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Diagua(2,2'-bipyridine- $\kappa^2 N, N'$)bis- $(perchlorato - \kappa O) copper(II)$

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.080; data-to-parameter ratio = 21.6.

The central CuN₂O₄ motif of the title compound, [Cu(ClO₄)₂(C₁₀H₈N₂)(H₂O)₂], exhibits a Jahn–Teller-distorted octahedral geometry around the metal atom, showing a considerably long Cu-O bond distance of 2.5058 (12) Å towards the second perchlorate group, giving a (4 + 1+1)-type coordination mode. In the crystal, the components are linked *via* intermolecular $O-H \cdots O$ hydrogen bonds, forming layers parallel to (001). Additional stabilization within these layers is provided by $\pi - \pi$ [centroid–centroid distances of 3.7848 (9)– 4.4231 (9) Å] stacking interactions.

Related literature

For applications of related compounds, see: Kurzak et al. (1999). For the coordination spheres of copper in related compounds, see: Hathaway (1973). For hydrogen-bond motifs, see: Bernstein et al. (1995); Etter et al. (1990).



Experimental

Crystal data $[Cu(ClO_4)_2(C_{10}H_8N_2)(H_2O)_2]$

 $M_r = 454.67$

Data collection

Oxford Diffraction Xcalibur 16487 measured reflections Sapphire2 diffractometer 5135 independent reflections 4239 reflections with $I > 2\sigma(I)$ Absorption correction: multi-scan (CrysAlis RED; Oxford $R_{\rm int} = 0.034$ Diffraction, 2008) $T_{\min} = 0.580, \ T_{\max} = 1.000$

Refinement

| $R[F^2 > 2\sigma(F^2)] = 0.030$ | H atoms treated by a mixture of |
|---------------------------------|--|
| $wR(F^2) = 0.080$ | independent and constrained |
| S = 1.05 | refinement |
| 5135 reflections | $\Delta \rho_{\rm max} = 0.42 \text{ e } \text{\AA}^{-3}$ |
| 238 parameters | $\Delta \rho_{\rm min} = -0.63 \text{ e } \text{\AA}^{-3}$ |

| Table 1 | | | |
|---------------|----------|-----|-----|
| Hvdrogen-bond | geometry | (Å. | °). |

| $D - H \cdot \cdot \cdot A$ | D-H | $H \cdot \cdot \cdot A$ | $D \cdots A$ | $D - \mathbf{H} \cdots A$ |
|---|--|--|---|--|
| $\begin{array}{c} 01W - H1W \cdots 010^{i} \\ 01W - H2W \cdots 03^{ii} \\ 02W - H3W \cdots 03^{iii} \\ 02W - H4W \cdots 04 \\ 02W - H4W \cdots 07^{iv} \end{array}$ | 0.72 (2) 0.88 (2) 0.76 (2) 0.78 (2) 0.78 (2) | 2.04 (2) 1.89 (2) 2.13 (2) 2.37 (2) 2.26 (3) | 2.7078 (17) 2.7665 (17) 2.8802 (18) 2.9518 (19) 2.8349 (18) | 155 (3) 177.3 (18) 169 (2) 133 (2) 132 (2) |
| Symmetry codes: (i) -x+2, -y+1, -z. | x - 1, y, z; (ii) |) $-x+1, -y$ | x + 1, -z; (iii) x | +1, y, z; (iv) |

Data collection: CrysAlis CCD (Oxford Diffraction, 2008); cell refinement: CrysAlis CCD; data reduction: CrysAlis CCD; program(s) used to solve structure: SIR2002 (Burla et al., 2003); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008): molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and DIAMOND (Brandenburg & Berndt, 2001); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2292).

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Mo $K\alpha$ radiation

 $0.13 \times 0.07 \times 0.05 \; \rm mm$

 $\mu = 1.83 \text{ mm}^{-1}$

T = 296 K

Z = 4

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supporting information

Acta Cryst. (2011). E67, m611-m612 [doi:10.1107/S1600536811013808]

Diaqua(2,2'-bipyridine- $\kappa^2 N, N'$)bis(perchlorato- κO)copper(II)

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S1. Comment

Copper(II) complexes containing O, N-donor atoms are very important owing to their significant catalytic activity in the preparative oxygenation of phenols and other substances, and their significant antibacterial and anticancer activity (Kurzak *et al.*, 1999).

The asymmetric unit of (I), and the atomic numbering used, is illustrated in Fig. 1. The Cu^{II} atom is located in a Jahn-Teller distorted octahedral coordination environment with two N atoms from one 2,2'-bipyridine ligand (N1, N2) (d(Cu— N) = 1.9723 (13)–1.9805 (12) Å) and two O atoms from two water molecular adopting a planar arrangement (d(Cu—O) = 1.9621 (12)–1.9719 (12) Å). The Cu(II) center is displaced out of the N₂O₂ plane by 0.028 (2)Å in the direction of one of perchlorate ligand with d(Cu—O9) = 2.3287 (12) Å. The O atom of the second perchlorate group occupies a sixth coordination site at a longer distance of 2.5058 (12) Å, completing the overall (4 + 1 + 1) type coordination. O9 is situated slightly off the axial direct of the square pyramid, nevertheless it is close enough to the Cu atom (Hathaway, 1973). The bipyridine rings of the 2,2'-bipyridine ligand are twisted relative to each other at 2.2 (8)°.

The crystal structure can be described as alternating layers of polyhedral (ClO_4 tetrahedrals and CuN_2O_4 octahedrals) perpendicular to *c* axis (Fig. 2).

The crystal packing in (I) is governed by classical hydrogen bond, *viz*. water molecules and perchlorate (Table 1, Fig. 3). All water H atoms are involved in these hydrogen bonds In the crystal, the components of the structure are linked *via* intermolecular O—H···O hydrogen bonds to form a two-dimensional layers parallel to (001) plane (Fig. 3). Additional stabilization within these layers is provided by π – π [3.7848 (9)Å to 4.4231 (9) Å] stacking interactions. These interaction bonds link the molecules within the layers and also link the layers together and reinforcing the cohesion of the structure.

The combination of these hydrogen bonds generates an alternating centrosymmetric rings in two-dimensional network which can be described by the graph-set motif $R_4^2(12)$ and $R_4^4(16)$ (Bernstein *et al.* 1995; Etter *et al.*, 1990).

S2. Experimental

The title compound was prepared by adding a methanol solution (10 ml) of copper (II) acetate monohydrate (0.1 mmol) to a methanol solution (10 ml) of 2,2'-bipyridine (0.1 mmol) and (1 ml) the perchloric acid. The mixture was stirred for about 2 h at 323 K and filtered. The filtrate was slowly evaporated at room temperature to yield blue crystals of (I) suitable for X-ray analysis.

S3. Refinement

H atoms of water molecule were located in difference Fourier maps and refined isotropically using restraints $U_{iso}(H) = 1.5U_{eq}(O)$. The remaining H atoms were localized on Fourier maps but introduced in calculated positions and treated as riding on their parent atoms (C_{aryl}) with C_{aryl}=0.93Å and $U_{iso}(H_{aryl})=1.2U_{eq}(C_{aryl})$.



Figure 1

(Farrugia, 1997) The asymmetric unit of the title compound with the atomic labeling scheme. Displacements are drawn at the 50% probability level.



Figure 2

(Brandenburg & Berndt, 2001) A diagram of the layered crystal packing in (I), viewed down the *b* axis, showing layers parallel to (001) with alterning polyhedrals (ClO₄ and CuN₂O₄).



Figure 3

(Brandenburg & Berndt, 2001) A part of crystal packing of (I) showing hydrogen bond connections in the same layer as dashed line.

Diaqua(2,2'-bipyridine- $\kappa^2 N, N'$)bis(perchlorato- κO)copper(II)

Crystal data

 $\begin{bmatrix} \text{Cu}(\text{ClO}_4)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2 \end{bmatrix}$ $M_r = 454.67$ Monoclinic, $P2_1/n$ a = 7.1378 (4) Å b = 12.7853 (7) Å c = 16.8033 (11) Å $\beta = 92.025$ (6)° V = 1532.49 (16) Å³ Z = 4

Data collection

| Oxford Diffraction Xcalibur Sapphire2 | 16487 measured reflections |
|---|---|
| diffractometer | 5135 independent reflections |
| Radiation source: Enhance (Mo) X-ray Source | 4239 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{\rm int} = 0.034$ |
| Detector resolution: 8.2632 pixels mm ⁻¹ | $\theta_{\text{max}} = 32.3^{\circ}, \ \theta_{\text{min}} = 3.1^{\circ}$ |
| ω scans | $h = -10 \rightarrow 6$ |
| Absorption correction: multi-scan | $k = -19 \rightarrow 19$ |
| (CrysAlis RED; Oxford Diffraction, 2008) | $l = -25 \rightarrow 25$ |
| $T_{\min} = 0.580, \ T_{\max} = 1.000$ | |
| Refinement | |
| Refinement on F^2 | Secondary atom site location: difference Fourier |
| Least-squares matrix: full | map |
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | Hydrogen site location: inferred from |

F(000) = 916

 $\theta = 3.0 - 32.3^{\circ}$

 $\mu = 1.83 \text{ mm}^{-1}$ T = 296 K

Needle, blue

 $0.13 \times 0.07 \times 0.05$ mm

 $D_{\rm x} = 1.971 {\rm Mg} {\rm m}^{-3}$

Mo Ka radiation, $\lambda = 0.7107$ Å

Cell parameters from 9763 reflections

| 1 |
|--|
| Hydrogen site location: inferred from |
| neighbouring sites |
| H atoms treated by a mixture of independent |
| and constrained refinement |
| $w = 1/[\sigma^2(F_o^2) + (0.0469P)^2]$ |
| where $P = (F_o^2 + 2F_c^2)/3$ |
| $(\Delta/\sigma)_{\rm max} = 0.001$ |
| $\Delta \rho_{\rm max} = 0.42 \text{ e } \text{\AA}^{-3}$ |
| $\Delta \rho_{\rm min} = -0.63 \ {\rm e} \ {\rm \AA}^{-3}$ |
| |

Special details

Experimental. CrysAlis RED, Oxford Diffraction Ltd. (Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm).

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 (A^2)

| | x | У | Ζ | $U_{ m iso}$ */ $U_{ m eq}$ |
|----|------------|--------------|--------------|-----------------------------|
| C1 | 0.8677 (2) | 0.16080 (13) | 0.14228 (10) | 0.0255 (3) |
| H1 | 0.8893 | 0.2282 | 0.1613 | 0.031* |

| C2 | 0.8928 (3) | 0.07755 (15) | 0.19373 (11) | 0.0302 (4) |
|-----|--------------|---------------|----------------|-------------|
| H2 | 0.9318 | 0.0886 | 0.2465 | 0.036* |
| C3 | 0.8593 (3) | -0.02215 (14) | 0.16589 (11) | 0.0299 (4) |
| H3 | 0.8759 | -0.0794 | 0.1995 | 0.036* |
| C4 | 0.8012 (2) | -0.03613 (13) | 0.08784 (11) | 0.0263 (3) |
| H4 | 0.7765 | -0.1029 | 0.0681 | 0.032* |
| C5 | 0.7797 (2) | 0.05028 (11) | 0.03897 (10) | 0.0189 (3) |
| C6 | 0.7203 (2) | 0.04419 (11) | -0.04548 (9) | 0.0181 (3) |
| C7 | 0.6861 (2) | -0.04880 (12) | -0.08553 (11) | 0.0244 (3) |
| H7 | 0.6975 | -0.1125 | -0.059 | 0.029* |
| C8 | 0.6349 (2) | -0.04559 (13) | -0.16509 (11) | 0.0283 (4) |
| H8 | 0.6092 | -0.1071 | -0.1929 | 0.034* |
| C9 | 0.6220 (2) | 0.04947 (14) | -0.20331 (11) | 0.0269 (3) |
| H9 | 0.589 | 0.0529 | -0.2573 | 0.032* |
| C10 | 0.6588 (2) | 0.13967 (12) | -0.16024 (10) | 0.0226 (3) |
| H10 | 0.6518 | 0.2039 | -0.1861 | 0.027* |
| N1 | 0.81339 (18) | 0.14762 (10) | 0.06591 (8) | 0.0196 (2) |
| N2 | 0.70407 (17) | 0.13722 (9) | -0.08243 (8) | 0.0186 (2) |
| O1W | 0.66836 (17) | 0.36086 (9) | -0.09192 (8) | 0.0237 (2) |
| H1W | 0.568 (3) | 0.3587 (18) | -0.0987 (14) | 0.036* |
| H2W | 0.691 (3) | 0.4275 (19) | -0.0820 (14) | 0.036* |
| O2W | 0.86002 (18) | 0.37137 (9) | 0.05755 (9) | 0.0274 (3) |
| H3W | 0.958 (3) | 0.394 (2) | 0.0544 (15) | 0.041* |
| H4W | 0.805 (3) | 0.415 (2) | 0.0787 (15) | 0.041* |
| O3 | 0.24885 (18) | 0.43183 (9) | 0.05923 (9) | 0.0361 (3) |
| O4 | 0.51492 (18) | 0.41771 (11) | 0.14266 (8) | 0.0363 (3) |
| 05 | 0.2632 (2) | 0.30038 (12) | 0.15559 (9) | 0.0406 (3) |
| O6 | 0.45262 (17) | 0.28891 (10) | 0.04596 (8) | 0.0313 (3) |
| 07 | 1.1044 (2) | 0.43059 (10) | -0.13244 (9) | 0.0389 (3) |
| 08 | 1.02596 (19) | 0.27740 (10) | -0.20091 (8) | 0.0322 (3) |
| O9 | 1.06594 (16) | 0.27377 (10) | -0.06166 (7) | 0.0256 (2) |
| O10 | 1.32354 (16) | 0.29465 (11) | -0.14184 (8) | 0.0324 (3) |
| Cu1 | 0.76523 (3) | 0.258975 (14) | -0.013428 (12) | 0.01792 (6) |
| Cl1 | 0.37148 (5) | 0.35902 (3) | 0.10177 (2) | 0.02055 (8) |
| C12 | 1.12857 (5) | 0.32027 (3) | -0.13482 (2) | 0.01947 (8) |

Atomic displacement parameters $(Å^2)$

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|------------|------------|------------|-------------|-------------|-------------|
| C1 | 0.0304 (8) | 0.0241 (8) | 0.0220 (8) | 0.0019 (6) | -0.0012 (7) | -0.0029 (6) |
| C2 | 0.0336 (9) | 0.0365 (9) | 0.0204 (8) | 0.0073 (7) | 0.0003 (7) | 0.0032 (7) |
| C3 | 0.0333 (9) | 0.0288 (8) | 0.0279 (9) | 0.0083 (7) | 0.0037 (7) | 0.0103 (7) |
| C4 | 0.0307 (8) | 0.0175 (7) | 0.0308 (9) | 0.0039 (6) | 0.0037 (7) | 0.0051 (6) |
| C5 | 0.0184 (6) | 0.0152 (6) | 0.0233 (7) | 0.0020 (5) | 0.0016 (6) | 0.0006 (5) |
| C6 | 0.0178 (6) | 0.0126 (6) | 0.0237 (7) | -0.0008 (5) | 0.0010 (5) | -0.0004 (5) |
| C7 | 0.0276 (8) | 0.0130 (6) | 0.0326 (9) | -0.0012 (6) | 0.0015 (7) | -0.0030 (6) |
| C8 | 0.0293 (8) | 0.0220 (7) | 0.0334 (9) | -0.0058 (6) | 0.0005 (7) | -0.0109 (7) |
| C9 | 0.0281 (8) | 0.0286 (8) | 0.0239 (8) | -0.0041 (6) | -0.0028 (6) | -0.0053 (6) |
| | | | | | | |

| C10 | 0.0230 (7) | 0.0215 (7) | 0.0230 (8) | -0.0012 (6) | -0.0027 (6) | 0.0001 (6) |
|-----|--------------|--------------|--------------|---------------|---------------|---------------|
| N1 | 0.0219 (6) | 0.0160 (5) | 0.0209 (6) | 0.0015 (5) | -0.0011 (5) | -0.0007 (5) |
| N2 | 0.0195 (6) | 0.0139 (5) | 0.0222 (6) | -0.0011 (4) | -0.0013 (5) | 0.0000 (4) |
| O1W | 0.0211 (5) | 0.0150 (5) | 0.0345 (7) | -0.0007 (4) | -0.0064 (5) | 0.0023 (4) |
| O2W | 0.0233 (6) | 0.0193 (6) | 0.0394 (7) | 0.0001 (4) | -0.0027 (5) | -0.0115 (5) |
| 03 | 0.0356 (7) | 0.0183 (6) | 0.0527 (9) | 0.0008 (5) | -0.0205 (6) | 0.0035 (5) |
| 04 | 0.0308 (6) | 0.0373 (7) | 0.0398 (8) | -0.0013 (6) | -0.0138 (6) | -0.0121 (6) |
| 05 | 0.0461 (8) | 0.0378 (8) | 0.0386 (8) | -0.0010 (6) | 0.0145 (7) | 0.0068 (6) |
| 06 | 0.0275 (6) | 0.0290 (6) | 0.0379 (7) | -0.0014 (5) | 0.0065 (5) | -0.0122 (5) |
| 07 | 0.0552 (9) | 0.0157 (6) | 0.0452 (8) | 0.0009 (6) | -0.0055 (7) | -0.0011 (5) |
| 08 | 0.0338 (7) | 0.0316 (6) | 0.0302 (7) | -0.0026 (5) | -0.0140 (6) | -0.0030 (5) |
| 09 | 0.0221 (5) | 0.0294 (6) | 0.0254 (6) | -0.0003 (5) | 0.0015 (5) | 0.0040 (5) |
| O10 | 0.0187 (5) | 0.0460 (8) | 0.0325 (7) | 0.0012 (5) | 0.0009 (5) | 0.0046 (6) |
| Cu1 | 0.02028 (10) | 0.01089 (9) | 0.02227 (10) | -0.00087 (6) | -0.00360 (7) | -0.00050 (6) |
| Cl1 | 0.02118 (16) | 0.01651 (15) | 0.02369 (18) | 0.00116 (12) | -0.00293 (13) | -0.00168 (13) |
| Cl2 | 0.01900 (16) | 0.01621 (15) | 0.02290 (17) | -0.00066 (12) | -0.00351 (13) | 0.00004 (12) |
| | | | | | | |

Geometric parameters (Å, °)

| C1—N1 | 1.338 (2) | C10—N2 | 1.336 (2) |
|----------|-------------|-------------|-------------|
| C1—C2 | 1.379 (2) | C10—H10 | 0.93 |
| C1—H1 | 0.93 | N1—Cu1 | 1.9723 (13) |
| С2—С3 | 1.376 (3) | N2—Cu1 | 1.9805 (12) |
| С2—Н2 | 0.93 | O1W—Cu1 | 1.9621 (12) |
| C3—C4 | 1.373 (3) | O2W—Cu1 | 1.9719 (12) |
| С3—Н3 | 0.93 | O1W—H1W | 0.72 (2) |
| C4—C5 | 1.382 (2) | O1W—H2W | 0.88 (2) |
| C4—H4 | 0.93 | O2W—H3W | 0.76 (2) |
| C5—N1 | 1.3432 (19) | O2W—H4W | 0.78 (3) |
| C5—C6 | 1.469 (2) | O3—Cl1 | 1.4490 (12) |
| C6—N2 | 1.3448 (18) | O4—Cl1 | 1.4260 (12) |
| C6—C7 | 1.384 (2) | O5—Cl1 | 1.4236 (15) |
| С7—С8 | 1.374 (3) | O6—Cl1 | 1.4342 (13) |
| С7—Н7 | 0.93 | O7—Cl2 | 1.4217 (13) |
| С8—С9 | 1.376 (3) | O8—Cl2 | 1.4187 (12) |
| С8—Н8 | 0.93 | O9—Cl2 | 1.4503 (13) |
| C9—C10 | 1.382 (2) | O10—Cl2 | 1.4386 (12) |
| С9—Н9 | 0.93 | O9—Cul | 2.3287 (12) |
| N1—C1—C2 | 122.07 (16) | C10—N2—C6 | 119.10 (13) |
| N1-C1-H1 | 119 | C10—N2—Cu1 | 126.53 (10) |
| C2 | 119 | C6—N2—Cu1 | 114.28 (10) |
| C3—C2—C1 | 119.00 (16) | Cu1—O1W—H1W | 113.8 (19) |
| С3—С2—Н2 | 120.5 | Cu1—O1W—H2W | 117.2 (15) |
| C1—C2—H2 | 120.5 | H1W—O1W—H2W | 104 (2) |
| C4—C3—C2 | 119.23 (16) | Cu1—O2W—H3W | 122.0 (19) |
| С4—С3—Н3 | 120.4 | Cu1—O2W—H4W | 129.3 (17) |
| С2—С3—Н3 | 120.4 | H3W—O2W—H4W | 104 (2) |

| C3—C4—C5 | 119.14 (16) | Cl2—O9—Cu1 | 130.08 (7) |
|----------------------------|-------------|-----------------------------|--------------|
| C3—C4—H4 | 120.4 | O1W—Cu1—O2W | 91.60 (6) |
| C5—C4—H4 | 120.4 | O1W—Cu1—N1 | 169.24 (5) |
| N1—C5—C4 | 121.71 (15) | O2W—Cu1—N1 | 93.97 (6) |
| N1—C5—C6 | 114.64 (13) | O1W—Cu1—N2 | 93.62 (5) |
| C4—C5—C6 | 123.65 (14) | O2W—Cu1—N2 | 172.19 (5) |
| N2—C6—C7 | 121.64 (14) | N1—Cu1—N2 | 81.83 (6) |
| N2—C6—C5 | 114.61 (12) | O1W—Cu1—O9 | 91.11 (5) |
| C7—C6—C5 | 123.74 (14) | O2W—Cu1—O9 | 81.41 (5) |
| C8—C7—C6 | 118.94 (15) | N1—Cu1—O9 | 98.81 (5) |
| С8—С7—Н7 | 120.5 | N2—Cu1—O9 | 92.69 (5) |
| С6—С7—Н7 | 120.5 | O5—Cl1—O4 | 111.57 (9) |
| C7—C8—C9 | 119.45 (15) | O5—C11—O6 | 109.09 (9) |
| С7—С8—Н8 | 120.3 | O4—C11—O6 | 110.14 (8) |
| С9—С8—Н8 | 120.3 | O5—C11—O3 | 108.65 (9) |
| C8—C9—C10 | 118.96 (16) | O4—C11—O3 | 108.10 (8) |
| C8—C9—H9 | 120.5 | 06—C11—O3 | 109.25 (9) |
| C10—C9—H9 | 120.5 | 08-012-07 | 110.21 (8) |
| N2-C10-C9 | 121.87 (15) | 08-C12-010 | 108 78 (8) |
| $N_2 - C_{10} - H_{10}$ | 119.1 | 07 - C12 - 010 | 110 30 (9) |
| C9-C10-H10 | 119.1 | 08-C12-09 | 109.82 (8) |
| C1-N1-C5 | 118 84 (14) | 07 | 109.02 (0) |
| C1-N1-Cu1 | 126 52 (11) | 010-012-09 | 107.71(7) |
| C_{5} N1— C_{11} | 114 59 (10) | | 107.71(7) |
| | 111.35 (10) | | |
| N1—C1—C2—C3 | -0.6 (3) | C7—C6—N2—Cu1 | -178.80 (12) |
| C1—C2—C3—C4 | -0.3 (3) | C5—C6—N2—Cu1 | 0.18 (17) |
| C2—C3—C4—C5 | 0.7 (3) | C1—N1—Cu1—O1W | -113.5 (3) |
| C3—C4—C5—N1 | -0.3 (3) | C5—N1—Cu1—O1W | 63.8 (3) |
| C3—C4—C5—C6 | 179.30 (16) | C1—N1—Cu1—O2W | 7.58 (15) |
| N1-C5-C6-N2 | -1.7 (2) | C5—N1—Cu1—O2W | -175.14 (11) |
| C4—C5—C6—N2 | 178.72 (15) | C1—N1—Cu1—N2 | -179.04 (15) |
| N1—C5—C6—C7 | 177.30 (15) | C5—N1—Cu1—N2 | -1.76 (11) |
| C4—C5—C6—C7 | -2.3(3) | C1—N1—Cu1—O9 | 89.49 (14) |
| N2-C6-C7-C8 | 0.2 (3) | C5—N1—Cu1—O9 | -93.24(11) |
| C5-C6-C7-C8 | -178.64(16) | C10-N2-Cu1-O1W | 13.96 (14) |
| C6-C7-C8-C9 | 1.1 (3) | C6-N2-Cu1-O1W | -169.38(11) |
| C7—C8—C9—C10 | -0.8(3) | C10 - N2 - Cu1 - N1 | -175.84(14) |
| C8-C9-C10-N2 | -0.9(3) | C6-N2-Cu1-N1 | 0.82 (11) |
| $C_2 - C_1 - N_1 - C_5$ | 1.0(3) | C10 - N2 - Cu1 - O9 | -77.32(14) |
| C_2 C_1 N_1 C_{u1} | 178 17 (13) | C6-N2-Cu1-O9 | 99 34 (11) |
| C4-C5-N1-C1 | -0.5(2) | C12 - C9 - C11 - O1W | -13.93(10) |
| C6-C5-N1-C1 | 179.83 (14) | C12 - 09 - Cu1 - 02W | -105.38(10) |
| C4-C5-N1-Cu1 | -178.04(13) | C12 - 09 - C11 - N1 | 161.89 (10) |
| C6 - C5 - N1 - Cu1 | 2 33 (18) | C12 - O9 - Cu1 - N2 | 79 74 (10) |
| $C9-C10-N^2-C6$ | 2.2.(2) | $C_{11} = 09 = C_{12} = 08$ | -52.93 (12) |
| C9-C10-N2-C11 | 178 71 (12) | Cu1 - 09 - Cl2 - 07 | 68 52 (11) |
| C7 - C6 - N2 - C10 | -19(2) | $C_{11} = 09 = 012 = 07$ | -171 24 (9) |
| 07 00 112 010 | 1.7 (2) | 011 07 012 -010 | 1,1.27()) |

C5—C6—N2—C10 177.11 (14)

Hydrogen-bond geometry (Å, °)

| D—H···A | <i>D</i> —Н | H···A | $D \cdots A$ | D—H···A |
|---|-------------|----------|--------------|------------|
| O1 <i>W</i> —H1 <i>W</i> ···O10 ⁱ | 0.72 (2) | 2.04 (2) | 2.7078 (17) | 155 (3) |
| O1 <i>W</i> —H2 <i>W</i> ···O3 ⁱⁱ | 0.88 (2) | 1.89 (2) | 2.7665 (17) | 177.3 (18) |
| O2 <i>W</i> —H3 <i>W</i> ···O3 ⁱⁱⁱ | 0.76 (2) | 2.13 (2) | 2.8802 (18) | 169 (2) |
| O2 <i>W</i> —H4 <i>W</i> ···O4 | 0.78 (2) | 2.37 (2) | 2.9518 (19) | 133 (2) |
| O2W—H4 W ···O7 ^{iv} | 0.78 (2) | 2.26 (3) | 2.8349 (18) | 132 (2) |

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