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catena-Poly[[diaquabis(4-formylbenzoato- κO^1)copper(II)]- μ -pyrazine- $\kappa^2 N:N'$]

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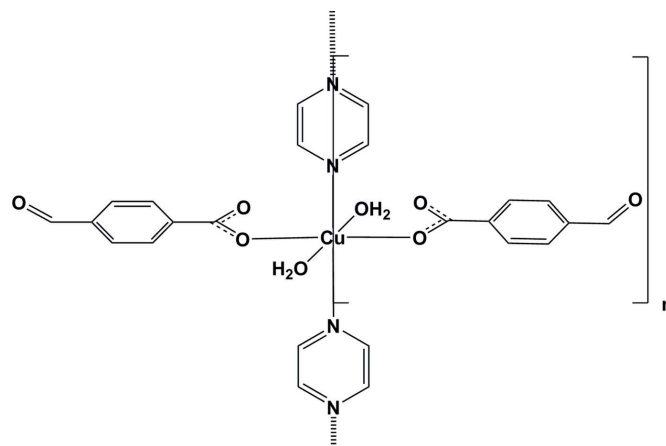
Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.028; wR factor = 0.089; data-to-parameter ratio = 16.0.

In the title polymeric compound, $[Cu(C_8H_5O_3)_2(C_4H_4N_2)(H_2O)_2]_n$, the Cu^{II} atom is located on a twofold rotation axis and has a slightly distorted octahedral coordination sphere. In the equatorial plane, it is coordinated by two carboxylate O atoms of two symmetry-related monodentate formylbenzoate anions and by two N atoms of the bridging pyrazine ligand, which is bisected by the twofold rotation axis. The axial positions are occupied by two O atoms of the coordinating water molecules. In the formylbenzoate anion, the carboxylate group is twisted away from the attached benzene ring by $6.2(2)^\circ$, while the benzene and pyrazine rings are oriented at a dihedral angle of $68.91(8)^\circ$. The pyrazine ligands bridge the Cu^{II} cations, forming polymeric chains running along the b -axis direction. Strong intramolecular $O-H\cdots O$ hydrogen bonds link the water molecules to the carboxylate O atoms. In the crystal, $O-H_{water}\cdots O_{water}$ hydrogen bonds link adjacent chains into layers parallel to the bc plane. The layers are linked *via* $C-H_{pyrazine}\cdots O_{formyl}$ hydrogen bonds, forming a three-dimensional network. There are also weak $C-H\cdots\pi$ interactions present.

Related literature

For structural functions and coordination relationships of arylcarboxylate ions in transition metal complexes of benzoic acid derivatives, see: Nadzhafov *et al.* (1981); Shnulin *et al.* (1981). For applications of transition metal complexes with biochemical molecules in biological systems, see: Antolini *et al.* (1982). Some benzoic acid derivatives, such as 4-amino-benzoic acid, have been extensively reported in coordination chemistry, as bifunctional organic ligands, due to the variety of their coordination modes, see: Chen & Chen (2002); Amir-

aslanov *et al.* (1979); Hauptmann *et al.* (2000). For a related structure involving 4-formylbenzoate, see: Hökelek *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(C_8H_5O_3)_2(C_4H_4N_2)(H_2O)_2]$
 $M_r = 477.90$
Monoclinic, $C2/c$
 $a = 21.7514(4)$ Å
 $b = 6.8794(2)$ Å
 $c = 12.9048(3)$ Å
 $\beta = 93.621(3)^\circ$

$V = 1927.17(8)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.19$ mm⁻¹
 $T = 294$ K
 $0.42 \times 0.22 \times 0.13$ mm

Data collection

Bruker SMART BREEZE CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2012)
 $T_{min} = 0.738$, $T_{max} = 0.857$

14917 measured reflections
2398 independent reflections
2231 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.089$
 $S = 1.14$
2398 reflections
150 parameters
2 restraints

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{max} = 0.47$ e Å⁻³
 $\Delta\rho_{min} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C2–C7 ring.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------|----------|-------------|-------------|---------------|
| $O4-H42\cdots O2$ | 0.80 (2) | 1.86 (2) | 2.640 (2) | 163 (3) |
| $O4-H41\cdots O4^i$ | 0.79 (2) | 2.41 (3) | 2.778 (2) | 110 (3) |
| $C9-H9\cdots O3^{ii}$ | 0.93 | 2.49 | 3.335 (3) | 152 |
| $C7-H7\cdots Cg^{iii}$ | 0.93 | 2.66 | 3.433 (2) | 141 |

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

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine

structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* for Windows (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2669).

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supporting information

Acta Cryst. (2014). E70, m4–m5 [https://doi.org/10.1107/S1600536813032297]

catena-Poly[[diaquabis(4-formylbenzoato- κ O¹)copper(II)]- μ -pyrazine- κ^2 N:N']

Fatih Çelik, Nefise Dilek, Nagihan Çaylak Delibaş, Hacali Necefoğlu and Tuncer Hökelek

S1. Comment

The structural functions and coordination relationships of the arylcarboxylate ion in transition metal complexes of benzoic acid derivatives change depending on the nature and position of the substituent groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the medium of the synthesis (Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981). Transition metal complexes with biochemically active ligands frequently show interesting physical and/or chemical properties, as a result they may find applications in biological systems (Antolini *et al.*, 1982). Some benzoic acid derivatives, such as 4-aminobenzoic acid, have been extensively reported in coordination chemistry, as bifunctional organic ligands, due to the varieties of their coordination modes (Chen & Chen, 2002; Amiraslanov *et al.*, 1979; Hauptmann *et al.*, 2000). The title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title compound contains half a Cu^{II} ion, one formylbenzoate (FB) anion, one water molecule and half of a pyrazine molecule. Atoms Cu1, and N1 and N2 of the pyrazine ligand, are located on a two-fold rotation axis (Fig. 1). The pyrazine ligands bridge adjacent Cu^{II} ions forming polymeric chains running along the *b*-axis direction (Fig. 2). The distances between the symmetry related Cu^{II} ions [Cu1ⁱ...Cu1ⁱ; symmetry code (i) = x, y-1, z] is 6.879 (3) Å.

In the equatorial plane of the Cu^{II} coordination sphere is composed of two carboxylate O atoms (O1 and O1ⁱⁱ; symmetry code: (ii) -x+1, y, -z+0.5) of two symmetry related monodentate formylbenzoate anions and two N atoms (N1 and N2ⁱ) of the bridging pyrazine ligand, which is bisected by the two-fold rotation axis. The axial positions are occupied by two O atoms (O4 and O4ⁱⁱ) of the coordinated water molecules.

The near equality of the C1—O1 [1.278 (2) Å] and C1—O2 [1.234 (2) Å] bonds in the carboxylate group indicate a delocalized bonding arrangement, rather than localized single and double bonds. The average Cu—N bond length is 2.0497 (19) Å, while the Cu—O bond lengths are 1.9546 (12) Å (for benzoate oxygen O1) and 2.4768 (12) Å (for water oxygen O4), close to standard values (Allen *et al.*, 1987). The dihedral angle between the planar carboxylate group (O1/C1/O2) and the adjacent benzene ring (C2—C7) is 6.2 (2)°, while the benzene and pyrazine rings are oriented at a dihedral angle of 68.91 (8)°. Strong intramolecular O—H...O hydrogen bonds (Table 1) link the water molecules to the carboxylate oxygens.

In the crystal, O—H_{water}...O_{water} hydrogen bonds (Table 1) link adjacent chains into layers parallel to the *bc* plane. The layers are linked via C—H_{pyrazine}...O_{formyl} hydrogen bonds forming a three-dimensional network. There also weak C—H... π interactions present.

S2. Experimental

The title compound was prepared by the reaction of CuSO₄·5H₂O (1.25 g, 5 mmol) in H₂O (250 ml) and pyrazine (0.40 g, 5 mmol) in H₂O (30 ml) with sodium 4-formylbenzoate (1.72 g, 10 mmol) in H₂O (100 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving blue block-like crystals.

S3. Refinement

The water H atoms (H41 and H42) were located in a difference Fourier map and freely refined. The C-bound H-atoms were positioned geometrically and constrained to ride on their parent atoms: C—H = 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

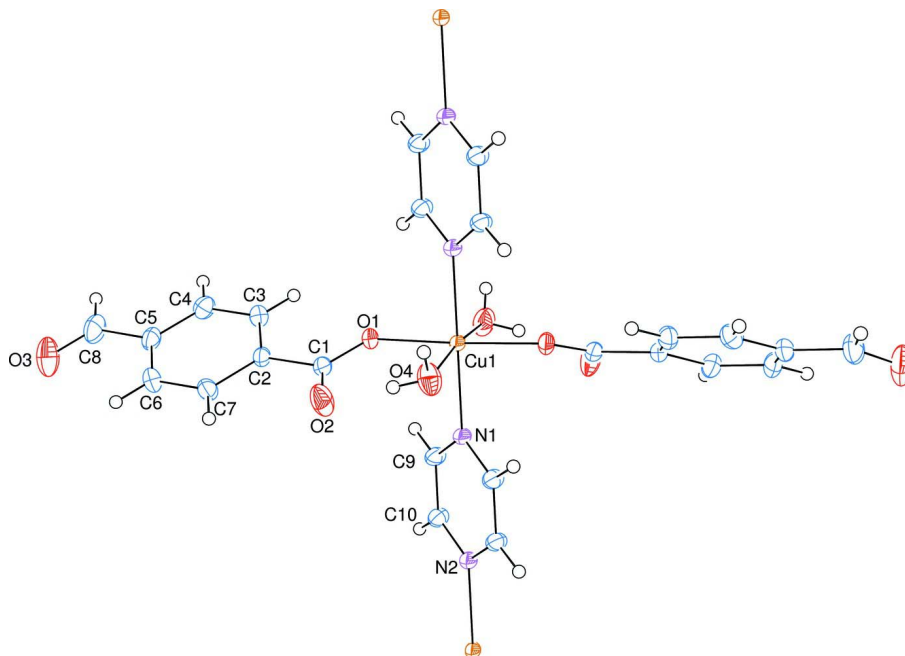


Figure 1

A view of the coordination geometry around the Cu^{II} atom of the title molecule, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The two-fold rotation axis bisects atoms Cu1, N1 and N2.

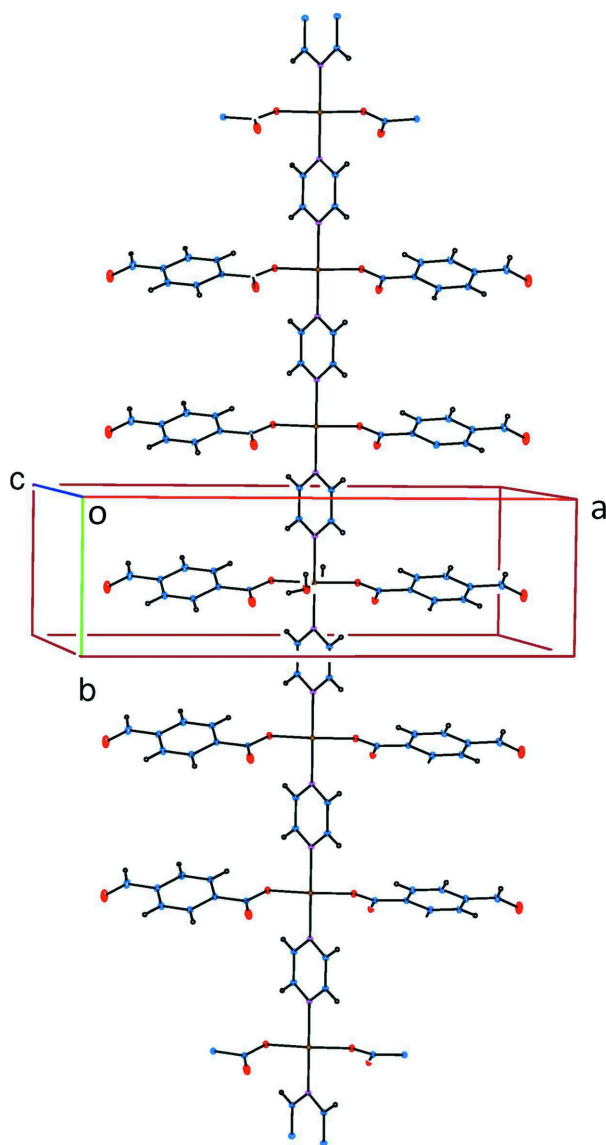


Figure 2

A partial view along the *c* axis of the crystal packing of the title compound.

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Crystal data

[Cu(C₈H₅O₃)₂(C₄H₄N₂)(H₂O)₂]

M_r = 477.90

Monoclinic, *C2/c*

Hall symbol: -C 2yc

a = 21.7514 (4) Å

b = 6.8794 (2) Å

c = 12.9048 (3) Å

β = 93.621 (3)°

V = 1927.17 (8) Å³

Z = 4

F(000) = 980

D_x = 1.647 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 9971 reflections

θ = 2.4–28.4°

μ = 1.19 mm⁻¹

T = 294 K

Block, blue

0.42 × 0.22 × 0.13 mm

Data collection

Bruker SMART BREEZE CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2012)
 $T_{\min} = 0.738$, $T_{\max} = 0.857$

14917 measured reflections
2398 independent reflections
2231 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -28 \rightarrow 27$
 $k = -8 \rightarrow 9$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.089$
 $S = 1.14$
2398 reflections
150 parameters
2 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
 $w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 1.6638P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.47 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 | 0.50000 | 0.56167 (4) | 0.25000 | 0.0226 (1) |
| O1 | 0.58159 (6) | 0.55545 (17) | 0.19469 (11) | 0.0283 (3) |
| O2 | 0.63771 (7) | 0.6755 (3) | 0.33131 (11) | 0.0478 (5) |
| O3 | 0.90018 (8) | 0.6186 (4) | 0.03875 (15) | 0.0643 (7) |
| O4 | 0.54054 (7) | 0.5818 (3) | 0.43338 (12) | 0.0429 (5) |
| N1 | 0.50000 | 0.8590 (3) | 0.25000 | 0.0222 (5) |
| N2 | 0.50000 | 1.2632 (3) | 0.25000 | 0.0228 (5) |
| C1 | 0.63185 (7) | 0.6123 (2) | 0.24173 (13) | 0.0255 (4) |
| C2 | 0.68848 (7) | 0.5984 (2) | 0.18010 (13) | 0.0233 (4) |
| C3 | 0.68624 (8) | 0.5098 (3) | 0.08295 (13) | 0.0278 (4) |
| C4 | 0.73941 (8) | 0.4934 (3) | 0.02948 (13) | 0.0311 (5) |
| C5 | 0.79501 (8) | 0.5656 (3) | 0.07299 (15) | 0.0298 (5) |
| C6 | 0.79729 (8) | 0.6554 (3) | 0.16972 (14) | 0.0322 (5) |
| C7 | 0.74435 (8) | 0.6718 (3) | 0.22284 (13) | 0.0286 (5) |
| C8 | 0.85122 (10) | 0.5472 (3) | 0.01458 (19) | 0.0433 (7) |
| C9 | 0.52244 (8) | 0.9602 (2) | 0.17228 (13) | 0.0263 (5) |

| | | | | |
|-----|-------------|------------|--------------|-------------|
| C10 | 0.52268 (8) | 1.1618 (2) | 0.17257 (13) | 0.0265 (5) |
| H3 | 0.64910 | 0.46150 | 0.05390 | 0.0330* |
| H4 | 0.73790 | 0.43420 | -0.03540 | 0.0370* |
| H6 | 0.83440 | 0.70420 | 0.19860 | 0.0390* |
| H7 | 0.74590 | 0.73200 | 0.28750 | 0.0340* |
| H8 | 0.84820 | 0.47380 | -0.04600 | 0.0520* |
| H9 | 0.53820 | 0.89410 | 0.11700 | 0.0310* |
| H10 | 0.53900 | 1.22800 | 0.11770 | 0.0320* |
| H41 | 0.5464 (15) | 0.485 (3) | 0.465 (2) | 0.065 (10)* |
| H42 | 0.5738 (10) | 0.609 (5) | 0.414 (2) | 0.064 (9)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|------------|-------------|
| Cu1 | 0.0165 (2) | 0.0139 (2) | 0.0382 (2) | 0.0000 | 0.0076 (1) | 0.0000 |
| O1 | 0.0170 (5) | 0.0258 (6) | 0.0428 (7) | -0.0016 (4) | 0.0076 (5) | -0.0036 (5) |
| O2 | 0.0327 (7) | 0.0712 (11) | 0.0413 (8) | -0.0153 (7) | 0.0155 (6) | -0.0173 (7) |
| O3 | 0.0307 (8) | 0.0990 (15) | 0.0650 (11) | -0.0003 (9) | 0.0176 (7) | 0.0074 (11) |
| O4 | 0.0330 (8) | 0.0558 (10) | 0.0408 (8) | -0.0057 (7) | 0.0086 (6) | 0.0119 (7) |
| N1 | 0.0214 (8) | 0.0149 (9) | 0.0308 (9) | 0.0000 | 0.0065 (7) | 0.0000 |
| N2 | 0.0206 (8) | 0.0160 (8) | 0.0322 (9) | 0.0000 | 0.0055 (7) | 0.0000 |
| C1 | 0.0211 (7) | 0.0212 (7) | 0.0350 (8) | -0.0011 (6) | 0.0079 (6) | 0.0000 (6) |
| C2 | 0.0186 (7) | 0.0219 (7) | 0.0298 (8) | 0.0006 (6) | 0.0046 (6) | 0.0021 (6) |
| C3 | 0.0215 (7) | 0.0302 (8) | 0.0316 (8) | -0.0002 (6) | 0.0002 (6) | -0.0008 (7) |
| C4 | 0.0312 (9) | 0.0340 (9) | 0.0284 (8) | 0.0045 (7) | 0.0045 (7) | -0.0018 (7) |
| C5 | 0.0236 (8) | 0.0307 (9) | 0.0359 (9) | 0.0038 (6) | 0.0093 (7) | 0.0044 (7) |
| C6 | 0.0204 (7) | 0.0372 (10) | 0.0391 (9) | -0.0049 (7) | 0.0032 (6) | 0.0000 (8) |
| C7 | 0.0245 (8) | 0.0312 (9) | 0.0305 (8) | -0.0054 (7) | 0.0044 (6) | -0.0046 (7) |
| C8 | 0.0317 (10) | 0.0525 (14) | 0.0475 (11) | 0.0065 (8) | 0.0170 (9) | 0.0027 (9) |
| C9 | 0.0301 (8) | 0.0206 (8) | 0.0293 (8) | 0.0001 (6) | 0.0114 (6) | -0.0016 (6) |
| C10 | 0.0298 (8) | 0.0200 (8) | 0.0308 (8) | 0.0006 (6) | 0.0111 (6) | 0.0029 (6) |

Geometric parameters (Å, °)

| | | | |
|----------------------|-------------|--------|-------------|
| Cu1—O1 | 1.9547 (13) | C2—C3 | 1.392 (2) |
| Cu1—O4 | 2.4766 (15) | C2—C7 | 1.397 (2) |
| Cu1—N1 | 2.046 (2) | C3—C4 | 1.388 (2) |
| Cu1—N2 ⁱ | 2.053 (2) | C4—C5 | 1.392 (3) |
| Cu1—O1 ⁱⁱ | 1.9547 (13) | C5—C6 | 1.391 (3) |
| Cu1—O4 ⁱⁱ | 2.4766 (15) | C5—C8 | 1.482 (3) |
| O1—C1 | 1.278 (2) | C6—C7 | 1.381 (2) |
| O2—C1 | 1.234 (2) | C9—C10 | 1.3869 (19) |
| O3—C8 | 1.196 (3) | C3—H3 | 0.9300 |
| O4—H42 | 0.80 (2) | C4—H4 | 0.9300 |
| O4—H41 | 0.79 (2) | C6—H6 | 0.9300 |
| N1—C9 ⁱⁱ | 1.3382 (19) | C7—H7 | 0.9300 |
| N1—C9 | 1.3382 (19) | C8—H8 | 0.9300 |
| N2—C10 | 1.3382 (19) | C9—H9 | 0.9300 |

| | | | |
|--|--------------|-------------|--------------|
| N2—C10 ⁱⁱ | 1.3382 (19) | C10—H10 | 0.9300 |
| C1—C2 | 1.511 (2) | | |
| O1—Cu1—O4 | 94.21 (5) | C3—C2—C7 | 119.60 (15) |
| O1—Cu1—N1 | 91.25 (4) | C1—C2—C7 | 119.15 (14) |
| O1—Cu1—N2 ⁱ | 88.75 (4) | C1—C2—C3 | 121.23 (14) |
| O1—Cu1—O1 ⁱⁱ | 177.49 (5) | C2—C3—C4 | 120.02 (16) |
| O1—Cu1—O4 ⁱⁱ | 85.93 (5) | C3—C4—C5 | 120.01 (16) |
| O4—Cu1—N1 | 86.80 (5) | C4—C5—C6 | 120.08 (16) |
| O4—Cu1—N2 ⁱ | 93.21 (5) | C4—C5—C8 | 119.21 (18) |
| O1 ⁱⁱ —Cu1—O4 | 85.93 (5) | C6—C5—C8 | 120.71 (17) |
| O4—Cu1—O4 ⁱⁱ | 173.59 (7) | C5—C6—C7 | 119.87 (17) |
| N1—Cu1—N2 ⁱ | 180.00 | C2—C7—C6 | 120.41 (16) |
| O1 ⁱⁱ —Cu1—N1 | 91.25 (4) | O3—C8—C5 | 125.6 (2) |
| O4 ⁱⁱ —Cu1—N1 | 86.80 (5) | N1—C9—C10 | 121.31 (16) |
| O1 ⁱⁱ —Cu1—N2 ⁱ | 88.75 (4) | N2—C10—C9 | 121.45 (16) |
| O4 ⁱⁱ —Cu1—N2 ⁱ | 93.21 (5) | C2—C3—H3 | 120.00 |
| O1 ⁱⁱ —Cu1—O4 ⁱⁱ | 94.21 (5) | C4—C3—H3 | 120.00 |
| Cu1—O1—C1 | 126.09 (12) | C3—C4—H4 | 120.00 |
| Cu1—O4—H41 | 119.0 (18) | C5—C4—H4 | 120.00 |
| Cu1—O4—H42 | 89.4 (18) | C5—C6—H6 | 120.00 |
| H41—O4—H42 | 104 (3) | C7—C6—H6 | 120.00 |
| C9—N1—C9 ⁱⁱ | 117.30 (18) | C2—C7—H7 | 120.00 |
| Cu1—N1—C9 | 121.35 (10) | C6—C7—H7 | 120.00 |
| Cu1—N1—C9 ⁱⁱ | 121.35 (10) | O3—C8—H8 | 117.00 |
| Cu1 ⁱⁱⁱ —N2—C10 | 121.42 (10) | C5—C8—H8 | 117.00 |
| C10—N2—C10 ⁱⁱ | 117.16 (18) | N1—C9—H9 | 119.00 |
| Cu1 ⁱⁱⁱ —N2—C10 ⁱⁱ | 121.42 (10) | C10—C9—H9 | 119.00 |
| O1—C1—O2 | 125.98 (16) | N2—C10—H10 | 119.00 |
| O2—C1—C2 | 118.42 (15) | C9—C10—H10 | 119.00 |
| O1—C1—C2 | 115.60 (14) | | |
| O4—Cu1—O1—C1 | -20.13 (13) | O1—C1—C2—C7 | 174.99 (15) |
| N1—Cu1—O1—C1 | 66.75 (12) | O2—C1—C2—C3 | 173.20 (18) |
| N2 ⁱ —Cu1—O1—C1 | -113.26 (12) | O2—C1—C2—C7 | -5.2 (2) |
| O4 ⁱⁱ —Cu1—O1—C1 | 153.44 (13) | C1—C2—C3—C4 | -177.90 (16) |
| O1—Cu1—N1—C9 | 39.77 (10) | C7—C2—C3—C4 | 0.5 (3) |
| O1—Cu1—N1—C9 ⁱⁱ | -140.23 (10) | C1—C2—C7—C6 | 177.88 (16) |
| O4—Cu1—N1—C9 | 133.92 (9) | C3—C2—C7—C6 | -0.6 (3) |
| O4—Cu1—N1—C9 ⁱⁱ | -46.08 (9) | C2—C3—C4—C5 | 0.0 (3) |
| O1 ⁱⁱ —Cu1—N1—C9 | -140.23 (10) | C3—C4—C5—C6 | -0.4 (3) |
| O4 ⁱⁱ —Cu1—N1—C9 | -46.08 (9) | C3—C4—C5—C8 | -179.83 (19) |
| Cu1—O1—C1—O2 | 2.3 (2) | C4—C5—C6—C7 | 0.4 (3) |
| Cu1—O1—C1—C2 | -177.93 (9) | C8—C5—C6—C7 | 179.77 (19) |
| Cu1—N1—C9—C10 | -179.70 (12) | C4—C5—C8—O3 | 172.6 (2) |
| C9 ⁱⁱ —N1—C9—C10 | 0.3 (2) | C6—C5—C8—O3 | -6.8 (4) |
| Cu1 ⁱⁱⁱ —N2—C10—C9 | -179.70 (12) | C5—C6—C7—C2 | 0.1 (3) |

| | | | |
|------------------------------|----------|--------------|----------|
| C10 ⁱⁱ —N2—C10—C9 | 0.3 (2) | N1—C9—C10—N2 | -0.6 (2) |
| O1—C1—C2—C3 | -6.6 (2) | | |

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

Hydrogen-bond geometry (Å, °)

C_g is the centroid of the C2–C7 ring.

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|---|-------------|---------------------|----------------------------|-------------------------------|
| O4—H42 \cdots O2 | 0.80 (2) | 1.86 (2) | 2.640 (2) | 163 (3) |
| O4—H41 \cdots O4 ^{iv} | 0.79 (2) | 2.41 (3) | 2.778 (2) | 110 (3) |
| C9—H9 \cdots O3 ^v | 0.93 | 2.49 | 3.335 (3) | 152 |
| C7—H7 \cdots C _g ^{vi} | 0.93 | 2.66 | 3.433 (2) | 141 |

Symmetry codes: (iv) $-x+1, -y+1, -z+1$; (v) $-x+3/2, -y+3/2, -z$; (vi) $-x+3/2, y+1/2, -z+1/2$.