Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[[bis(isonicotinamide)copper(II)]-μ-benzene-1,2-dicarboxylato] monohydrate]

Xiao-Guang Zhou

College of Environmental Engineering, Jilin Normal University, Siping 136000, People's Republic of China
Correspondence e-mail: 03170924@sina.com

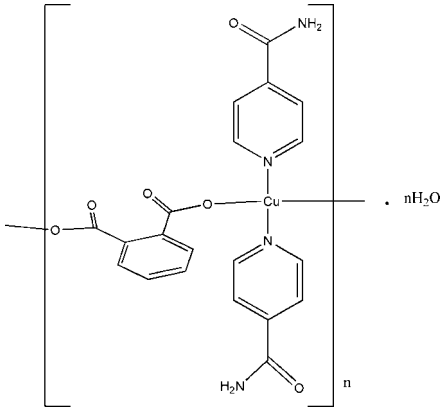
Received 29 October 2007; accepted 17 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.088; data-to-parameter ratio = 14.1.

In the title compound, $\{[Cu(C_6H_6N_2O)_2(C_8H_4O_4)]\cdot H_2O\}_n$, the Cu^{II} center exhibits a *trans*-CuN_2O_2 square-planar geometry arising from two O atoms of two benzene-1,2-dicarboxylate (bdc) dianions and two N atoms of two isonicotinamide molecules. The bdc dianions link the Cu centres into a zigzag chain. O—H···O and N—H···O hydrogen bonds generate a three-dimensional network.

Related literature

For related literature, see: Aakeroy *et al.* (2002); Abourahma *et al.* (2002); Bhogala *et al.* (2004); Eddaoudi *et al.* (2002); Lehn (1995).



Experimental

Crystal data

$[Cu(C_6H_6N_2O)_2(C_8H_4O_4)]\cdot H_2O$
M_r = 489.92
Monoclinic, $P2_1/n$
a = 8.023 (2) Å
b = 22.903 (6) Å
c = 11.473 (3) Å
β = 97.128 (3)°
V = 2091.7 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 293 (2) K
0.38 × 0.16 × 0.09 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.813, T_{max} = 0.903
17837 measured reflections
4106 independent reflections
3171 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.088
S = 1.04
4106 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O6^{i}	1.9409 (18)	Cu1—N1	2.006 (2)
Cu1—O3	1.9610 (17)	Cu1—N3	2.008 (2)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
OW1—HW1A···O5^{i}	0.89	1.87	2.735 (3)	163
OW1—HW1B···O4^{ii}	0.92	2.12	3.042 (3)	176
N4—H4A···O1^{iii}	0.86	2.18	3.015 (3)	165
N4—H4B···O3^{iv}	0.86	2.31	3.112 (3)	155
N2—H2A···O2^{v}	0.86	2.13	2.946 (3)	159
N2—H2B···OW1^{vi}	0.86	2.46	3.175 (3)	141

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by Jilin Normal University Innovative Foundation (research grant No. 20060051056).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2621).

References

Aakeroy, C. B., Beatty, A. M. & Helfrich, B. A. (2002). *J. Am. Chem. Soc.* **124**, 14425–14432.
Abourahma, H., Moulton, B., Kravtsov, V. & Zaworotko, M. J. (2002). *J. Am. Chem. Soc.* **124**, 9990–9991.
Bhogala, B. R., Thallapally, P. K. & Nangia, A. (2004). *Cryst. Growth Des.* **4**, 215–218.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SMART* (Version 5.611), *SAINT* (Version 6.0) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Eddaoudi, M., Kim, J., Rosi, N., Vodak, D., Wachter, J., O'Keeffe, M. & Yaghi, O. M. (2002). *Science*, **295**, 469–472.
Lehn, J. M. (1995). *Supramolecular Chemistry: Concepts and Perspectives*. Weinheim: VCH.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807060217

supplementary materials

Acta Cryst. (2007). E**63**, m3166 [**doi:10.1107/S1600536807060217**]

Poly[[[bis(isonicotinamide)copper(II)]-μ-benzene-1,2-dicarboxylato] monohydrate]

X.-G. Zhou

Comment

Organic amides have proved to be useful in self-assembling coordination compounds through hydrogen bonding (*e.g.* Bhogala *et al.*, 2004). To augment this family, we obtained the title compound, (I), (Fig. 1), by choosing benzene-1,2-dicarboxylate, isonicotinamide and Cu^{II} as the staring materials.

Compound (I) is constructed from the basic unit $[Cu(C_6H_6N_2O)_2(C_8H_4O_4)]\cdot H_2O$. The Cu^{II} center shows a square planar coordination geometry, being coordinated by two N atoms of two isonicotinamide molecules and two O atoms from two benzene-1,2-dicarboxylate dianions (Table 1). Each benzene-1,2-dicarboxylate ligand bridges two Cu^{II} centers to form an infinite zigzag chain.

Hydrogen-bonding interactions generate a three-dimensional network in the crystal strcture of (I) (Table 2, Fig. 2). Thus, compound (I) can be considered as a three-dimensional supramolecular array stabilized by hydrogen-bonding interactions.

Experimental

A mixture of $CuSO_4$ (0.5 mmol), benzene-1,2-dicarboxylic acid (0.5 mmol), NaOH (1.0 mmol) and isonicotinamide (1.0 mmol) was heated in water/ethanol (20 ml, 1:1 *v*/*v*) mixture and continually stirred about 30 min at 333 K. The mixture was filtered and the filtrate was allowed to stand. One week later, blue blocks of (I) were obtained.

Refinement

The water H atoms were located in a difference map and refined as riding in their as-found relative positions. The U_{iso} values were freely refined.

The C– and N-bound H atoms were positioned geometrically (C—H = 0.93 Å, N—H = 0.86 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}$(carrier).

Figures

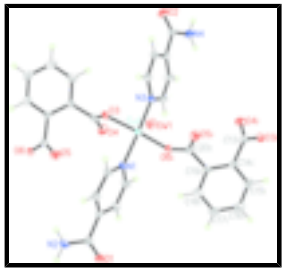


Fig. 1. View of (I) showing the local coordination environment of Cu(II) with 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry code: (i) *x*- 1/2, 1/2 − *y*, 1/2 + *z*.

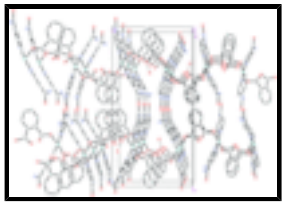


Fig. 2. The packing for (I). H atoms have been omitted for clarity.

Poly[[[bis(isonicotinamide)copper(II)]-μ-benzene-1,2-dicarboxylato] monohydrate]

Crystal data

$[Cu(C_6H_6N_2O)_2(C_8H_4O_4)]\cdot H_2O$	F_{000} = 1004
M_r = 489.92	D_x = 1.556 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3211 reflections
a = 8.023 (2) Å	θ = 2.5–23.0º
b = 22.903 (6) Å	μ = 1.10 mm^{-1}
c = 11.473 (3) Å	T = 293 (2) K
β = 97.128 (3)º	Block, blue
V = 2091.7 (9) Å^3	0.38 × 0.16 × 0.09 mm
Z = 4	

Data collection

Bruker APEX I CCD diffractometer	4106 independent reflections
Radiation source: fine-focus sealed tube	3171 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 293(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −9→9
T_{min} = 0.813, T_{max} = 0.903	k = −28→28
17837 measured reflections	l = −14→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.088	$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.975P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4106 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
291 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.54119 (4)	0.233735 (13)	0.83422 (3)	0.03007 (11)
O3	0.6678 (2)	0.17280 (7)	0.76335 (15)	0.0312 (4)
O2	0.0383 (2)	−0.01116 (8)	0.8689 (2)	0.0481 (5)
O5	0.9281 (3)	0.22272 (9)	0.57311 (18)	0.0487 (5)
O6	0.8999 (2)	0.20366 (8)	0.38014 (16)	0.0364 (4)
OW1	0.7108 (3)	0.21483 (9)	1.0445 (2)	0.0541 (6)
HW1A	0.6272	0.2354	1.0693	0.068 (11)*
HW1B	0.8019	0.2389	1.0644	0.109 (17)*
O4	0.5213 (3)	0.20936 (9)	0.60265 (17)	0.0460 (5)
O1	0.9730 (2)	0.47765 (8)	0.6720 (2)	0.0511 (6)
N4	−0.1684 (3)	0.05588 (10)	0.8562 (2)	0.0434 (6)
H4A	−0.2454	0.0300	0.8588	0.052*
H4B	−0.1948	0.0923	0.8505	0.052*
N1	0.7024 (3)	0.29483 (9)	0.79177 (19)	0.0314 (5)
N2	1.1750 (3)	0.41113 (10)	0.6543 (2)	0.0438 (6)
H2A	1.2418	0.4367	0.6309	0.053*
H2B	1.2055	0.3752	0.6612	0.053*
N3	0.3642 (3)	0.17358 (9)	0.85260 (19)	0.0298 (5)
C13	0.6209 (3)	0.17375 (11)	0.6516 (2)	0.0315 (6)
C16	0.6908 (4)	0.02106 (13)	0.5449 (3)	0.0529 (8)
H16A	0.6550	−0.0165	0.5604	0.063*
C5	0.7409 (3)	0.38399 (12)	0.6910 (3)	0.0391 (7)
H5A	0.6936	0.4158	0.6487	0.047*
C4	1.0243 (3)	0.42715 (12)	0.6799 (2)	0.0357 (6)
C1	0.8677 (3)	0.29098 (11)	0.8185 (2)	0.0342 (6)
H1A	0.9113	0.2594	0.8634	0.041*
C3	0.9141 (3)	0.37930 (11)	0.7179 (2)	0.0311 (6)
C8	0.0795 (4)	0.14272 (12)	0.8104 (3)	0.0423 (7)
H8A	−0.0303	0.1516	0.7796	0.051*
C14	0.6898 (3)	0.12431 (11)	0.5849 (2)	0.0309 (6)
C18	0.8577 (4)	0.08515 (12)	0.4431 (3)	0.0429 (7)

H18A	0.9314	0.0908	0.3876	0.051*
C9	0.1188 (3)	0.08828 (11)	0.8575 (2)	0.0301 (6)
C15	0.6331 (4)	0.06837 (12)	0.6035 (3)	0.0430 (7)
H15A	0.5552	0.0625	0.6560	0.052*
C10	−0.0085 (3)	0.03971 (12)	0.8608 (2)	0.0348 (6)
C19	0.8055 (3)	0.13276 (11)	0.5048 (2)	0.0312 (6)
C2	0.9782 (3)	0.33170 (11)	0.7827 (2)	0.0344 (6)
H2C	1.0935	0.3271	0.8019	0.041*
C11	0.2846 (3)	0.07746 (11)	0.9010 (2)	0.0346 (6)
H11A	0.3159	0.0412	0.9328	0.042*
C12	0.4028 (3)	0.12067 (11)	0.8968 (2)	0.0338 (6)
H12A	0.5139	0.1127	0.9259	0.041*
C20	0.8826 (3)	0.19152 (11)	0.4871 (3)	0.0316 (6)
C7	0.2050 (3)	0.18376 (12)	0.8097 (3)	0.0424 (7)
H7A	0.1772	0.2203	0.7778	0.051*
C6	0.6409 (3)	0.34095 (12)	0.7279 (3)	0.0393 (7)
H6A	0.5253	0.3438	0.7079	0.047*
C17	0.8012 (4)	0.02959 (13)	0.4637 (3)	0.0518 (8)
H17A	0.8376	−0.0020	0.4228	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02659 (18)	0.02751 (18)	0.0382 (2)	−0.00159 (14)	0.01255 (14)	0.00079 (14)
O3	0.0280 (10)	0.0329 (10)	0.0340 (11)	0.0018 (8)	0.0089 (8)	0.0003 (8)
O2	0.0328 (12)	0.0275 (11)	0.0845 (16)	0.0015 (9)	0.0098 (11)	0.0008 (10)
O5	0.0579 (14)	0.0435 (12)	0.0451 (13)	−0.0152 (10)	0.0078 (10)	−0.0065 (10)
O6	0.0382 (11)	0.0318 (10)	0.0425 (11)	−0.0025 (8)	0.0184 (9)	0.0016 (9)
OW1	0.0533 (14)	0.0437 (12)	0.0687 (16)	−0.0015 (12)	0.0218 (12)	−0.0039 (11)
O4	0.0449 (13)	0.0430 (12)	0.0478 (13)	0.0133 (10)	−0.0033 (10)	0.0019 (10)
O1	0.0408 (13)	0.0271 (11)	0.0886 (17)	0.0001 (9)	0.0202 (11)	0.0062 (11)
N4	0.0260 (13)	0.0307 (13)	0.0737 (18)	−0.0010 (10)	0.0072 (12)	0.0092 (12)
N1	0.0271 (12)	0.0293 (12)	0.0393 (13)	−0.0007 (10)	0.0100 (10)	0.0025 (10)
N2	0.0298 (13)	0.0299 (12)	0.0738 (18)	−0.0033 (10)	0.0151 (12)	0.0074 (12)
N3	0.0230 (11)	0.0278 (11)	0.0399 (13)	0.0002 (9)	0.0090 (9)	0.0010 (10)
C13	0.0240 (14)	0.0312 (14)	0.0401 (16)	−0.0065 (11)	0.0070 (12)	−0.0002 (12)
C16	0.064 (2)	0.0283 (16)	0.065 (2)	−0.0086 (15)	0.0030 (18)	0.0004 (15)
C5	0.0317 (16)	0.0346 (15)	0.0520 (18)	0.0057 (12)	0.0092 (13)	0.0137 (13)
C4	0.0297 (15)	0.0312 (15)	0.0465 (17)	−0.0051 (12)	0.0054 (12)	−0.0009 (13)
C1	0.0318 (15)	0.0286 (14)	0.0418 (16)	0.0027 (12)	0.0032 (12)	0.0055 (12)
C3	0.0295 (15)	0.0263 (13)	0.0383 (15)	−0.0021 (11)	0.0072 (12)	−0.0015 (11)
C8	0.0250 (15)	0.0365 (16)	0.064 (2)	−0.0017 (12)	−0.0021 (13)	0.0107 (14)
C14	0.0294 (14)	0.0298 (14)	0.0331 (15)	−0.0022 (11)	0.0018 (11)	0.0012 (11)
C18	0.0459 (18)	0.0385 (17)	0.0461 (18)	0.0050 (14)	0.0131 (14)	−0.0026 (14)
C9	0.0266 (14)	0.0265 (13)	0.0381 (15)	−0.0005 (11)	0.0078 (11)	0.0004 (11)
C15	0.0460 (18)	0.0387 (17)	0.0457 (18)	−0.0117 (14)	0.0114 (14)	0.0018 (14)
C10	0.0304 (15)	0.0303 (15)	0.0444 (17)	−0.0018 (12)	0.0069 (12)	0.0017 (12)
C19	0.0284 (15)	0.0276 (14)	0.0374 (15)	0.0015 (11)	0.0037 (12)	−0.0004 (12)

C2	0.0258 (14)	0.0317 (15)	0.0451 (17)	−0.0001 (12)	0.0017 (12)	0.0017 (12)
C11	0.0298 (15)	0.0275 (14)	0.0470 (17)	0.0044 (11)	0.0065 (12)	0.0050 (12)
C12	0.0229 (14)	0.0359 (15)	0.0429 (16)	0.0038 (12)	0.0053 (12)	0.0047 (12)
C20	0.0239 (14)	0.0297 (14)	0.0421 (17)	0.0030 (11)	0.0080 (12)	0.0006 (12)
C7	0.0319 (16)	0.0289 (15)	0.066 (2)	0.0002 (12)	0.0029 (14)	0.0139 (14)
C6	0.0240 (14)	0.0426 (17)	0.0526 (19)	0.0024 (12)	0.0095 (13)	0.0123 (14)
C17	0.061 (2)	0.0308 (16)	0.065 (2)	0.0040 (15)	0.0106 (17)	−0.0119 (15)

Geometric parameters (Å, °)

Cu1—O6^{i}	1.9409 (18)	C5—C6	1.371 (4)
Cu1—O3	1.9610 (17)	C5—C3	1.390 (4)
Cu1—N1	2.006 (2)	C5—H5A	0.9300
Cu1—N3	2.008 (2)	C4—C3	1.506 (4)
O3—C13	1.291 (3)	C1—C2	1.384 (4)
O2—C10	1.224 (3)	C1—H1A	0.9300
O5—C20	1.237 (3)	C3—C2	1.382 (4)
O6—C20	1.282 (3)	C8—C7	1.379 (4)
O6—Cu1^{ii}	1.9409 (18)	C8—C9	1.379 (4)
OW1—HW1A	0.8939	C8—H8A	0.9300
OW1—HW1B	0.9207	C14—C15	1.385 (4)
O4—C13	1.228 (3)	C14—C19	1.399 (4)
O1—C4	1.227 (3)	C18—C17	1.381 (4)
N4—C10	1.330 (3)	C18—C19	1.392 (4)
N4—H4A	0.8600	C18—H18A	0.9300
N4—H4B	0.8600	C9—C11	1.384 (4)
N1—C1	1.326 (3)	C9—C10	1.514 (4)
N1—C6	1.344 (3)	C15—H15A	0.9300
N2—C4	1.331 (3)	C19—C20	1.505 (4)
N2—H2A	0.8600	C2—H2C	0.9300
N2—H2B	0.8600	C11—C12	1.375 (4)
N3—C7	1.331 (3)	C11—H11A	0.9300
N3—C12	1.335 (3)	C12—H12A	0.9300
C13—C14	1.509 (4)	C7—H7A	0.9300
C16—C17	1.377 (4)	C6—H6A	0.9300
C16—C15	1.385 (4)	C17—H17A	0.9300
C16—H16A	0.9300		
O6^{i}—Cu1—O3	171.25 (8)	C9—C8—H8A	120.4
O6^{i}—Cu1—N1	88.08 (8)	C15—C14—C19	119.1 (2)
O3—Cu1—N1	90.75 (8)	C15—C14—C13	117.9 (2)
O6^{i}—Cu1—N3	91.93 (8)	C19—C14—C13	123.0 (2)
O3—Cu1—N3	87.98 (8)	C17—C18—C19	120.6 (3)
N1—Cu1—N3	171.72 (9)	C17—C18—H18A	119.7
C13—O3—Cu1	107.33 (16)	C19—C18—H18A	119.7
C20—O6—Cu1^{ii}	123.79 (18)	C8—C9—C11	117.8 (2)
HW1A—OW1—HW1B	102.2	C8—C9—C10	123.5 (2)
C10—N4—H4A	120.0	C11—C9—C10	118.7 (2)
C10—N4—H4B	120.0	C16—C15—C14	120.9 (3)

H4A—N4—H4B	120.0	C16—C15—H15A	119.6
C1—N1—C6	117.8 (2)	C14—C15—H15A	119.6
C1—N1—Cu1	123.62 (18)	O2—C10—N4	123.6 (3)
C6—N1—Cu1	118.47 (18)	O2—C10—C9	120.0 (2)
C4—N2—H2A	120.0	N4—C10—C9	116.4 (2)
C4—N2—H2B	120.0	C18—C19—C14	119.4 (2)
H2A—N2—H2B	120.0	C18—C19—C20	118.5 (2)
C7—N3—C12	117.8 (2)	C14—C19—C20	122.0 (2)
C7—N3—Cu1	119.97 (18)	C3—C2—C1	118.8 (2)
C12—N3—Cu1	121.91 (17)	C3—C2—H2C	120.6
O4—C13—O3	123.9 (2)	C1—C2—H2C	120.6
O4—C13—C14	121.7 (2)	C12—C11—C9	119.7 (2)
O3—C13—C14	114.3 (2)	C12—C11—H11A	120.2
C17—C16—C15	120.0 (3)	C9—C11—H11A	120.2
C17—C16—H16A	120.0	N3—C12—C11	122.5 (2)
C15—C16—H16A	120.0	N3—C12—H12A	118.7
C6—C5—C3	118.9 (3)	C11—C12—H12A	118.7
C6—C5—H5A	120.6	O5—C20—O6	125.6 (3)
C3—C5—H5A	120.6	O5—C20—C19	119.7 (2)
O1—C4—N2	123.3 (3)	O6—C20—C19	114.7 (2)
O1—C4—C3	120.2 (2)	N3—C7—C8	123.1 (3)
N2—C4—C3	116.4 (2)	N3—C7—H7A	118.4
N1—C1—C2	123.1 (2)	C8—C7—H7A	118.4
N1—C1—H1A	118.5	N1—C6—C5	123.0 (3)
C2—C1—H1A	118.5	N1—C6—H6A	118.5
C2—C3—C5	118.4 (2)	C5—C6—H6A	118.5
C2—C3—C4	122.5 (2)	C16—C17—C18	119.9 (3)
C5—C3—C4	119.1 (2)	C16—C17—H17A	120.0
C7—C8—C9	119.1 (3)	C18—C17—H17A	120.0
C7—C8—H8A	120.4		
N1—Cu1—O3—C13	−81.57 (16)	C8—C9—C10—N4	−23.4 (4)
N3—Cu1—O3—C13	90.24 (16)	C11—C9—C10—N4	158.3 (3)
O6^{i}—Cu1—N1—C1	136.7 (2)	C17—C18—C19—C14	−2.4 (4)
O3—Cu1—N1—C1	−52.0 (2)	C17—C18—C19—C20	174.6 (3)
O6^{i}—Cu1—N1—C6	−46.6 (2)	C15—C14—C19—C18	1.7 (4)
O3—Cu1—N1—C6	124.8 (2)	C13—C14—C19—C18	−177.3 (3)
O6^{i}—Cu1—N3—C7	45.0 (2)	C15—C14—C19—C20	−175.2 (3)
O3—Cu1—N3—C7	−126.2 (2)	C13—C14—C19—C20	5.8 (4)
O6^{i}—Cu1—N3—C12	−141.7 (2)	C5—C3—C2—C1	−0.3 (4)
O3—Cu1—N3—C12	47.1 (2)	C4—C3—C2—C1	177.2 (2)
Cu1—O3—C13—O4	3.4 (3)	N1—C1—C2—C3	1.2 (4)
Cu1—O3—C13—C14	−172.49 (16)	C8—C9—C11—C12	0.5 (4)
C6—N1—C1—C2	−0.7 (4)	C10—C9—C11—C12	178.8 (2)
Cu1—N1—C1—C2	176.0 (2)	C7—N3—C12—C11	−1.0 (4)
C6—C5—C3—C2	−1.1 (4)	Cu1—N3—C12—C11	−174.5 (2)
C6—C5—C3—C4	−178.6 (3)	C9—C11—C12—N3	0.4 (4)
O1—C4—C3—C2	−147.1 (3)	Cu1^{ii}—O6—C20—O5	12.9 (4)

N2—C4—C3—C2	34.1 (4)	Cu1^{ii}—O6—C20—C19	−164.68 (16)
O1—C4—C3—C5	30.4 (4)	C18—C19—C20—O5	−135.5 (3)
N2—C4—C3—C5	−148.4 (3)	C14—C19—C20—O5	41.5 (4)
O4—C13—C14—C15	−107.9 (3)	C18—C19—C20—O6	42.3 (3)
O3—C13—C14—C15	68.1 (3)	C14—C19—C20—O6	−140.8 (3)
O4—C13—C14—C19	71.2 (4)	C12—N3—C7—C8	0.9 (4)
O3—C13—C14—C19	−112.8 (3)	Cu1—N3—C7—C8	174.5 (2)
C7—C8—C9—C11	−0.6 (4)	C9—C8—C7—N3	−0.1 (5)
C7—C8—C9—C10	−178.9 (3)	C1—N1—C6—C5	−0.8 (4)
C17—C16—C15—C14	−2.5 (5)	Cu1—N1—C6—C5	−177.7 (2)
C19—C14—C15—C16	0.7 (4)	C3—C5—C6—N1	1.7 (4)
C13—C14—C15—C16	179.8 (3)	C15—C16—C17—C18	1.8 (5)
C8—C9—C10—O2	157.5 (3)	C19—C18—C17—C16	0.7 (5)
C11—C9—C10—O2	−20.8 (4)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
OW1—HW1A···O5^{i}	0.89	1.87	2.735 (3)	163
OW1—HW1B···O4^{iii}	0.92	2.12	3.042 (3)	176
N4—H4A···O1^{iv}	0.86	2.18	3.015 (3)	165
N4—H4B···O3^{v}	0.86	2.31	3.112 (3)	155
N2—H2A···O2^{vi}	0.86	2.13	2.946 (3)	159
N2—H2B···OW1^{ii}	0.86	2.46	3.175 (3)	141

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

Fig. 1

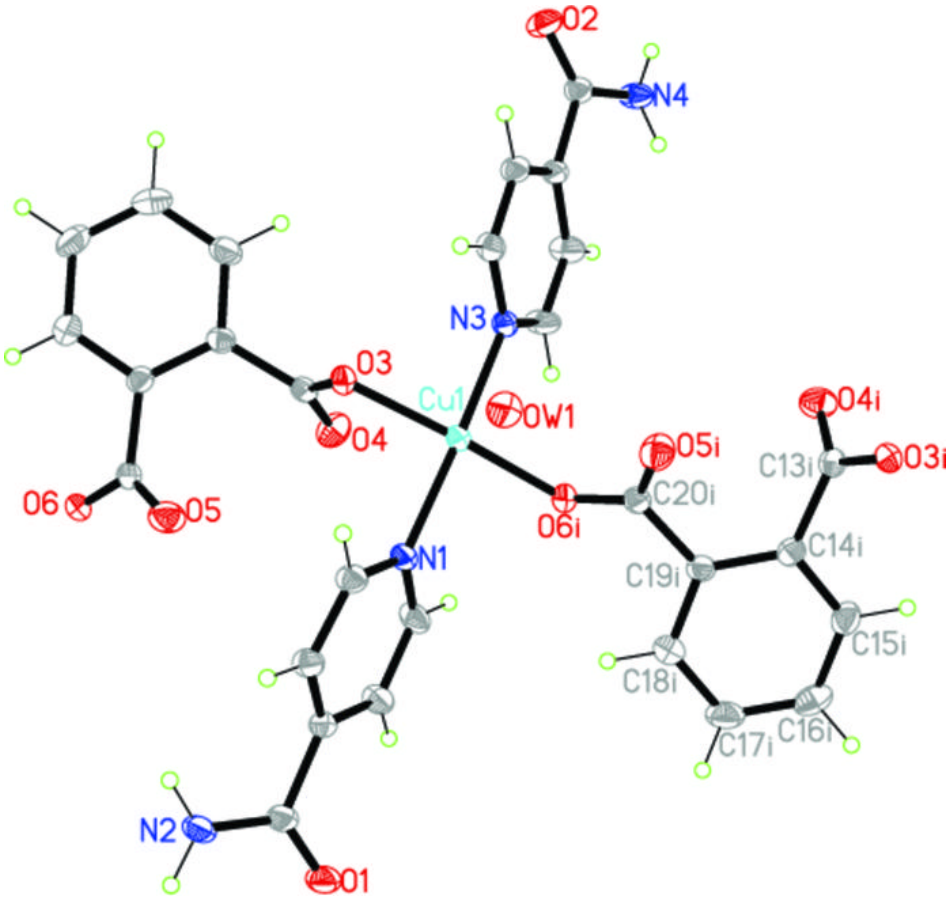

O2
N4
N3
O3
Cu1
OW1
O4
O5i
C13i
O4i
O3i
O6
O5
O6i
C20i
N1
C14i
C19i
C15i
C18i
C17i
C16i
N2
O1

Fig. 2