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catena-Poly[[(μ-4,4′-bipyridine-κ^2N:N')-bis[aqua(dimethylformamide-κO)-copper(II)]]-di-μ-terephthalato-κ^4O^1:O^4]

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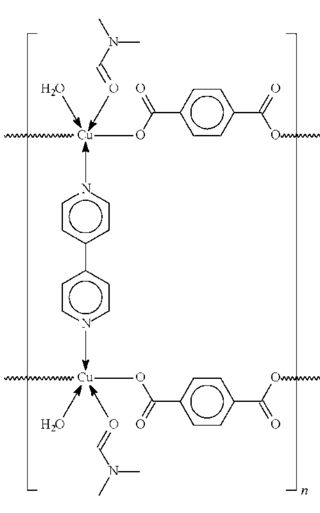
Key indicators: single-crystal X-ray study; *T* = 173 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.033; *wR* factor = 0.086; data-to-parameter ratio = 18.7.

The title coordination polymer, $[Cu_2(C_8H_4O_4)_2(C_{10}H_8N_2)(C_3H_7NO)_2(H_2O)_2]_n$, adopts a ladder structure in which terephthalate functions as the rails and bipyridine, lying on inversion centres, as the rungs. The Cu atom is also coordinated by water and dimethylformamide molecules in a square-pyramidal environment. Hydrogen bonds link the ladders into a three-dimensional network.

Related literature

For the crystal structure of a copper terephthalate-4,4′-bipyridine cocrystal with terephthalic acid, see Baeg & Lee (2003).



Experimental

Crystal data

$[Cu_2(C_8H_4O_4)_2(C_{10}H_8N_2)(C_3H_7NO)_2(H_2O)_2]$
M_r = 793.71
Monoclinic, $P2_1/n$
a = 10.8424 (2) Å
b = 14.3465 (3) Å
c = 11.1929 (2) Å
β = 108.741 (1)°
V = 1648.75 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 173 (2) K
0.15 × 0.03 × 0.02 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.813, T_{max} = 0.973
21007 measured reflections
4415 independent reflections
3131 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.086
S = 1.04
4415 reflections
236 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.943 (1)	Cu1—O1*w*	1.975 (2)
Cu1—O4^i	1.946 (1)	Cu1—N1	2.008 (2)
Cu1—O5	2.312 (1)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{ii}	0.83 (1)	1.83 (1)	2.658 (2)	175 (3)
O1*W*—H1*W*2···O3^{iii}	0.84 (1)	1.85 (1)	2.684 (2)	168 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2124).

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supplementary materials

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catena-Poly[[(*μ*-4,4'-bipyridine-*κ*^{2}*N*:*N*')bis[aqua(dimethylformamide-*κO*)copper(II)]]-di-*μ*-terephthalato-*κ*^{4}*O*^{1}:*O*^{4}]

J.-Y. Xu, B.-L. Chen and S. W. Ng

Comment

The hydrothermal reaction of copper(II) nitrate, terephthalic acid and 4,4'-bipyridine furnishes the expected copper terephthalate adduct with 4,4'-bipyridine as a 1/1 cocrystal with terephthalic acid. The compound adopts a layer structure and the terephthalic acid behaves as a guest molecule in the porous host (Baeg & Lee, 2003). With the addition of DMF in the hydrothermal synthesis, the dimensionality of the product is lowered to a ladder structure in the present study. The compound is formally $(C_{10}H_8N_2)(C_8H_4O_4)_2(C_3H_7NO)_2(H_2O)_2Cu_2$; the terephthalate represents the rails of the ladder and the *N*-heterocycle the rungs. The copper atom is also coordinated by water and DMF in a square-pyramidal geometry. Although the ladder appears to have voids (Fig. 2), these are actually occupied by the DMF ligands of adjacent ladders, and there are no empty spaces in the crystal structure.

Experimental

Copper(II) nitrate 2.5-hydrate (0.025 g, 0.11 mmol), terephthalic acid (0.018 g, 0.11 mmol) and 4,4'-bipyridine (0.009 g, 0.06 mmol) in DMF/ethanol/water (3 ml/3 ml/2 ml) were heated at 348 K for several days. Small, dark blue crystals were collected from the cooled solution in 70% yield.

Refinement

Carbon-bound hydrogen atoms were placed at calculated positions (C—H = 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2–1.5 times U_{eq}(C). The water H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.84 (1) Å; the displacement parameters were freely refined.

Figures

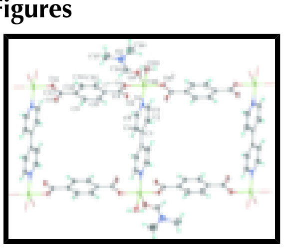

Fig. 1. A portion of the ladder structure; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. [Translational code (i): *x*, 1 + *y*, *z*.]

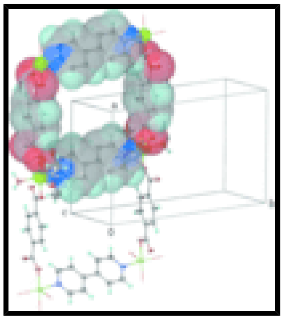

Fig. 2. Space-filling plot depicting the square grid formed from the bipyridine and terephthalate linkages that make up the ladder structure.

catena-Poly[[(μ-4,4'-bipyridine-κ^2*N*:*N'*)bis[aqua(dimethylformamide-\ κ*O*)copper(II)]]-di-μ-terephthalato-κ^4*O*^{1}:*O*^{4}]

Crystal data

$[Cu_2(C_8H_4O_4)_2(C_{10}H_8N_2)(C_3H_7NO)_2(H_2O)_2]$	F_{000} = 816
M_r = 793.71	D_x = 1.599 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4717 reflections
a = 10.8424 (2) Å	θ = 2.4–27.3°
b = 14.3465 (3) Å	μ = 1.36 mm^{-1}
c = 11.1929 (2) Å	*T* = 173 (2) K
β = 108.741 (1)°	Prism, blue
V = 1648.75 (5) Å^3	0.15 × 0.03 × 0.02 mm
Z = 2	

Data collection

Bruker X8 APEXII diffractometer	4415 independent reflections
Radiation source: fine-focus sealed tube	3131 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 173(2) K	θ_{max} = 29.4°
φ and ω scans	θ_{min} = 2.3°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 14$
T_{min} = 0.813, T_{max} = 0.973	$k = -19 \rightarrow 19$
21007 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.086	$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.0236P]$

	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4415 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
236 parameters	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.53837 (2)	0.371184 (17)	0.64815 (2)	0.01513 (8)
O1	0.35686 (13)	0.37764 (9)	0.64009 (13)	0.0196 (3)
O2	0.27817 (13)	0.40992 (10)	0.43389 (12)	0.0198 (3)
O3	−0.35170 (13)	0.37559 (10)	0.45053 (13)	0.0222 (3)
O4	−0.27850 (13)	0.36803 (9)	0.66048 (13)	0.0192 (3)
O5	0.59539 (14)	0.34997 (10)	0.86385 (13)	0.0250 (3)
O1w	0.55072 (14)	0.50852 (10)	0.65718 (13)	0.0183 (3)
H1w1	0.6064 (19)	0.5313 (18)	0.629 (2)	0.050 (9)*
H1w2	0.4812 (15)	0.5389 (15)	0.625 (2)	0.037 (7)*
N1	0.52007 (16)	0.23600 (12)	0.59914 (15)	0.0169 (4)
N2	0.5139 (2)	0.37178 (13)	1.02550 (16)	0.0292 (4)
C1	0.6080 (2)	0.17317 (15)	0.66171 (18)	0.0218 (5)
H1	0.6770	0.1931	0.7336	0.026*
C2	0.6031 (2)	0.08068 (15)	0.62679 (18)	0.0227 (5)
H2	0.6676	0.0384	0.6747	0.027*
C3	0.50411 (19)	0.04921 (14)	0.52162 (17)	0.0165 (4)
C4	0.4123 (2)	0.11503 (14)	0.45831 (19)	0.0232 (5)
H4	0.3416	0.0972	0.3866	0.028*
C5	0.4237 (2)	0.20588 (15)	0.49936 (19)	0.0239 (5)
H5	0.3596	0.2494	0.4543	0.029*
C6	0.26399 (19)	0.39180 (13)	0.53743 (18)	0.0164 (4)
C7	0.12944 (18)	0.38330 (13)	0.54406 (18)	0.0158 (4)
C8	0.02418 (19)	0.39287 (14)	0.43468 (18)	0.0188 (4)
H8	0.0387	0.4034	0.3565	0.023*
C9	−0.10098 (19)	0.38726 (14)	0.43854 (18)	0.0196 (4)
H9	−0.1722	0.3932	0.3628	0.024*
C10	−0.12433 (19)	0.37297 (13)	0.55176 (18)	0.0164 (4)
C11	−0.0189 (2)	0.36227 (15)	0.66153 (19)	0.0238 (5)
H11	−0.0335	0.3517	0.7397	0.029*
C12	0.1059 (2)	0.36693 (15)	0.65759 (19)	0.0231 (5)
H12	0.1771	0.3589	0.7330	0.028*
C13	−0.26200 (19)	0.37214 (13)	0.55229 (19)	0.0173 (4)
C14	0.5048 (2)	0.35112 (15)	0.90772 (19)	0.0236 (5)
H14	0.4208	0.3358	0.8520	0.028*
C15	0.4001 (3)	0.37555 (17)	1.0660 (2)	0.0390 (6)
H15A	0.3244	0.3522	0.9984	0.058*
H15B	0.3844	0.4401	1.0856	0.058*

H15C	0.4145	0.3368	1.1414	0.058*
C16	0.6383 (3)	0.3923 (2)	1.1183 (2)	0.0481 (7)
H16A	0.7072	0.3867	1.0796	0.072*
H16B	0.6548	0.3483	1.1887	0.072*
H16C	0.6373	0.4560	1.1497	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.00697 (13)	0.02238 (14)	0.01633 (13)	−0.00036 (10)	0.00415 (9)	−0.00054 (10)
O1	0.0070 (7)	0.0310 (8)	0.0204 (7)	−0.0001 (6)	0.0038 (6)	−0.0001 (6)
O2	0.0123 (7)	0.0279 (8)	0.0207 (7)	−0.0020 (6)	0.0076 (6)	0.0006 (6)
O3	0.0092 (7)	0.0330 (9)	0.0233 (7)	0.0020 (6)	0.0037 (6)	0.0009 (6)
O4	0.0108 (7)	0.0275 (8)	0.0207 (7)	−0.0001 (6)	0.0070 (6)	0.0002 (6)
O5	0.0178 (8)	0.0371 (9)	0.0197 (7)	−0.0011 (7)	0.0054 (6)	0.0013 (6)
O1w	0.0109 (8)	0.0234 (8)	0.0219 (7)	−0.0002 (6)	0.0069 (6)	0.0013 (6)
N1	0.0108 (8)	0.0241 (9)	0.0161 (8)	0.0004 (7)	0.0046 (6)	0.0004 (7)
N2	0.0340 (12)	0.0355 (11)	0.0175 (9)	0.0008 (9)	0.0075 (8)	−0.0031 (8)
C1	0.0176 (11)	0.0270 (12)	0.0175 (10)	−0.0003 (9)	0.0008 (8)	0.0003 (9)
C2	0.0187 (11)	0.0243 (12)	0.0200 (10)	0.0020 (9)	−0.0008 (9)	0.0021 (9)
C3	0.0125 (10)	0.0247 (11)	0.0140 (9)	0.0000 (8)	0.0063 (8)	0.0028 (8)
C4	0.0154 (10)	0.0266 (12)	0.0217 (10)	0.0023 (9)	−0.0024 (9)	−0.0030 (9)
C5	0.0158 (11)	0.0256 (12)	0.0249 (11)	0.0040 (9)	−0.0010 (9)	−0.0013 (9)
C6	0.0122 (10)	0.0158 (10)	0.0224 (10)	−0.0008 (8)	0.0073 (8)	−0.0017 (8)
C7	0.0097 (9)	0.0183 (10)	0.0206 (10)	0.0008 (8)	0.0066 (8)	0.0010 (8)
C8	0.0147 (10)	0.0259 (11)	0.0174 (9)	−0.0005 (9)	0.0075 (8)	−0.0012 (8)
C9	0.0096 (9)	0.0283 (12)	0.0192 (10)	0.0012 (8)	0.0023 (8)	−0.0022 (8)
C10	0.0089 (9)	0.0180 (10)	0.0238 (10)	−0.0001 (8)	0.0075 (8)	−0.0007 (8)
C11	0.0140 (11)	0.0383 (13)	0.0212 (10)	0.0021 (9)	0.0088 (8)	0.0067 (9)
C12	0.0109 (10)	0.0372 (13)	0.0199 (10)	0.0016 (9)	0.0031 (8)	0.0043 (9)
C13	0.0105 (9)	0.0169 (10)	0.0259 (10)	−0.0001 (8)	0.0077 (8)	−0.0005 (8)
C14	0.0251 (12)	0.0275 (12)	0.0159 (10)	−0.0003 (9)	0.0036 (9)	0.0012 (8)
C15	0.0495 (17)	0.0443 (16)	0.0333 (13)	0.0032 (13)	0.0275 (12)	−0.0036 (11)
C16	0.0508 (18)	0.0621 (19)	0.0228 (12)	−0.0050 (14)	−0.0001 (12)	−0.0094 (12)

Geometric parameters (Å, °)

Cu1—O1	1.943 (1)	C3—C3^{iii}	1.486 (4)
Cu1—O4^{i}	1.946 (1)	C4—C5	1.374 (3)
Cu1—O5	2.312 (1)	C4—H4	0.950
Cu1—O1w	1.975 (2)	C5—H5	0.950
Cu1—N1	2.008 (2)	C6—C7	1.489 (3)
O1—C6	1.277 (2)	C7—C8	1.387 (3)
O2—C6	1.245 (2)	C7—C12	1.394 (3)
O3—C13	1.238 (2)	C8—C9	1.374 (3)
O4—C13	1.281 (2)	C8—H8	0.950
O4—Cu1^{ii}	1.9462 (14)	C9—C10	1.385 (3)
O5—C14	1.231 (3)	C9—H9	0.950

O1w—H1w1	0.83 (1)	C10—C11	1.392 (3)
O1w—H1w2	0.84 (1)	C10—C13	1.495 (3)
N1—C5	1.333 (3)	C11—C12	1.369 (3)
N1—C1	1.335 (3)	C11—H11	0.950
N2—C14	1.324 (3)	C12—H12	0.950
N2—C16	1.444 (3)	C14—H14	0.950
N2—C15	1.445 (3)	C15—H15A	0.980
C1—C2	1.379 (3)	C15—H15B	0.980
C1—H1	0.950	C15—H15C	0.980
C2—C3	1.389 (3)	C16—H16A	0.980
C2—H2	0.950	C16—H16B	0.980
C3—C4	1.390 (3)	C16—H16C	0.980

O1—Cu1—O4^{i}	178.07 (6)	O2—C6—C7	118.66 (17)
O1—Cu1—O1w	90.33 (6)	O1—C6—C7	116.35 (17)
O4^{i}—Cu1—O1w	88.21 (6)	C8—C7—C12	118.79 (18)
O1—Cu1—N1	91.36 (6)	C8—C7—C6	119.31 (17)
O4^{i}—Cu1—N1	90.34 (6)	C12—C7—C6	121.90 (17)
O1w—Cu1—N1	167.58 (6)	C9—C8—C7	120.50 (18)
O1—Cu1—O5	88.96 (6)	C9—C8—H8	119.8
O4^{i}—Cu1—O5	89.91 (5)	C7—C8—H8	119.8
O1w—Cu1—O5	94.98 (5)	C8—C9—C10	120.69 (18)
N1—Cu1—O5	97.35 (6)	C8—C9—H9	119.7
C6—O1—Cu1	122.90 (13)	C10—C9—H9	119.7
C13—O4—Cu1^{ii}	112.40 (12)	C9—C10—C11	118.94 (18)
C14—O5—Cu1	115.77 (13)	C9—C10—C13	118.77 (17)
Cu1—O1w—H1w1	114.6 (19)	C11—C10—C13	122.27 (18)
Cu1—O1w—H1w2	117.2 (17)	C12—C11—C10	120.41 (19)
H1w1—O1w—H1w2	107 (3)	C12—C11—H11	119.8
C5—N1—C1	117.13 (18)	C10—C11—H11	119.8
C5—N1—Cu1	121.62 (14)	C11—C12—C7	120.65 (19)
C1—N1—Cu1	121.18 (14)	C11—C12—H12	119.7
C14—N2—C16	121.0 (2)	C7—C12—H12	119.7
C14—N2—C15	121.5 (2)	O3—C13—O4	124.35 (18)
C16—N2—C15	117.4 (2)	O3—C13—C10	119.09 (18)
N1—C1—C2	123.03 (18)	O4—C13—C10	116.56 (17)
N1—C1—H1	118.5	O5—C14—N2	125.9 (2)
C2—C1—H1	118.5	O5—C14—H14	117.0
C1—C2—C3	120.10 (19)	N2—C14—H14	117.0
C1—C2—H2	120.0	N2—C15—H15A	109.5
C3—C2—H2	120.0	N2—C15—H15B	109.5
C2—C3—C4	116.30 (19)	H15A—C15—H15B	109.5
C2—C3—C3^{iii}	122.3 (2)	N2—C15—H15C	109.5
C4—C3—C3^{iii}	121.4 (2)	H15A—C15—H15C	109.5
C5—C4—C3	120.08 (18)	H15B—C15—H15C	109.5
C5—C4—H4	120.0	N2—C16—H16A	109.5
C3—C4—H4	120.0	N2—C16—H16B	109.5
N1—C5—C4	123.35 (19)	H16A—C16—H16B	109.5

N1—C5—H5	118.3	N2—C16—H16C	109.5
C4—C5—H5	118.3	H16A—C16—H16C	109.5
O2—C6—O1	124.98 (18)	H16B—C16—H16C	109.5
O1w—Cu1—O1—C6	83.52 (14)	Cu1—O1—C6—O2	−5.7 (3)
N1—Cu1—O1—C6	−84.17 (15)	Cu1—O1—C6—C7	172.75 (12)
O5—Cu1—O1—C6	178.50 (14)	O2—C6—C7—C8	2.0 (3)
O1—Cu1—O5—C14	−1.64 (15)	O1—C6—C7—C8	−176.58 (17)
O4^{i}—Cu1—O5—C14	176.79 (15)	O2—C6—C7—C12	−177.32 (19)
O1w—Cu1—O5—C14	88.60 (15)	O1—C6—C7—C12	4.1 (3)
N1—Cu1—O5—C14	−92.88 (15)	C12—C7—C8—C9	0.7 (3)
O1—Cu1—N1—C5	50.14 (17)	C6—C7—C8—C9	−178.65 (18)
O4^{i}—Cu1—N1—C5	−130.78 (17)	C7—C8—C9—C10	0.7 (3)
O1w—Cu1—N1—C5	−47.6 (4)	C8—C9—C10—C11	−1.4 (3)
O5—Cu1—N1—C5	139.27 (16)	C8—C9—C10—C13	176.95 (18)
O1—Cu1—N1—C1	−133.23 (16)	C9—C10—C11—C12	0.8 (3)
O4^{i}—Cu1—N1—C1	45.85 (16)	C13—C10—C11—C12	−177.54 (19)
O1w—Cu1—N1—C1	129.0 (3)	C10—C11—C12—C7	0.6 (3)
O5—Cu1—N1—C1	−44.10 (16)	C8—C7—C12—C11	−1.3 (3)
C5—N1—C1—C2	0.6 (3)	C6—C7—C12—C11	177.98 (19)
Cu1—N1—C1—C2	−176.20 (16)	Cu1^{ii}—O4—C13—O3	−1.6 (2)
N1—C1—C2—C3	0.5 (3)	Cu1^{ii}—O4—C13—C10	178.28 (12)
C1—C2—C3—C4	−1.3 (3)	C9—C10—C13—O3	6.6 (3)
C1—C2—C3—C3^{iii}	178.7 (2)	C11—C10—C13—O3	−175.09 (19)
C2—C3—C4—C5	1.1 (3)	C9—C10—C13—O4	−173.25 (17)
C3^{iii}—C3—C4—C5	−178.9 (2)	C11—C10—C13—O4	5.1 (3)
C1—N1—C5—C4	−0.8 (3)	Cu1—O5—C14—N2	−155.75 (18)
Cu1—N1—C5—C4	175.95 (16)	C16—N2—C14—O5	−2.5 (3)
C3—C4—C5—N1	0.0 (3)	C15—N2—C14—O5	176.9 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O2^{iv}	0.83 (1)	1.83 (1)	2.658 (2)	175 (3)
O1w—H1w2···O3^{v}	0.84 (1)	1.85 (1)	2.684 (2)	168 (3)

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

Fig. 1

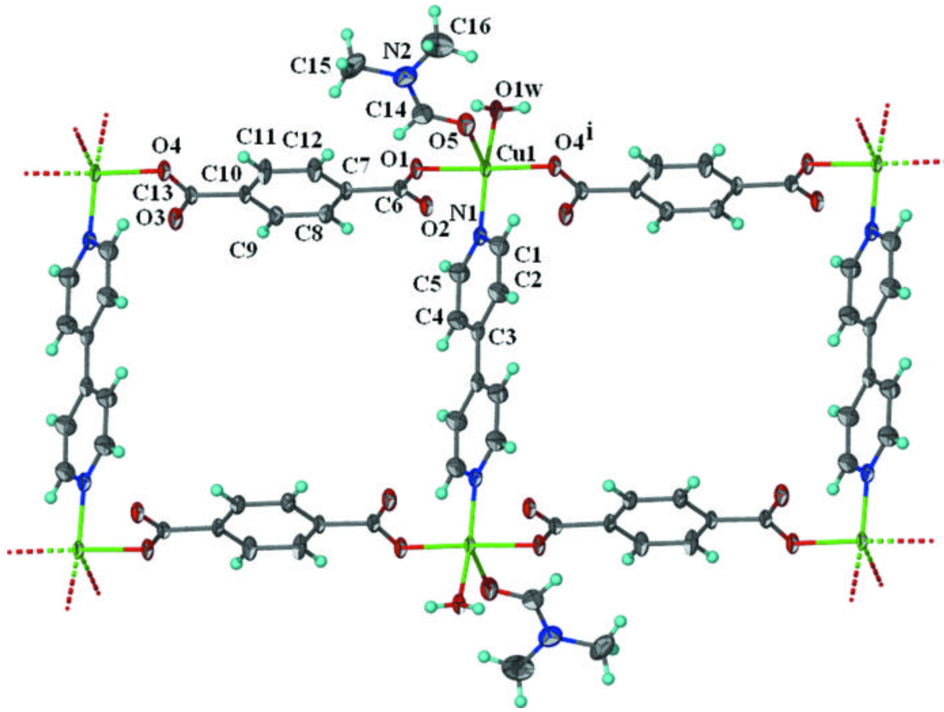
C16
N2
C15
O1w
C14
O5
Cu1
O4i
O4
C11
C12
C7
O1
C10
C13
O3
C6
O2
N1
C9
C8
C1
C5
C2
C4
C3

Fig. 2