

Diaquabis(4-bromobenzoato- κ O)-bis(nicotinamide- κ N¹)copper(II)

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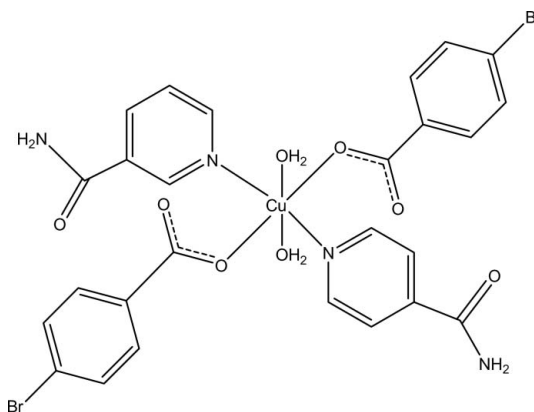
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 17.3.

The asymmetric unit of the title mononuclear Cu^{II} complex, [Cu(C₇H₄BrO₂)₂(C₆H₆N₂O)₂(H₂O)₂], contains one half-molecule, the Cu^{II} atom being located on an inversion center. The unit cell contains two nicotinamide (NA), two 4-bromobenzoate (PBB) ligands and two coordinated water molecules. The four O atoms in the equatorial plane around the Cu^{II} ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands in the axial positions. The dihedral angle between the carboxylate group and the adjacent benzene ring is 22.17 (16)°, while the pyridine ring and the benzene ring are oriented at a dihedral angle of 82.80 (6)°. In the crystal, N—H...O, O—H...O and C—H...O hydrogen bonds link the molecules into a three-dimensional network. A weak C—H... π interaction is also observed.

Related literature

For literature on niacin, see: Krishnamachari (1974). For information on the nicotinic acid derivative *N,N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009*a,b*); Hökelek & Necefoğlu (1998, 2007); Necefoğlu *et al.* (2011). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

[Cu(C₇H₄BrO₂)₂(C₆H₆N₂O)₂(H₂O)₂]
 $M_r = 743.84$
 Triclinic, $P\bar{1}$
 $a = 7.7072$ (3) Å
 $b = 9.7536$ (5) Å
 $c = 9.8471$ (4) Å
 $\alpha = 76.273$ (2)°

$\beta = 74.240$ (2)°
 $\gamma = 85.024$ (3)°
 $V = 691.86$ (5) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 3.73$ mm⁻¹
 $T = 100$ K
 $0.41 \times 0.38 \times 0.35$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.236$, $T_{\max} = 0.271$

11758 measured reflections
 3515 independent reflections
 3172 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.108$
 $S = 1.13$
 3515 reflections
 203 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.86$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the N1/C8–C12 pyridine ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H21...O2 ⁱ	0.85 (3)	2.06 (3)	2.831 (2)	151 (3)
N2—H22...O3 ⁱⁱ	0.88 (3)	2.03 (3)	2.893 (3)	166 (3)
O4—H41...O2 ⁱⁱⁱ	0.87 (4)	1.86 (4)	2.718 (2)	167 (4)
O4—H42...O3 ^{iv}	0.78 (4)	2.17 (4)	2.911 (2)	159 (4)
C6—H6...O2 ^v	0.95	2.43	3.377 (3)	172
C4—H4...C _g ^{vi}	0.95	2.63	3.581 (3)	176

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: WinGX publication routines (Farrugia, 1999) and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2279).

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supplementary materials

Acta Cryst. (2011). E67, m900-m901 [doi:10.1107/S1600536811021696]

Diaquabis(4-bromobenzoato- κO)bis(nicotinamide- κN^1)copper(II)

H. Necefoğlu, F. E. Özbek, V. Öztürk, B. Tercan and T. Hökelek

Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N,N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title mononuclear Cu^{II} complex, (Fig. 1), contains one-half molecule. It consists of two nicotinamide (NA), two 4-bromobenzoate (PBB) ligands and two coordinated water molecules, all ligands coordinating in a monodentate manner. Atom Cu1 is located on an inversion center. The crystal structures of similar complexes of Cu^{II}, Co^{II}, Ni^{II}, Mn^{II} and Zn^{II} ions, [Cu(C₇H₅O₂)₂(C₁₀H₁₄N₂O)₂] (Hökelek *et al.*, 1996), [Co(C₆H₆N₂O)₂(C₇H₄NO₄)₂(H₂O)₂] (Hökelek & Necefoğlu, 1998), [Co(C₉H₉O₂)₂(C₁₀H₁₄N₂O)₂(H₂O)₂] (Necefoğlu *et al.*, 2011), [Ni(C₇H₄ClO₂)₂(C₆H₆N₂O)₂(H₂O)₂] (Hökelek *et al.*, 2009a), [Mn(C₉H₁₀NO₂)₂(H₂O)₄].2H₂O (Hökelek & Necefoğlu, 2007) and [Zn(C₇H₄BrO₂)₂(C₆H₆N₂O)₂(H₂O)₂] (Hökelek *et al.*, 2009b) have also been reported. In the copper(II) complex mentioned above the two benzoate ions coordinate to the Cu^{II} atom as bidentate ligands, while in the other structures all the ligands coordinate in a monodentate manner.

In the title complex, the four symmetry related O atoms (O1, O1', O4 and O4') in the equatorial plane around the Cu^{II} ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two symmetry related N atoms of the NA ligands (N1 and N1') in the axial positions. The near equalities of the C1—O1 [1.272 (3) Å] and C1—O2 [1.246 (3) Å] bonds in the carboxylate group indicate delocalized bonding arrangement, rather than localized single and double bonds. The Cu—O bond lengths are 1.9756 (16) Å (for benzoate oxygens) and 2.4199 (16) Å (for water oxygens), and the Cu—N bond length is 2.0116 (16) Å, close to standard values (Allen *et al.*, 1987). The Cu atom is displaced out of the mean-plane of the carboxylate group (O1/C1/O2) by -0.5279 (1) Å. The dihedral angle between the planar carboxylate group and the adjacent benzene ring A (C2—C7) is 22.17 (16)°. The benzene A (C2—C7) and the pyridine B (N1/C8—C12) rings are oriented at a dihedral angle of A/B = 82.80 (6)°.

In the crystal, intermolecular N—H...O, O—H...O and C—H...O hydrogen bonds link the molecules into a three-dimensional network (Table 1). There also exists a weak C-H... π interaction (Table 1).

Experimental

The title compound was prepared by the reaction of CuSO₄·5H₂O (1.23 g, 5 mmol) in H₂O (20 ml) and NA (1.22 g, 10 mmol) in H₂O (20 ml) with sodium 4-bromobenzoate (2.23 g, 10 mmol) in H₂O (100 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for three weeks, giving blue single crystals.

Refinement

Atoms H21 and H22 (for NH₂) and H41 and H42 (for H₂O) were located in a difference Fourier map and were freely refined. The C-bound H-atoms were positioned geometrically with C—H = 0.95 Å for aromatic H-atoms, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

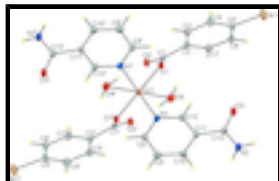


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (') $-x, -y, -z+1$].

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Crystal data

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$M_r = 743.84$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.7072$ (3) Å

$b = 9.7536$ (5) Å

$c = 9.8471$ (4) Å

$\alpha = 76.273$ (2)°

$\beta = 74.240$ (2)°

$\gamma = 85.024$ (3)°

$V = 691.86$ (5) Å³

$Z = 1$

$F(000) = 371$

$D_x = 1.785$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7694 reflections

$\theta = 2.2$ – 28.7 °

$\mu = 3.73$ mm⁻¹

$T = 100$ K

Block, blue

$0.41 \times 0.38 \times 0.35$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{\text{min}} = 0.236$, $T_{\text{max}} = 0.271$

11758 measured reflections

3515 independent reflections

3172 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$

$\theta_{\text{max}} = 28.7$ °, $\theta_{\text{min}} = 2.2$ °

$h = -10 \rightarrow 10$

$k = -12 \rightarrow 13$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.039$$

$$wR(F^2) = 0.108$$

$$S = 1.13$$

3515 reflections

203 parameters

0 restraints

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

$$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.169P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.29 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > 2\sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.50803 (3)	0.60173 (3)	0.78887 (3)	0.02585 (11)
Cu1	0.0000	0.0000	0.5000	0.00979 (12)
O1	0.1042 (2)	0.17464 (16)	0.50913 (16)	0.0123 (3)
O2	-0.1351 (2)	0.26522 (18)	0.64918 (17)	0.0160 (3)
O3	0.4297 (2)	-0.00851 (18)	0.84131 (16)	0.0182 (4)
O4	0.3099 (2)	-0.0838 (2)	0.43625 (18)	0.0172 (4)
H41	0.271 (5)	-0.146 (4)	0.402 (4)	0.036 (9)*
H42	0.383 (5)	-0.042 (4)	0.371 (4)	0.043 (11)*
N1	-0.0003 (2)	-0.08494 (19)	0.70725 (18)	0.0111 (4)
N2	0.3330 (3)	-0.1428 (2)	1.0661 (2)	0.0176 (4)
H21	0.251 (4)	-0.189 (3)	1.134 (3)	0.028 (10)*
H22	0.417 (4)	-0.110 (3)	1.094 (3)	0.016 (7)*
C1	0.0294 (3)	0.2585 (2)	0.5904 (2)	0.0103 (4)
C2	0.1508 (3)	0.3509 (2)	0.6240 (2)	0.0116 (4)
C3	0.0789 (3)	0.4675 (2)	0.6809 (2)	0.0149 (4)
H3	-0.0442	0.4943	0.6883	0.018*
C4	0.1860 (3)	0.5448 (3)	0.7267 (3)	0.0174 (5)
H4	0.1375	0.6251	0.7644	0.021*
C5	0.3644 (3)	0.5032 (2)	0.7167 (2)	0.0145 (4)
C6	0.4403 (3)	0.3898 (2)	0.6570 (2)	0.0158 (5)
H6	0.5638	0.3638	0.6490	0.019*
C7	0.3328 (3)	0.3151 (2)	0.6094 (2)	0.0144 (4)

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H7	0.3837	0.2384	0.5663	0.017*
C8	-0.1393 (3)	-0.1592 (2)	0.8002 (2)	0.0132 (4)
H8	-0.2407	-0.1721	0.7675	0.016*
C9	-0.1386 (3)	-0.2178 (3)	0.9430 (2)	0.0170 (5)
H9	-0.2382	-0.2703	1.0072	0.020*
C10	0.0077 (3)	-0.1992 (2)	0.9903 (2)	0.0150 (4)
H10	0.0101	-0.2388	1.0877	0.018*
C11	0.1524 (3)	-0.1221 (2)	0.8948 (2)	0.0109 (4)
C12	0.1421 (3)	-0.0671 (2)	0.7527 (2)	0.0122 (4)
H12	0.2405	-0.0151	0.6859	0.015*
C13	0.3162 (3)	-0.0880 (2)	0.9325 (2)	0.0137 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02453 (18)	0.03006 (18)	0.03230 (18)	-0.00115 (12)	-0.01163 (13)	-0.01980 (13)
Cu1	0.0109 (2)	0.0129 (2)	0.00714 (19)	0.00162 (14)	-0.00356 (14)	-0.00453 (14)
O1	0.0122 (7)	0.0149 (8)	0.0112 (7)	-0.0005 (6)	-0.0023 (6)	-0.0064 (6)
O2	0.0104 (8)	0.0214 (9)	0.0164 (8)	0.0013 (6)	-0.0016 (6)	-0.0073 (6)
O3	0.0165 (8)	0.0292 (9)	0.0101 (7)	-0.0054 (7)	-0.0030 (6)	-0.0053 (7)
O4	0.0150 (8)	0.0222 (9)	0.0147 (8)	0.0026 (7)	-0.0015 (7)	-0.0085 (7)
N1	0.0115 (9)	0.0131 (9)	0.0100 (8)	0.0037 (7)	-0.0032 (7)	-0.0062 (7)
N2	0.0172 (10)	0.0277 (11)	0.0090 (9)	-0.0027 (9)	-0.0044 (8)	-0.0043 (8)
C1	0.0091 (9)	0.0127 (10)	0.0087 (9)	-0.0004 (7)	-0.0024 (8)	-0.0014 (8)
C2	0.0141 (10)	0.0129 (10)	0.0083 (9)	0.0016 (8)	-0.0027 (8)	-0.0038 (8)
C3	0.0132 (10)	0.0162 (11)	0.0152 (10)	0.0034 (8)	-0.0025 (8)	-0.0057 (9)
C4	0.0200 (12)	0.0152 (11)	0.0189 (11)	0.0042 (9)	-0.0040 (9)	-0.0102 (9)
C5	0.0151 (11)	0.0175 (11)	0.0139 (10)	-0.0030 (8)	-0.0044 (8)	-0.0075 (8)
C6	0.0117 (10)	0.0192 (11)	0.0179 (10)	0.0029 (8)	-0.0045 (9)	-0.0070 (9)
C7	0.0157 (11)	0.0150 (11)	0.0131 (10)	0.0030 (8)	-0.0024 (8)	-0.0072 (8)
C8	0.0112 (10)	0.0169 (11)	0.0129 (10)	0.0037 (8)	-0.0030 (8)	-0.0073 (8)
C9	0.0175 (12)	0.0190 (11)	0.0129 (10)	0.0011 (9)	0.0000 (9)	-0.0055 (9)
C10	0.0153 (11)	0.0189 (11)	0.0097 (9)	0.0008 (9)	-0.0009 (8)	-0.0045 (8)
C11	0.0107 (10)	0.0140 (10)	0.0094 (9)	0.0019 (8)	-0.0025 (8)	-0.0061 (8)
C12	0.0136 (10)	0.0143 (10)	0.0100 (9)	0.0037 (8)	-0.0030 (8)	-0.0065 (8)
C13	0.0153 (11)	0.0187 (11)	0.0090 (10)	0.0043 (9)	-0.0035 (8)	-0.0082 (8)

Geometric parameters (\AA , $^\circ$)

Br1—C5	1.895 (2)	C3—H3	0.9500
Cu1—O1	1.9756 (16)	C4—C5	1.383 (3)
Cu1—O1 ⁱ	1.9756 (16)	C4—H4	0.9500
Cu1—N1	2.0116 (16)	C6—C5	1.386 (3)
Cu1—N1 ⁱ	2.0116 (16)	C6—C7	1.384 (3)
Cu1—O4	2.4199 (16)	C6—H6	0.9500
Cu1—O4 ⁱ	2.4199 (16)	C7—H7	0.9500
O1—C1	1.272 (3)	C8—N1	1.340 (3)
O2—C1	1.246 (3)	C8—H8	0.9500

O3—C13	1.238 (3)	C9—C8	1.388 (3)
O4—H41	0.87 (4)	C9—H9	0.9500
O4—H42	0.79 (4)	C10—C9	1.371 (3)
N2—C13	1.334 (3)	C10—C11	1.391 (3)
N2—H21	0.85 (3)	C10—H10	0.9500
N2—H22	0.88 (3)	C11—C12	1.396 (3)
C1—C2	1.502 (3)	C11—C13	1.493 (3)
C2—C7	1.393 (3)	C12—N1	1.331 (3)
C3—C2	1.392 (3)	C12—H12	0.9500
C3—C4	1.387 (3)		
O1—Cu1—O1 ⁱ	180.0	C4—C3—C2	120.4 (2)
O1—Cu1—O4	85.01 (6)	C4—C3—H3	119.8
O1 ⁱ —Cu1—O4	94.99 (6)	C3—C4—H4	120.5
O1—Cu1—O4 ⁱ	94.99 (6)	C5—C4—C3	119.0 (2)
O1 ⁱ —Cu1—O4 ⁱ	85.01 (6)	C5—C4—H4	120.5
O1—Cu1—N1	90.51 (7)	C4—C5—Br1	119.31 (17)
O1 ⁱ —Cu1—N1	89.49 (7)	C4—C5—C6	121.7 (2)
O1—Cu1—N1 ⁱ	89.49 (7)	C6—C5—Br1	119.02 (17)
O1 ⁱ —Cu1—N1 ⁱ	90.51 (7)	C5—C6—H6	120.6
O4 ⁱ —Cu1—O4	180.0	C7—C6—C5	118.7 (2)
N1 ⁱ —Cu1—N1	180.0	C7—C6—H6	120.6
N1—Cu1—O4	86.82 (6)	C2—C7—H7	119.6
N1 ⁱ —Cu1—O4	93.18 (6)	C6—C7—C2	120.8 (2)
N1—Cu1—O4 ⁱ	93.18 (6)	C6—C7—H7	119.6
N1 ⁱ —Cu1—O4 ⁱ	86.82 (6)	N1—C8—C9	121.6 (2)
C1—O1—Cu1	125.94 (15)	N1—C8—H8	119.2
Cu1—O4—H41	87 (2)	C9—C8—H8	119.2
Cu1—O4—H42	122 (3)	C8—C9—H9	120.4
H41—O4—H42	105 (3)	C10—C9—C8	119.3 (2)
C8—N1—Cu1	121.83 (14)	C10—C9—H9	120.4
C12—N1—Cu1	118.84 (15)	C9—C10—C11	119.6 (2)
C12—N1—C8	119.33 (18)	C9—C10—H10	120.2
C13—N2—H21	124.3 (19)	C11—C10—H10	120.2
C13—N2—H22	118.4 (19)	C10—C11—C12	117.8 (2)
H22—N2—H21	115 (3)	C10—C11—C13	125.52 (19)
O1—C1—C2	117.12 (18)	C12—C11—C13	116.7 (2)
O2—C1—O1	125.2 (2)	N1—C12—C11	122.5 (2)
O2—C1—C2	117.63 (19)	N1—C12—H12	118.8
C3—C2—C1	119.91 (19)	C11—C12—H12	118.8
C3—C2—C7	119.4 (2)	O3—C13—N2	122.1 (2)
C7—C2—C1	120.53 (19)	O3—C13—C11	119.74 (18)
C2—C3—H3	119.8	N2—C13—C11	118.2 (2)
O4—Cu1—O1—C1	-150.09 (16)	C4—C3—C2—C7	-1.9 (3)
O4 ⁱ —Cu1—O1—C1	29.91 (16)	C2—C3—C4—C5	-0.8 (3)
N1—Cu1—O1—C1	-63.33 (16)	C3—C4—C5—Br1	-176.52 (17)
N1 ⁱ —Cu1—O1—C1	116.67 (16)	C3—C4—C5—C6	2.5 (4)

supplementary materials

O1—Cu1—N1—C12	-42.00 (15)	C7—C6—C5—Br1	177.63 (17)
O1 ⁱ —Cu1—N1—C12	138.00 (15)	C7—C6—C5—C4	-1.4 (4)
O1—Cu1—N1—C8	138.32 (16)	C5—C6—C7—C2	-1.4 (3)
O1 ⁱ —Cu1—N1—C8	-41.68 (16)	C9—C8—N1—Cu1	179.86 (16)
O4—Cu1—N1—C12	42.98 (15)	C9—C8—N1—C12	0.2 (3)
O4 ⁱ —Cu1—N1—C12	-137.02 (15)	C10—C9—C8—N1	0.1 (3)
O4—Cu1—N1—C8	-136.71 (16)	C11—C10—C9—C8	0.0 (3)
O4 ⁱ —Cu1—N1—C8	43.29 (16)	C9—C10—C11—C12	-0.4 (3)
Cu1—O1—C1—O2	-19.3 (3)	C9—C10—C11—C13	177.1 (2)
Cu1—O1—C1—C2	157.31 (13)	C10—C11—C12—N1	0.7 (3)
O1—C1—C2—C3	164.19 (19)	C13—C11—C12—N1	-177.08 (18)
O1—C1—C2—C7	-20.9 (3)	C10—C11—C13—O3	-174.0 (2)
O2—C1—C2—C3	-19.0 (3)	C10—C11—C13—N2	4.7 (3)
O2—C1—C2—C7	156.0 (2)	C12—C11—C13—O3	3.6 (3)
C1—C2—C7—C6	-171.9 (2)	C12—C11—C13—N2	-177.76 (19)
C3—C2—C7—C6	3.0 (3)	C11—C12—N1—Cu1	179.75 (15)
C4—C3—C2—C1	173.1 (2)	C11—C12—N1—C8	-0.6 (3)

Symmetry codes: (i) $-x, -y, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

Cg is the centroid of the N1/C8–C12 pyridine ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H21 \cdots O2 ⁱⁱ	0.85 (3)	2.06 (3)	2.831 (2)	151 (3)
N2—H22 \cdots O3 ⁱⁱⁱ	0.88 (3)	2.03 (3)	2.893 (3)	166 (3)
O4—H41 \cdots O2 ⁱ	0.87 (4)	1.86 (4)	2.718 (2)	167 (4)
O4—H42 \cdots O3 ^{iv}	0.78 (4)	2.17 (4)	2.911 (2)	159 (4)
C6—H6 \cdots O2 ^v	0.95	2.43	3.377 (3)	172
C4—H4 \cdots Cg ^{vi}	0.95	2.63	3.581 (3)	176

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

Fig. 1

