.6 | C12—C11—H11A | 105.1 |
| C2—C1—H1C | 119.6 | C10—C11—H11B | 105.1 |
| C3—C2—C1 | 116.7 (4) | C12—C11—H11B | 105.1 |
| C3—C2—H2 | 121.7 | H11A—C11—H11B | 105.9 |
| C1—C2—H2 | 121.7 | O4—C12—O5 | 123.2 (4) |
| N3—C3—C2 | 123.6 (4) | O4—C12—C11 | 115.7 (4) |
| N3—C3—H3 | 118.2 | O5—C12—C11 | 121.1 (4) |
| C2—C3—H3 | 118.2 | | |

| | | | |
|---|---|---|---|
| O5—Cu1—O2—C9 | 51.3 (4) | C3—N3—C4—C5 | −177.7 (4) |
| N2—Cu1—O2—C9 | −137.8 (4) | C1—N1—C4—N3 | −2.0 (6) |
| N1—Cu1—O2—C9 | −174.3 (6) | Cu1—N1—C4—N3 | 173.5 (4) |
| O1—Cu1—O2—C9 | −46.1 (4) | C1—N1—C4—C5 | 176.0 (4) |
| O2—Cu1—O5—C12 | −50.4 (3) | Cu1—N1—C4—C5 | −8.5 (4) |
| N2—Cu1—O5—C12 | −171.8 (6) | C6—N4—C5—N2 | −0.5 (7) |
| N1—Cu1—O5—C12 | 137.5 (3) | C6—N4—C5—C4 | 177.1 (4) |
| O1—Cu1—O5—C12 | 50.9 (3) | C8—N2—C5—N4 | 0.7 (6) |
| O2—Cu1—N1—C4 | 43.9 (8) | Cu1—N2—C5—N4 | 177.8 (3) |
| O5—Cu1—N1—C4 | 178.4 (3) | C8—N2—C5—C4 | −177.1 (4) |
| N2—Cu1—N1—C4 | 6.7 (3) | Cu1—N2—C5—C4 | 0.0 (5) |
| O1—Cu1—N1—C4 | −85.5 (3) | N3—C4—C5—N4 | 5.8 (6) |
| O2—Cu1—N1—C1 | −141.1 (6) | N1—C4—C5—N4 | −172.3 (4) |
| O5—Cu1—N1—C1 | −6.6 (4) | N3—C4—C5—N2 | −176.3 (4) |
| N2—Cu1—N1—C1 | −178.3 (4) | N1—C4—C5—N2 | 5.6 (5) |
| O1—Cu1—N1—C1 | 89.5 (4) | C5—N4—C6—C7 | 0.5 (7) |
| O2—Cu1—N2—C5 | −176.8 (3) | N4—C6—C7—C8 | −0.6 (8) |
| O5—Cu1—N2—C5 | −55.1 (8) | C5—N2—C8—C7 | −0.8 (6) |
| N1—Cu1—N2—C5 | −3.5 (3) | Cu1—N2—C8—C7 | −177.4 (3) |
| O1—Cu1—N2—C5 | 82.5 (3) | C6—C7—C8—N2 | 0.8 (7) |
| O2—Cu1—N2—C8 | 0.0 (4) | Cu1—O2—C9—O3 | −178.8 (3) |
| O5—Cu1—N2—C8 | 121.6 (7) | Cu1—O2—C9—C10 | 3.2 (6) |
| N1—Cu1—N2—C8 | 173.2 (4) | O3—C9—C10—C11 | 137.1 (5) |
| O1—Cu1—N2—C8 | −100.8 (4) | O2—C9—C10—C11 | −44.9 (7) |
| C4—N1—C1—C2 | 1.6 (6) | C9—C10—C11—C12 | −3.2 (7) |
| Cu1—N1—C1—C2 | −173.3 (3) | Cu1—O5—C12—O4 | 177.3 (3) |
| N1—C1—C2—C3 | 0.5 (7) | Cu1—O5—C12—C11 | −3.5 (5) |
| C4—N3—C3—C2 | 2.2 (7) | C10—C11—C12—O4 | −131.7 (4) |
| C1—C2—C3—N3 | −2.5 (7) | C10—C11—C12—O5 | 49.0 (6) |
| C3—N3—C4—N1 | 0.2 (6) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···O1*W* | 0.85 (4) | 1.89 (4) | 2.703 (5) | 162 (4) |
| O1—H1*B*···O4$^{i}$ | 0.85 (4) | 2.05 (4) | 2.903 (4) | 178 (4) |
| O1*W*—H1*WA*···O2*W*$^{ii}$ | 0.85 (4) | 1.95 (2) | 2.790 (6) | 169 (5) |

| | | | | |
|---|---|---|---|---|
| O1*W*—H1*WB*···N3$^{iii}$ | 0.84 (4) | 2.45 (5) | 3.216 (5) | 152 (4) |
| O1*W*—H1*WB*···N4$^{iii}$ | 0.84 (4) | 2.46 (4) | 3.130 (5) | 137 (5) |
| O2*W*—H2*WA*···O3$^{iii}$ | 0.85 (4) | 2.04 (4) | 2.876 (6) | 167 (5) |
| O2*W*—H2*WB*···O3$^{iv}$ | 0.85 (4) | 1.94 (4) | 2.777 (5) | 168 (4) |

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*; (ii) −*x*+1, *y*+1/2, −*z*+1/2; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) *x*, *y*−1, *z*.