

Bis(isonicotinamide- κN^1)bis(4-methylbenzoato- κO)copper(II) dihydrate

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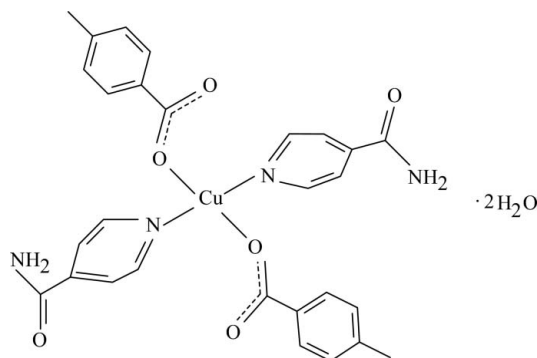
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.035; wR factor = 0.080; data-to-parameter ratio = 15.7.

In the centrosymmetric title compound, $[Cu(C_8H_7O_2)_2(C_6H_6N_2O)_2] \cdot 2H_2O$, the Cu^{II} ion is located on a crystallographic inversion center. The asymmetric unit is completed by one 4-methylbenzoate anion, one isonicotinamide (INA) ligand and one uncoordinated water molecule; all the ligands are monodentate. The two O and the two N atoms around the Cu^{II} ion form a slightly distorted square-planar arrangement. The dihedral angle between the carboxylate group and the attached benzene ring is $13.86(9)^\circ$, while the pyridine and benzene rings are oriented at a dihedral angle of $86.08(5)^\circ$. The uncoordinated water molecules are linked to the INA ligands by $O-H \cdots O$ hydrogen bonds. In the crystal structure, intermolecular $O-H \cdots O$, $N-H \cdots O$ and $C-H \cdots O$ hydrogen bonds link the molecules into a three-dimensional network.

Related literature

For niacin, see: Krishnamachari (1974) and for N,N -diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009a,b,c); Hökelek & Necefoğlu (1998); Necefoğlu *et al.* (2010a,b).



Experimental

Crystal data

$[Cu(C_8H_7O_2)_2(C_6H_6N_2O)_2] \cdot 2H_2O$	$V = 1291.92(6) \text{ \AA}^3$
$M_r = 614.11$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.7138(2) \text{ \AA}$	$\mu = 0.91 \text{ mm}^{-1}$
$b = 18.9948(4) \text{ \AA}$	$T = 100 \text{ K}$
$c = 11.9671(3) \text{ \AA}$	$0.29 \times 0.27 \times 0.25 \text{ mm}$
$\beta = 95.906(3)^\circ$	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	11754 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	3199 independent reflections
$T_{\min} = 0.763$, $T_{\max} = 0.959$	2637 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	
$S = 1.08$	
3199 reflections	$\Delta\rho_{\text{max}} = 0.63 \text{ e \AA}^{-3}$
204 parameters	$\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H21 \cdots O1^i$	0.82 (2)	2.46 (2)	3.283 (2)	177 (2)
$N2-H22 \cdots O4^{ii}$	0.86 (2)	2.14 (2)	2.983 (2)	171 (2)
$O4-H41 \cdots O3$	0.77 (3)	2.10 (3)	2.866 (2)	178 (3)
$O4-H42 \cdots O1^{iii}$	0.78 (3)	2.04 (3)	2.813 (2)	173 (3)
$C3-H3 \cdots O3^{iv}$	0.93	2.48	3.324 (2)	151
$C10-H10 \cdots O1^{iii}$	0.93	2.50	3.242 (2)	137
$C12-H12 \cdots O4^{ii}$	0.93	2.34	3.253 (2)	169

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

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: ORTEP-3 for Windows (Farrugia, 1997); 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: SU2197).

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supporting information

Acta Cryst. (2010). E66, m955–m956 [https://doi.org/10.1107/S1600536810028060]

Bis(isonicotinamide- κ N¹)bis(4-methylbenzoato- κ O)copper(II) dihydrate**Tuncer Hökelek, Güner Saka, Barış Tercan, Efdal Çimen and Hacali Necefoğlu****S1. Comment**

As a part of our ongoing investigation on 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 title compound is a mononuclear complex, where the Cu^{II} ion is located on a crystallographic inversion center (Fig. 1). The asymmetric unit contains one 4-methylbenzoate (PMB) anion, one isonicotinamide (INA) ligand and one uncoordinated water molecule, and all the ligands are coordinated in a monodentate manner. The crystal structures of some NA and/or DENA complexes of Cu^{II}, Co^{II}, Ni^{II}, Mn^{II} and Zn^{II} ions have been reported on recently (Hökelek *et al.*, 1996; Necefoğlu *et al.*, 2010*a,b*; Hökelek & Necefoğlu, 1998; Hökelek *et al.*, 2009*a,b,c*). In the copper(II) complex, *trans*-Bis(benzoato-O,O')bis(*N,N*-diethylnicotinamide-N1)copper(II) [Hökelek *et al.*, 1996], the two benzoate ions are coordinated to the Cu atom as bidentate ligands, while in the other structures all the ligands are coordinated in a monodentate manner.

The two O atoms (O2, and the symmetry-related atom, O2') and the two N atoms (N1, and the symmetry-related atom, N1') around the Cu^{II} ion form a slightly distorted square-planar arrangement (Fig. 1). The Cu1—O2 bond length is 1.9192 (13) Å, and the Cu1—N1 bond length is 2.0562 (15) Å. The near equality of the C1—O1 [1.249 (2) Å] and C1—O2 [1.287 (2) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds. The Cu^{II} ion is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by 0.3593 (1) Å. The dihedral angle between the planar carboxylate group and the benzene ring A (= C2—C7) is 13.86 (9)°, while that between rings A and B (= N1/C9—C13) is 86.08 (5)°. The uncoordinated water molecules are linked to the INA groups by O—H \cdots O hydrogen bonds (Table 1 and Fig. 1).

In the crystal structure intermolecular O—H \cdots O, N—H \cdots O and C—H \cdots O hydrogen bonds (Table 1) link the molecules to form a three-dimensional network.

S2. Experimental

The title compound was prepared by the reaction of CuSO₄·5H₂O (1.25 g, 5 mmol) in H₂O (50 ml) and isonicotinamide (2.44 g, 20 mmol) in H₂O (15 ml) with sodium 4-methylbenzoate (1.58 g, 10 mmol) in H₂O (500 ml). The precipitated green mass was set aside in solution at ambient temperature. After three weeks it had transformed into purple crystals. These were separated off by filtration and dried at room temperature.

S3. Refinement

Atoms H21, H22 (for NH₂) and H41, H42 (for H₂O) were located in a difference Fourier map and were freely refined: N—H = 0.82 (2) - 0.86 (2) Å; O—H = 0.77 (3) - 0.78 (3) Å. The remaining H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å for aromatic and methyl H-atoms, respectively, and constrained to ride on their parent atoms, with

$U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C})$, where $k = 1.5$ for methyl H-atoms and $k = 1.2$ for aromatic H-atoms.

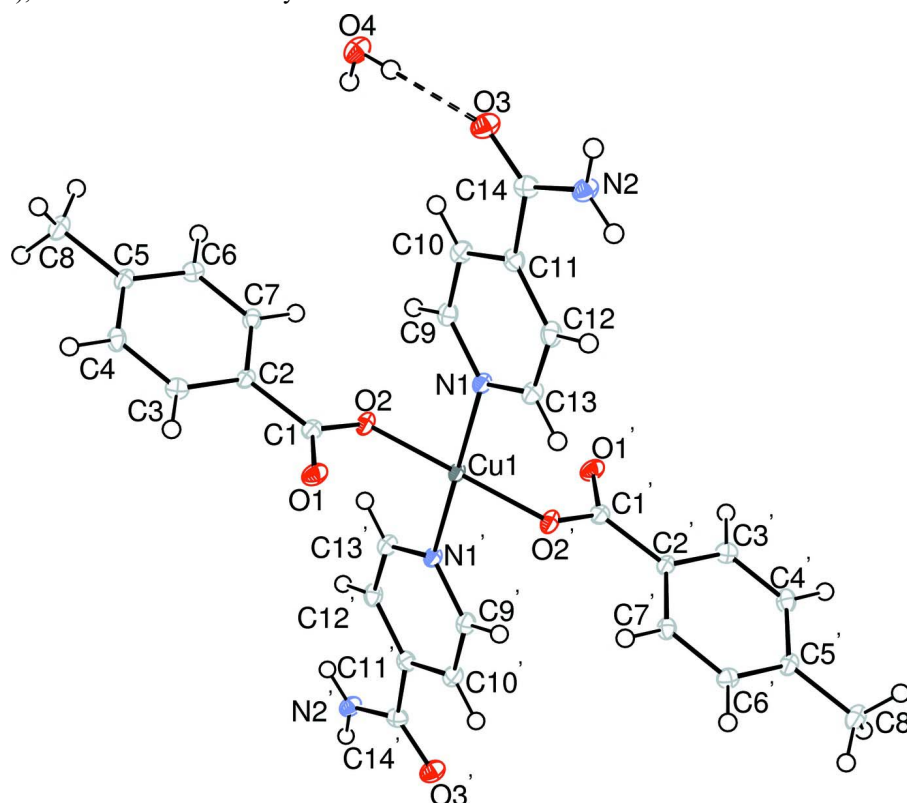


Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator: (') $-x, -y, -z$. Only one of the crystal water molecules is shown [dashed line indicates the O-H...O hydrogen-bond].

Bis(isonicotinamide- κN^1)bis(4-methylbenzoato- κO)copper(II) dihydrate

Crystal data

$[\text{Cu}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$

$M_r = 614.11$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 5.7138$ (2) Å

$b = 18.9948$ (4) Å

$c = 11.9671$ (3) Å

$\beta = 95.906$ (3)°

$V = 1291.92$ (6) Å³

$Z = 2$

$F(000) = 638$

$D_x = 1.579$ Mg m⁻³

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

Cell parameters from 5200 reflections

$\theta = 2.7\text{--}28.2^\circ$

$\mu = 0.91$ mm⁻¹

$T = 100$ K

Block, violet

$0.29 \times 0.27 \times 0.25$ mm

Data collection

Bruker Kappa APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

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

$T_{\text{min}} = 0.763$, $T_{\text{max}} = 0.959$

11754 measured reflections

3199 independent reflections

2637 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 28.4^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -7 \rightarrow 7$

$k = -20 \rightarrow 25$
 $l = -16 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.080$
 $S = 1.08$
 3199 reflections
 204 parameters
 0 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
 $w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 1.1079P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.63 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.51 \text{ e } \text{\AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.0000	0.0000	0.0000	0.01074 (9)
O1	0.0382 (2)	-0.09651 (7)	-0.17689 (11)	0.0173 (3)
O2	-0.1745 (2)	-0.00164 (6)	-0.14584 (11)	0.0140 (3)
O3	-0.8594 (2)	-0.25069 (7)	0.09449 (12)	0.0191 (3)
O4	-1.1555 (3)	-0.22382 (8)	-0.10917 (14)	0.0184 (3)
H41	-1.077 (5)	-0.2318 (14)	-0.055 (2)	0.027 (7)*
H42	-1.097 (5)	-0.1903 (14)	-0.132 (2)	0.028 (7)*
N1	-0.2249 (3)	-0.07406 (8)	0.05451 (13)	0.0124 (3)
N2	-0.6168 (3)	-0.27723 (9)	0.24930 (14)	0.0158 (3)
H21	-0.707 (4)	-0.3082 (12)	0.2657 (19)	0.016 (6)*
H22	-0.487 (4)	-0.2719 (10)	0.2909 (18)	0.007 (5)*
C1	-0.1300 (3)	-0.05595 (9)	-0.20439 (15)	0.0134 (4)
C2	-0.2973 (3)	-0.06975 (9)	-0.30646 (15)	0.0112 (3)
C3	-0.2437 (3)	-0.11966 (9)	-0.38569 (16)	0.0144 (4)
H3	-0.1009	-0.1435	-0.3763	0.017*
C4	-0.4027 (3)	-0.13357 (9)	-0.47810 (16)	0.0144 (4)
H4	-0.3645	-0.1665	-0.5308	0.017*
C5	-0.6202 (3)	-0.09904 (9)	-0.49401 (15)	0.0132 (4)
C6	-0.6723 (3)	-0.04968 (9)	-0.41381 (16)	0.0136 (4)
H6	-0.8162	-0.0264	-0.4225	0.016*
C7	-0.5137 (3)	-0.03481 (9)	-0.32179 (16)	0.0126 (4)

H7	-0.5510	-0.0013	-0.2697	0.015*
C8	-0.7908 (3)	-0.11485 (10)	-0.59515 (16)	0.0175 (4)
H8A	-0.8165	-0.1647	-0.6006	0.026*
H8B	-0.7274	-0.0984	-0.6616	0.026*
H8C	-0.9374	-0.0915	-0.5878	0.026*
C9	-0.4391 (3)	-0.08763 (10)	0.00027 (16)	0.0143 (4)
H9	-0.4908	-0.0604	-0.0621	0.017*
C10	-0.5851 (3)	-0.14000 (9)	0.03306 (16)	0.0149 (4)
H10	-0.7323	-0.1471	-0.0062	0.018*
C11	-0.5111 (3)	-0.18220 (9)	0.12538 (16)	0.0132 (4)
C12	-0.2892 (3)	-0.16896 (9)	0.18202 (16)	0.0149 (4)
H12	-0.2327	-0.1958	0.2440	0.018*
C13	-0.1551 (3)	-0.11484 (10)	0.14368 (16)	0.0150 (4)
H13	-0.0079	-0.1062	0.1820	0.018*
C14	-0.6762 (3)	-0.24014 (9)	0.15535 (16)	0.0145 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01320 (16)	0.01035 (15)	0.00829 (16)	-0.00275 (12)	-0.00076 (11)	-0.00013 (12)
O1	0.0140 (7)	0.0194 (7)	0.0172 (7)	0.0006 (5)	-0.0041 (5)	0.0042 (5)
O2	0.0181 (6)	0.0127 (6)	0.0103 (6)	-0.0040 (5)	-0.0020 (5)	0.0005 (5)
O3	0.0180 (7)	0.0167 (6)	0.0217 (8)	-0.0030 (5)	-0.0025 (6)	0.0026 (6)
O4	0.0205 (8)	0.0147 (7)	0.0189 (8)	-0.0022 (6)	-0.0036 (6)	0.0018 (6)
N1	0.0131 (8)	0.0128 (7)	0.0110 (8)	-0.0015 (6)	-0.0007 (6)	-0.0005 (6)
N2	0.0154 (9)	0.0143 (8)	0.0168 (9)	-0.0034 (6)	-0.0019 (7)	0.0021 (6)
C1	0.0144 (9)	0.0138 (8)	0.0118 (9)	-0.0058 (7)	0.0011 (7)	0.0037 (7)
C2	0.0129 (9)	0.0102 (8)	0.0102 (9)	-0.0029 (6)	-0.0004 (7)	0.0014 (6)
C3	0.0139 (9)	0.0128 (8)	0.0164 (10)	0.0011 (7)	0.0013 (7)	0.0016 (7)
C4	0.0195 (9)	0.0109 (8)	0.0131 (9)	-0.0004 (7)	0.0024 (7)	-0.0036 (7)
C5	0.0163 (9)	0.0117 (8)	0.0110 (9)	-0.0045 (7)	-0.0010 (7)	0.0016 (7)
C6	0.0130 (9)	0.0127 (8)	0.0149 (10)	0.0003 (6)	0.0003 (7)	0.0019 (7)
C7	0.0155 (9)	0.0106 (8)	0.0117 (9)	-0.0016 (6)	0.0014 (7)	-0.0011 (7)
C8	0.0205 (10)	0.0174 (9)	0.0136 (10)	-0.0034 (7)	-0.0032 (8)	-0.0003 (7)
C9	0.0161 (9)	0.0142 (9)	0.0124 (9)	0.0014 (6)	0.0000 (7)	-0.0001 (7)
C10	0.0148 (9)	0.0147 (9)	0.0149 (10)	0.0004 (7)	-0.0004 (7)	-0.0015 (7)
C11	0.0152 (9)	0.0110 (8)	0.0137 (10)	0.0005 (6)	0.0028 (7)	-0.0014 (7)
C12	0.0200 (10)	0.0130 (8)	0.0116 (9)	-0.0013 (7)	0.0012 (7)	0.0014 (7)
C13	0.0149 (9)	0.0164 (9)	0.0131 (9)	-0.0001 (7)	-0.0013 (7)	0.0001 (7)
C14	0.0133 (9)	0.0120 (8)	0.0183 (10)	0.0011 (7)	0.0027 (7)	-0.0012 (7)

Geometric parameters (Å, °)

Cu1—O2	1.9192 (13)	C4—H4	0.9300
Cu1—O2 ⁱ	1.9192 (13)	C5—C4	1.401 (3)
Cu1—N1	2.0562 (15)	C5—C6	1.396 (3)
Cu1—N1 ⁱ	2.0562 (15)	C5—C8	1.504 (3)
O1—C1	1.249 (2)	C6—H6	0.9300

O2—C1	1.287 (2)	C7—C6	1.382 (3)
O3—C14	1.228 (2)	C7—H7	0.9300
O4—H41	0.77 (3)	C8—H8A	0.9600
O4—H42	0.78 (3)	C8—H8B	0.9600
N1—C9	1.350 (2)	C8—H8C	0.9600
N1—C13	1.345 (2)	C9—H9	0.9300
N2—C14	1.341 (2)	C10—C9	1.381 (3)
N2—H21	0.82 (2)	C10—C11	1.395 (3)
N2—H22	0.86 (2)	C10—H10	0.9300
C2—C1	1.495 (3)	C11—C12	1.398 (3)
C2—C3	1.397 (2)	C11—C14	1.516 (2)
C2—C7	1.398 (3)	C12—C13	1.388 (2)
C3—C4	1.383 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—H13	0.9300
O2 ⁱ —Cu1—O2	180.00 (4)	C7—C6—C5	121.11 (17)
O2—Cu1—N1	89.67 (6)	C7—C6—H6	119.4
O2 ⁱ —Cu1—N1	90.33 (6)	C2—C7—H7	119.8
O2—Cu1—N1 ⁱ	90.33 (6)	C6—C7—C2	120.40 (17)
O2 ⁱ —Cu1—N1 ⁱ	89.67 (6)	C6—C7—H7	119.8
N1—Cu1—N1 ⁱ	180.00 (10)	C5—C8—H8A	109.5
C1—O2—Cu1	113.26 (12)	C5—C8—H8B	109.5
H42—O4—H41	103 (3)	C5—C8—H8C	109.5
C9—N1—Cu1	122.91 (12)	H8A—C8—H8B	109.5
C13—N1—Cu1	120.10 (12)	H8A—C8—H8C	109.5
C13—N1—C9	116.85 (16)	H8B—C8—H8C	109.5
C14—N2—H21	117.9 (16)	N1—C9—C10	123.05 (17)
C14—N2—H22	123.8 (14)	N1—C9—H9	118.5
H22—N2—H21	118 (2)	C10—C9—H9	118.5
O1—C1—O2	122.72 (18)	C9—C10—C11	119.75 (17)
O1—C1—C2	121.14 (17)	C9—C10—H10	120.1
O2—C1—C2	116.10 (16)	C11—C10—H10	120.1
C3—C2—C1	120.47 (16)	C10—C11—C12	117.82 (17)
C3—C2—C7	119.07 (17)	C10—C11—C14	117.32 (16)
C7—C2—C1	120.42 (16)	C12—C11—C14	124.85 (17)
C2—C3—H3	120.0	C11—C12—H12	120.7
C4—C3—C2	120.03 (17)	C13—C12—C11	118.51 (17)
C4—C3—H3	120.0	C13—C12—H12	120.7
C3—C4—C5	121.34 (17)	N1—C13—C12	124.04 (17)
C3—C4—H4	119.3	N1—C13—H13	118.0
C5—C4—H4	119.3	C12—C13—H13	118.0
C4—C5—C8	120.56 (16)	O3—C14—N2	122.56 (17)
C6—C5—C4	118.05 (17)	O3—C14—C11	119.40 (17)
C6—C5—C8	121.39 (17)	N2—C14—C11	118.03 (17)
C5—C6—H6	119.4		
O2 ⁱ —Cu1—N1—C9	161.86 (14)	C1—C2—C7—C6	-177.34 (16)
O2—Cu1—N1—C9	-18.14 (14)	C3—C2—C7—C6	0.2 (3)

O2 ⁱ —Cu1—N1—C13	-22.59 (14)	C2—C3—C4—C5	-0.7 (3)
O2—Cu1—N1—C13	157.41 (14)	C6—C5—C4—C3	0.2 (3)
N1—Cu1—O2—C1	-76.89 (12)	C8—C5—C4—C3	179.96 (17)
N1 ⁱ —Cu1—O2—C1	103.11 (12)	C4—C5—C6—C7	0.5 (3)
Cu1—O2—C1—O1	-11.8 (2)	C8—C5—C6—C7	-179.23 (16)
Cu1—O2—C1—C2	166.15 (11)	C2—C7—C6—C5	-0.7 (3)
Cu1—N1—C9—C10	176.28 (14)	C11—C10—C9—N1	-0.8 (3)
C13—N1—C9—C10	0.6 (3)	C9—C10—C11—C12	0.5 (3)
Cu1—N1—C13—C12	-175.86 (14)	C9—C10—C11—C14	-178.32 (16)
C9—N1—C13—C12	0.0 (3)	C10—C11—C12—C13	0.0 (3)
C3—C2—C1—O1	-13.1 (3)	C14—C11—C12—C13	178.73 (17)
C7—C2—C1—O1	164.51 (16)	C10—C11—C14—O3	4.5 (2)
C3—C2—C1—O2	169.00 (16)	C10—C11—C14—N2	-174.41 (17)
C7—C2—C1—O2	-13.4 (2)	C12—C11—C14—O3	-174.24 (18)
C7—C2—C3—C4	0.5 (3)	C12—C11—C14—N2	6.9 (3)
C1—C2—C3—C4	178.05 (16)	C11—C12—C13—N1	-0.3 (3)

Symmetry code: (i) $-x, -y, -z$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H21 \cdots O1 ⁱⁱ	0.82 (2)	2.46 (2)	3.283 (2)	177 (2)
N2—H22 \cdots O4 ⁱⁱⁱ	0.86 (2)	2.14 (2)	2.983 (2)	171 (2)
O4—H41 \cdots O3	0.77 (3)	2.10 (3)	2.866 (2)	178 (3)
O4—H42 \cdots O1 ^{iv}	0.78 (3)	2.04 (3)	2.813 (2)	173 (3)
C3—H3 \cdots O3 ^v	0.93	2.48	3.324 (2)	151
C10—H10 \cdots O1 ^{iv}	0.93	2.50	3.242 (2)	137
C12—H12 \cdots O4 ⁱⁱⁱ	0.93	2.34	3.253 (2)	169

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