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catena-Poly[[[(4,7-dimethyl-1,10-phenanthroline-κ^2N,N')copper(II)]-μ-terephthalato-$\kappa^2O:O'$] terephthalic acid hemisolvate]

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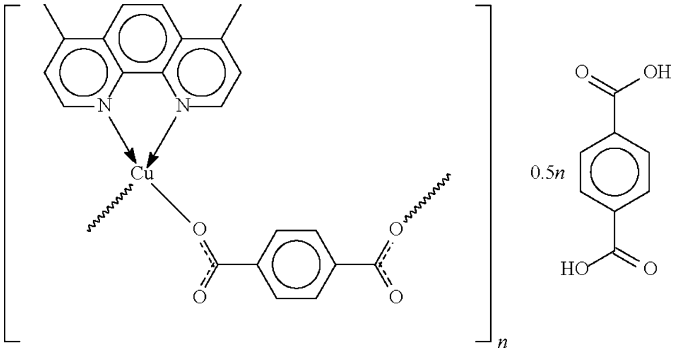
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.066; wR factor = 0.225; data-to-parameter ratio = 16.9.

In the title compound, $[Cu(C_8H_4O_4)(C_{14}H_{12}N_2)]_n\cdot 0.5nC_8H_6O_4$, the terephthalate dianion links adjacent Cu atoms into a zigzag chain. The kink at the metal linkage is nearly a right angle. The metal atom shows square-planar coordination. The solvent terephthalic acid molecule is disordered about a centre of inversion; it occupies the space between chains but is not hydrogen bonded to any.

Related literature

For copper terephthalate adducts with 1,10-phenanthroline, see: Sun *et al.* (2001); Marsh (2004); Rogan *et al.* (2004). For a discussion of the distortion of square-planar geometries of copper carboxylates, see: Li *et al.* (2005). For related literature, see: Bailey & Brown (1967); Li *et al.* (2006).



Experimental

Crystal data

$[Cu(C_8H_4O_4)(C_{14}H_{12}N_2)]\cdot 0.5C_8H_6O_4$
M_r = 518.97
Monoclinic, $C2/c$
a = 18.764 (5) Å
b = 17.769 (5) Å
c = 14.749 (5) Å
β = 117.841 (5)°
V = 4348 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 295 (2) K
0.33 × 0.20 × 0.08 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalStructure*; Rigaku, 2000)
T_{min} = 0.828, T_{max} = 0.921
16066 measured reflections
4914 independent reflections
4295 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.225
S = 1.15
4914 reflections
290 parameters
16 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.980 (3)	Cu1—O4	2.580 (4)
Cu1—O2	2.486 (3)	Cu1—N1	2.009 (3)
Cu1—O3	1.961 (3)	Cu1—N2	2.000 (3)
O1—Cu1—O3	95.4 (1)	O3—Cu1—N1	93.0 (1)
O1—Cu1—N1	165.7 (1)	O3—Cu1—N2	168.9 (1)
O1—Cu1—N2	91.9 (1)	N1—Cu1—N2	81.6 (1)

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: XU2271).

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supplementary materials

Acta Cryst. (2007). E**63**, m1865 [**doi:10.1107/S1600536807027663**]

catena-Poly[[[(4,7-dimethyl-1,10-phenanthroline-κ^2N,N')copper(II)]-μ-terephthalato-$\kappa^2O:O'$] terephthalic acid hemisolvate\]

Y.-H. Wen and S. W. Ng

Comment

Copper terephthalate forms adducts with 1,10-phenanthroline; the 1:1 adduct has been isolated as an anhydrous (Sun *et al.*, 2001; Marsh, 2004) as well as a monoaqua (Rogan *et al.*, 2004) compound in which the dicarboxylate dianion functions as a bridging entity. A 1:2 adduct is known having two monodeprotonated carboxylate groups (Li *et al.*, 2006). Copper(II) terephthalate–dimethylphenanthroline crystallizes as a 1:0.5 cocrystal, $(C_{14}H_{14}N_2)(C_8H_4O_4)Cu\cdot 0.5C_8H_6O_4$, the terephthalate dianion links adjacent copper atoms into a zigzag chain, the kink at the metal linkage being nearly a right angle. The metal atom shows square-planar coordination; if the long double-bonded oxygen atoms that are more than 2.5 Å away are considered, then the geometry is an octahedron. The lattice terephthalic acid molecule is disordered about a center-of-inversion; it occupies the space between chains but is not hydrogen bonded to any.

Experimental

A mixture of copper(II) hydoxide carbonate (0.203 g, 1 mmol)), terephthalic acid (0.164 g, 1 mmo1) and 4,7-dimethyl-1,10-phenanthroline (0.062 g, 0.3 mmol) and water (16 ml) was placed in a 25-ml, Teflon-lined, stainless steel Parr bomb. The bomb was heated to 453 K for 72 h. It was cooled to room temperature over 72 h to furnish several blue prismatic crystals.

Refinement

The structure when refined with only the atoms comprising the $(C_{14}H_{14}N_2)(C_8H_4O_4)Cu$ portion of the asymmetric refined to a satisfactory *R*-index but with two voids of 382 Å^3, each about a center-of-inversion. As the terephthalic acid itself is a centrosymmetric molecule displaying a volume of 174.8 Å^3 (Bailey & Brown, 1967), the voids of the unit cell should accommodate four terephthalic acid molecules.

The electron densities in the difference Fourier map were allowed to refine off the symmetry element, as a half-occupancy $C_8H_6O_4$ molecule. The aromatic ring was refined as a rigid hexagon of 1.39 Å sides; the C–C distances were restrained to 1.50±0.01 Å and the C–O distances to 1.25±0.01 Å. The two –C—C(=O)–OH units were restrained to be nearly flat, and other distances restraints were use to ensure sensible bond angles. The temperature factors of all C– and O-atoms were restrained to equal each other. The atoms were refined isotropically.

The H-atoms were placed in calculated positions (O–H 0.82 Å and C–H 0.93 Å), and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C,*O*).

The final difference Fourier map had a large peak near the disordered terephthalic acid molecule.

Figures

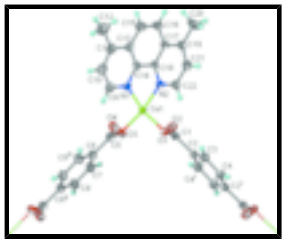

Fig. 1. **Figure 1**. Thermal ellipsoid plot of the polymeric $(C_{14}H_{14}N_2)(C_8H_4O_4)Cu$ chain; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. The hemiterephthalic acid molecule is not shown.

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Crystal data

$[Cu(C_8H_4O_4)(C_{14}H_{12}N_2)]\cdot 0.5C_8H_6O_4$	$F_{000} = 2128$
$M_r = 518.97$	$D_x = 1.585$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 5331 reflections
a = 18.764 (5) Å	θ = 2.7–27.5º
b = 17.769 (5) Å	μ = 1.05 mm^{-1}
c = 14.749 (5) Å	*T* = 295 (2) K
β = 117.841 (5)º	Prism, blue
V = 4348 (2) Å^3	0.33 × 0.20 × 0.08 mm
Z = 8	

Data collection

Rigaku Mercury CCD diffractometer	4914 independent reflections
Radiation source: fine-focus sealed tube	4295 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
T = 295(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (CrystalStructure; Rigaku, 2000)	*h* = −20→24
$T_{min} = 0.828$, $T_{max} = 0.921$	*k* = −23→23
16066 measured reflections	*l* = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.225$	$w = 1/[\sigma^2(F_o^2) + (0.1414P)^2 + 6.3201P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.15$	$(\Delta/\sigma)_{max} = 0.001$
4914 reflections	$\Delta\rho_{max} = 1.41$ e Å^{-3}
290 parameters	$\Delta\rho_{min} = -0.88$ e Å^{-3}
16 restraints	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.017 (2)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.25030 (3)	0.53888 (2)	0.62123 (3)	0.0363 (3)	
O1	0.30675 (15)	0.50921 (15)	0.76751 (19)	0.0415 (6)	
O2	0.39382 (18)	0.57136 (17)	0.7350 (2)	0.0514 (7)	
O3	0.28153 (19)	0.44917 (15)	0.5707 (2)	0.0483 (7)	
O4	0.1733 (2)	0.41283 (19)	0.5821 (3)	0.0599 (8)	
N1	0.20944 (18)	0.59243 (18)	0.4862 (2)	0.0375 (6)	
N2	0.19708 (19)	0.62594 (16)	0.6513 (2)	0.0377 (6)	
C1	0.3768 (2)	0.53507 (18)	0.7936 (3)	0.0376 (8)	
C2	0.4409 (2)	0.51817 (18)	0.9015 (3)	0.0339 (7)	
C3	0.4211 (2)	0.5079 (2)	0.9807 (3)	0.0395 (7)	
H3	0.3679	0.5139	0.9677	0.047*	
C4	0.4796 (2)	0.4888 (2)	1.0790 (3)	0.0396 (8)	
H4	0.4656	0.4808	1.1310	0.048*	
C5	0.2296 (3)	0.3998 (2)	0.5624 (3)	0.0429 (8)	
C6	0.2401 (2)	0.3225 (2)	0.5288 (3)	0.0400 (8)	
C7	0.3078 (3)	0.3049 (2)	0.5186 (3)	0.0433 (8)	
H7	0.3466	0.3416	0.5305	0.052*	
C8	0.3184 (3)	0.2329 (2)	0.4908 (3)	0.0440 (8)	
H8	0.3645	0.2213	0.4851	0.053*	
C9	0.2153 (2)	0.5730 (2)	0.4036 (3)	0.0455 (9)	
H9	0.2374	0.5264	0.4024	0.055*	
C10	0.1896 (3)	0.6197 (3)	0.3179 (3)	0.0512 (10)	
H10	0.1956	0.6040	0.2617	0.061*	
C11	0.1557 (2)	0.6885 (2)	0.3155 (3)	0.0471 (9)	
C12	0.1270 (4)	0.7387 (4)	0.2239 (4)	0.0724 (15)	
H12A	0.1454	0.7195	0.1776	0.109*	
H12B	0.1480	0.7885	0.2453	0.109*	
H12C	0.0692	0.7403	0.1899	0.109*	
C13	0.1481 (2)	0.7105 (2)	0.4034 (3)	0.0402 (8)	
C14	0.1757 (2)	0.6606 (2)	0.4854 (3)	0.0364 (7)	
C15	0.1137 (3)	0.7799 (2)	0.4124 (3)	0.0511 (10)	
H15	0.0966	0.8147	0.3593	0.061*	
C16	0.1053 (3)	0.7962 (2)	0.4971 (3)	0.0529 (10)	
H16	0.0818	0.8416	0.5000	0.063*	
C17	0.1317 (2)	0.7453 (2)	0.5817 (3)	0.0409 (8)	
C18	0.1680 (2)	0.67809 (19)	0.5755 (3)	0.0346 (7)	

C19	0.1238 (3)	0.7575 (2)	0.6720 (3)	0.0499 (10)	
C20	0.0834 (4)	0.8272 (3)	0.6848 (5)	0.0779 (17)	
H20A	0.0665	0.8184	0.7361	0.117*	
H20B	0.0373	0.8392	0.6208	0.117*	
H20C	0.1207	0.8685	0.7056	0.117*	
C21	0.1524 (3)	0.7029 (2)	0.7462 (3)	0.0511 (10)	
H21	0.1472	0.7092	0.8054	0.061*	
C22	0.1889 (3)	0.6385 (2)	0.7348 (3)	0.0465 (9)	
H22	0.2083	0.6029	0.7871	0.056*	
O5	−0.014 (2)	0.4403 (15)	0.4138 (17)	0.247 (5)*	0.50
H5O	−0.0152	0.4371	0.4758	0.297*	0.50
O6	0.002 (3)	0.5681 (15)	0.422 (2)	0.247 (5)*	0.50
O7	0.0155 (19)	0.5688 (17)	−0.0359 (17)	0.247 (5)*	0.50
H7O	0.0177	0.5738	−0.0973	0.297*	0.50
O8	−0.005 (3)	0.4375 (16)	−0.0488 (18)	0.247 (5)*	0.50
C23	−0.004 (3)	0.5035 (12)	0.2799 (17)	0.247 (5)*	0.50
C24	0.004 (3)	0.4358 (12)	0.2378 (19)	0.247 (5)*	0.50
H24	0.0072	0.3908	0.2715	0.297*	0.50
C25	0.007 (2)	0.4356 (12)	0.1453 (17)	0.247 (5)*	0.50
H25	0.0119	0.3904	0.1171	0.297*	0.50
C26	0.002 (2)	0.5030 (12)	0.0949 (16)	0.247 (5)*	0.50
C27	−0.005 (2)	0.5706 (12)	0.1371 (18)	0.247 (5)*	0.50
H27	−0.0086	0.6157	0.1034	0.297*	0.50
C28	−0.008 (2)	0.5708 (11)	0.2296 (18)	0.247 (5)*	0.50
H28	−0.0133	0.6161	0.2578	0.297*	0.50
C29	−0.0052 (14)	0.5040 (13)	0.3804 (12)	0.247 (5)*	0.50
C30	0.0043 (13)	0.5031 (15)	−0.0064 (11)	0.247 (5)*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0400 (4)	0.0313 (3)	0.0304 (3)	0.00531 (15)	0.0103 (2)	−0.00028 (14)
O1	0.0386 (13)	0.0412 (13)	0.0331 (12)	0.0006 (11)	0.0070 (10)	0.0026 (11)
O2	0.0572 (17)	0.0521 (16)	0.0401 (15)	0.0015 (13)	0.0189 (13)	0.0137 (13)
O3	0.0618 (18)	0.0342 (13)	0.0503 (16)	0.0024 (12)	0.0274 (14)	−0.0036 (11)
O4	0.0640 (19)	0.0554 (18)	0.066 (2)	0.0006 (15)	0.0347 (17)	−0.0190 (15)
N1	0.0362 (15)	0.0403 (15)	0.0307 (14)	0.0066 (12)	0.0113 (12)	−0.0007 (12)
N2	0.0447 (16)	0.0335 (14)	0.0296 (14)	0.0056 (12)	0.0130 (12)	−0.0009 (11)
C1	0.044 (2)	0.0295 (16)	0.0325 (17)	0.0036 (13)	0.0121 (15)	0.0007 (12)
C2	0.0324 (16)	0.0280 (14)	0.0324 (16)	−0.0005 (12)	0.0077 (13)	0.0009 (12)
C3	0.0345 (17)	0.0430 (18)	0.0371 (17)	−0.0027 (14)	0.0135 (14)	0.0006 (15)
C4	0.0405 (18)	0.0426 (19)	0.0364 (17)	−0.0049 (15)	0.0186 (15)	0.0020 (14)
C5	0.056 (2)	0.0376 (18)	0.0327 (17)	0.0049 (16)	0.0190 (16)	−0.0020 (14)
C6	0.058 (2)	0.0342 (16)	0.0301 (16)	0.0034 (15)	0.0224 (16)	−0.0017 (13)
C7	0.057 (2)	0.0391 (18)	0.0369 (18)	−0.0057 (16)	0.0250 (17)	−0.0035 (14)
C8	0.060 (2)	0.0399 (18)	0.0401 (19)	0.0023 (16)	0.0306 (18)	−0.0016 (15)
C9	0.0422 (19)	0.051 (2)	0.0390 (19)	0.0100 (16)	0.0154 (16)	−0.0019 (16)
C10	0.052 (2)	0.068 (3)	0.0363 (19)	0.005 (2)	0.0221 (17)	−0.0003 (18)

C11	0.046 (2)	0.055 (2)	0.0383 (19)	−0.0021 (17)	0.0181 (16)	0.0041 (17)
C12	0.099 (4)	0.078 (3)	0.044 (2)	0.012 (3)	0.037 (3)	0.018 (2)
C13	0.0395 (18)	0.0429 (18)	0.0334 (17)	−0.0022 (15)	0.0129 (14)	0.0026 (14)
C14	0.0354 (17)	0.0362 (17)	0.0337 (16)	−0.0010 (13)	0.0130 (14)	−0.0020 (13)
C15	0.063 (3)	0.042 (2)	0.046 (2)	0.0090 (18)	0.0241 (19)	0.0124 (17)
C16	0.067 (3)	0.0343 (18)	0.052 (2)	0.0121 (18)	0.024 (2)	0.0079 (17)
C17	0.049 (2)	0.0326 (17)	0.0380 (18)	0.0054 (15)	0.0178 (16)	−0.0004 (14)
C18	0.0378 (17)	0.0303 (15)	0.0317 (16)	−0.0001 (13)	0.0128 (13)	−0.0007 (12)
C19	0.062 (2)	0.0402 (19)	0.046 (2)	0.0099 (18)	0.0236 (19)	−0.0043 (16)
C20	0.118 (5)	0.052 (3)	0.071 (3)	0.033 (3)	0.051 (3)	0.001 (2)
C21	0.068 (3)	0.050 (2)	0.0363 (19)	0.005 (2)	0.0253 (19)	−0.0044 (17)
C22	0.062 (2)	0.0432 (19)	0.0322 (17)	0.0102 (18)	0.0198 (17)	0.0034 (15)

Geometric parameters (Å, °)

Cu1—O1	1.980 (3)	C12—H12C	0.9600
Cu1—O2	2.486 (3)	C13—C14	1.391 (5)
Cu1—O3	1.961 (3)	C13—C15	1.427 (6)
Cu1—O4	2.580 (4)	C14—C18	1.435 (5)
Cu1—N1	2.009 (3)	C15—C16	1.360 (6)
Cu1—N2	2.000 (3)	C15—H15	0.9300
Cu1—C1	2.543 (4)	C16—C17	1.430 (5)
O1—C1	1.271 (5)	C16—H16	0.9300
O2—C1	1.234 (5)	C17—C18	1.398 (5)
O3—C5	1.274 (5)	C17—C19	1.425 (6)
O4—C5	1.241 (5)	C19—C21	1.371 (6)
N1—C9	1.319 (5)	C19—C20	1.510 (6)
N1—C14	1.365 (5)	C20—H20A	0.9600
N2—C22	1.330 (5)	C20—H20B	0.9600
N2—C18	1.355 (4)	C20—H20C	0.9600
C1—C2	1.510 (5)	C21—C22	1.383 (6)
C2—C4^{i}	1.386 (5)	C21—H21	0.9300
C2—C3	1.395 (5)	C22—H22	0.9300
C3—C4	1.391 (5)	O5—C29	1.275 (10)
C3—H3	0.9300	O5—H5O	0.9300
C4—C2^{i}	1.386 (5)	O6—C29	1.273 (10)
C4—H4	0.9300	O7—C30	1.297 (10)
C5—C6	1.504 (5)	O7—H7O	0.9300
C6—C7	1.383 (6)	O8—C30	1.295 (10)
C6—C8^{ii}	1.401 (6)	C23—C24	1.3900
C7—C8	1.386 (5)	C23—C28	1.3900
C7—H7	0.9300	C23—C29	1.496 (6)
C8—C6^{ii}	1.401 (6)	C24—C25	1.3900
C8—H8	0.9300	C24—H24	0.9300
C9—C10	1.396 (6)	C25—C26	1.3900
C9—H9	0.9300	C25—H25	0.9300
C10—C11	1.371 (6)	C26—C27	1.3900
C10—H10	0.9300	C26—C30	1.514 (6)

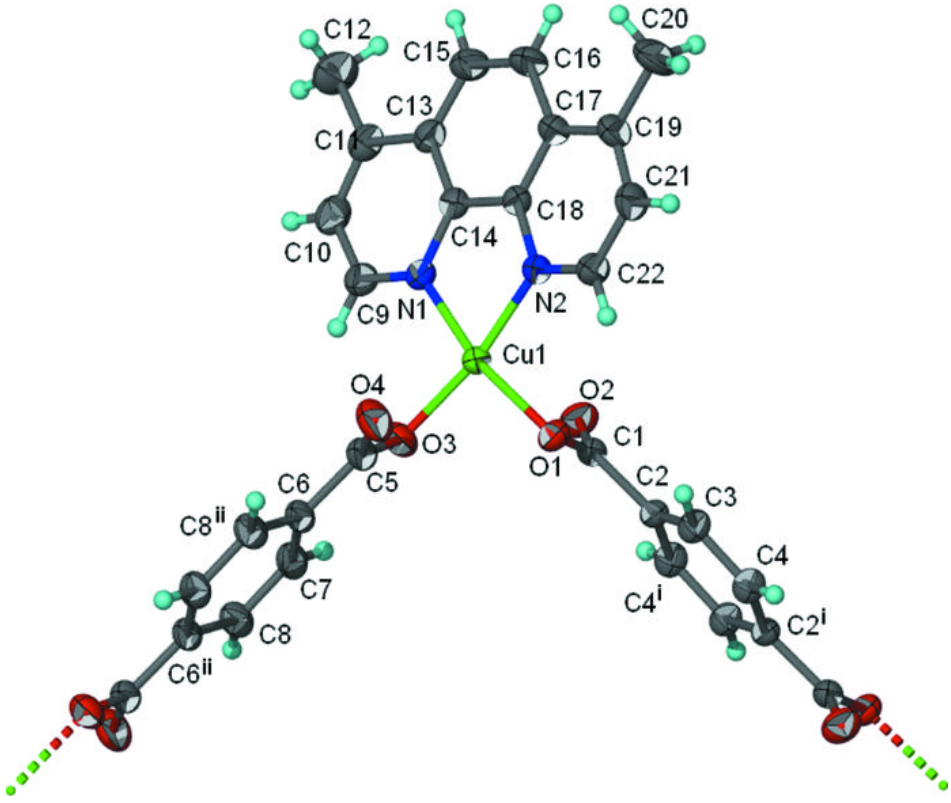
C11—C13	1.422 (5)	C27—C28	1.3900
C11—C12	1.493 (6)	C27—H27	0.9300
C12—H12A	0.9600	C28—H28	0.9300
C12—H12B	0.9600		
O1—Cu1—O3	95.4 (1)	C14—C13—C11	117.6 (4)
O1—Cu1—N1	165.7 (1)	C14—C13—C15	118.0 (3)
O1—Cu1—N2	91.9 (1)	C11—C13—C15	124.4 (4)
O3—Cu1—N1	93.0 (1)	N1—C14—C13	123.7 (3)
O3—Cu1—N2	168.9 (1)	N1—C14—C18	115.6 (3)
N1—Cu1—N2	81.6 (1)	C13—C14—C18	120.7 (3)
O3—Cu1—C1	93.05 (12)	C16—C15—C13	121.4 (4)
O1—Cu1—C1	29.41 (11)	C16—C15—H15	119.3
N2—Cu1—C1	97.39 (12)	C13—C15—H15	119.3
N1—Cu1—C1	138.58 (12)	C15—C16—C17	121.7 (4)
C1—O1—Cu1	100.7 (2)	C15—C16—H16	119.2
C5—O3—Cu1	104.2 (2)	C17—C16—H16	119.2
C9—N1—C14	117.6 (3)	C18—C17—C19	117.2 (3)
C9—N1—Cu1	129.3 (3)	C18—C17—C16	117.7 (4)
C14—N1—Cu1	112.9 (2)	C19—C17—C16	125.1 (3)
C22—N2—C18	118.2 (3)	N2—C18—C17	123.5 (3)
C22—N2—Cu1	128.4 (3)	N2—C18—C14	116.0 (3)
C18—N2—Cu1	113.4 (2)	C17—C18—C14	120.5 (3)
O2—C1—O1	123.1 (3)	C21—C19—C17	117.7 (4)
O2—C1—C2	120.2 (4)	C21—C19—C20	120.9 (4)
O1—C1—C2	116.7 (3)	C17—C19—C20	121.3 (4)
O2—C1—Cu1	73.2 (2)	C19—C20—H20A	109.5
O1—C1—Cu1	49.90 (17)	C19—C20—H20B	109.5
C2—C1—Cu1	166.2 (3)	H20A—C20—H20B	109.5
C4^{i}—C2—C3	119.8 (3)	C19—C20—H20C	109.5
C4^{i}—C2—C1	119.1 (3)	H20A—C20—H20C	109.5
C3—C2—C1	121.0 (3)	H20B—C20—H20C	109.5
C4—C3—C2	121.0 (3)	C19—C21—C22	121.4 (4)
C4—C3—H3	119.5	C19—C21—H21	119.3
C2—C3—H3	119.5	C22—C21—H21	119.3
C2^{i}—C4—C3	119.2 (3)	N2—C22—C21	121.9 (4)
C2^{i}—C4—H4	120.4	N2—C22—H22	119.0
C3—C4—H4	120.4	C21—C22—H22	119.0
O4—C5—O3	123.1 (4)	C29—O5—H5O	120.0
O4—C5—C6	120.3 (4)	C30—O7—H7O	120.0
O3—C5—C6	116.6 (3)	C24—C23—C28	120.0
C7—C6—C8^{ii}	119.3 (3)	C24—C23—C29	120.2 (6)
C7—C6—C5	120.8 (4)	C28—C23—C29	119.8 (6)
C8^{ii}—C6—C5	119.9 (3)	C23—C24—C25	120.0
C6—C7—C8	120.5 (4)	C23—C24—H24	120.0
C6—C7—H7	119.8	C25—C24—H24	120.0
C8—C7—H7	119.8	C24—C25—C26	120.0
C7—C8—C6^{ii}	120.2 (4)	C24—C25—H25	120.0

C7—C8—H8	119.9	C26—C25—H25	120.0
C6^{ii}—C8—H8	119.9	C25—C26—C27	120.0
N1—C9—C10	122.5 (4)	C25—C26—C30	120.3 (6)
N1—C9—H9	118.8	C27—C26—C30	119.7 (6)
C10—C9—H9	118.8	C28—C27—C26	120.0
C11—C10—C9	120.9 (4)	C28—C27—H27	120.0
C11—C10—H10	119.6	C26—C27—H27	120.0
C9—C10—H10	119.6	C27—C28—C23	120.0
C10—C11—C13	117.7 (4)	C27—C28—H28	120.0
C10—C11—C12	121.5 (4)	C23—C28—H28	120.0
C13—C11—C12	120.8 (4)	O6—C29—O5	127.6 (10)
C11—C12—H12A	109.5	O6—C29—C23	116.2 (9)
C11—C12—H12B	109.5	O5—C29—C23	116.1 (9)
H12A—C12—H12B	109.5	O8—C30—O7	131.0 (10)
C11—C12—H12C	109.5	O8—C30—C26	114.4 (9)
H12A—C12—H12C	109.5	O7—C30—C26	114.6 (9)
H12B—C12—H12C	109.5		
O3—Cu1—O1—C1	86.5 (2)	C9—C10—C11—C12	−179.2 (5)
N2—Cu1—O1—C1	−101.8 (2)	C10—C11—C13—C14	0.0 (5)
N1—Cu1—O1—C1	−39.1 (6)	C12—C11—C13—C14	179.5 (4)
O1—Cu1—O3—C5	83.7 (3)	C10—C11—C13—C15	−179.5 (4)
N2—Cu1—O3—C5	−47.5 (7)	C12—C11—C13—C15	0.0 (7)
N1—Cu1—O3—C5	−107.9 (3)	C9—N1—C14—C13	−0.7 (5)
C1—Cu1—O3—C5	113.1 (3)	Cu1—N1—C14—C13	175.4 (3)
O3—Cu1—N1—C9	−8.1 (4)	C9—N1—C14—C18	177.9 (3)
O1—Cu1—N1—C9	117.8 (5)	Cu1—N1—C14—C18	−6.0 (4)
N2—Cu1—N1—C9	−178.4 (4)	C11—C13—C14—N1	0.2 (5)
C1—Cu1—N1—C9	89.9 (4)	C15—C13—C14—N1	179.7 (4)
O3—Cu1—N1—C14	176.4 (2)	C11—C13—C14—C18	−178.3 (3)
O1—Cu1—N1—C14	−57.7 (6)	C15—C13—C14—C18	1.2 (5)
N2—Cu1—N1—C14	6.1 (2)	C14—C13—C15—C16	−2.1 (6)
C1—Cu1—N1—C14	−85.6 (3)	C11—C13—C15—C16	177.4 (4)
O3—Cu1—N2—C22	114.9 (7)	C13—C15—C16—C17	1.0 (7)
O1—Cu1—N2—C22	−16.6 (4)	C15—C16—C17—C18	1.0 (7)
N1—Cu1—N2—C22	176.2 (4)	C15—C16—C17—C19	−178.7 (4)
C1—Cu1—N2—C22	−45.6 (4)	C22—N2—C18—C17	1.8 (5)
O3—Cu1—N2—C18	−66.5 (7)	Cu1—N2—C18—C17	−176.9 (3)
O1—Cu1—N2—C18	162.0 (3)	C22—N2—C18—C14	−177.8 (3)
N1—Cu1—N2—C18	−5.2 (2)	Cu1—N2—C18—C14	3.5 (4)
C1—Cu1—N2—C18	133.0 (3)	C19—C17—C18—N2	−1.7 (6)
Cu1—O1—C1—O2	3.3 (4)	C16—C17—C18—N2	178.5 (4)
Cu1—O1—C1—C2	−175.6 (2)	C19—C17—C18—C14	177.9 (4)
O3—Cu1—C1—O2	87.2 (2)	C16—C17—C18—C14	−1.9 (6)
O1—Cu1—C1—O2	−177.1 (3)	N1—C14—C18—N2	1.8 (5)
N2—Cu1—C1—O2	−96.5 (2)	C13—C14—C18—N2	−179.6 (3)
N1—Cu1—C1—O2	−10.8 (3)	N1—C14—C18—C17	−177.9 (3)
O3—Cu1—C1—O1	−95.7 (2)	C13—C14—C18—C17	0.8 (5)
N2—Cu1—C1—O1	80.6 (2)	C18—C17—C19—C21	0.3 (6)

N1—Cu1—C1—O1	166.4 (2)	C16—C17—C19—C21	−180.0 (4)
O3—Cu1—C1—C2	−79.0 (11)	C18—C17—C19—C20	−178.2 (5)
O1—Cu1—C1—C2	16.6 (10)	C16—C17—C19—C20	1.5 (7)
N2—Cu1—C1—C2	97.3 (11)	C17—C19—C21—C22	0.9 (7)
N1—Cu1—C1—C2	−177.0 (10)	C20—C19—C21—C22	179.4 (5)
O2—C1—C2—C4^{i}	−29.4 (5)	C18—N2—C22—C21	−0.5 (6)
O1—C1—C2—C4^{i}	149.5 (3)	Cu1—N2—C22—C21	178.0 (3)
Cu1—C1—C2—C4^{i}	135.3 (10)	C19—C21—C22—N2	−0.9 (7)
O2—C1—C2—C3	152.0 (4)	C28—C23—C24—C25	0.0
O1—C1—C2—C3	−29.1 (5)	C29—C23—C24—C25	−179 (3)
Cu1—C1—C2—C3	−43.3 (12)	C23—C24—C25—C26	0.0
C4^{i}—C2—C3—C4	−1.7 (6)	C24—C25—C26—C27	0.0
C1—C2—C3—C4	176.9 (3)	C24—C25—C26—C30	−179 (3)
C2—C3—C4—C2^{i}	1.7 (6)	C25—C26—C27—C28	0.0
Cu1—O3—C5—O4	1.4 (5)	C30—C26—C27—C28	179 (3)
Cu1—O3—C5—C6	−177.5 (3)	C26—C27—C28—C23	0.0
O4—C5—C6—C7	−172.1 (4)	C24—C23—C28—C27	0.0
O3—C5—C6—C7	6.7 (5)	C29—C23—C28—C27	179 (3)
O4—C5—C6—C8^{ii}	6.7 (6)	C24—C23—C29—O6	168 (2)
O3—C5—C6—C8^{ii}	−174.4 (3)	C28—C23—C29—O6	−11 (2)
C8^{ii}—C6—C7—C8	−0.9 (6)	C24—C23—C29—O5	−12 (2)
C5—C6—C7—C8	178.0 (3)	C28—C23—C29—O5	169 (2)
C6—C7—C8—C6^{ii}	0.9 (6)	C25—C26—C30—O8	13 (2)
C14—N1—C9—C10	1.0 (6)	C27—C26—C30—O8	−166 (2)
Cu1—N1—C9—C10	−174.3 (3)	C25—C26—C30—O7	−167 (2)
N1—C9—C10—C11	−0.8 (7)	C27—C26—C30—O7	14 (2)
C9—C10—C11—C13	0.3 (6)		

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

Fig. 1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