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catena-Poly[[[(pyrazino[2,3-*f*][1,10]-phenanthroline)copper(II)]-μ-4,4′-oxydibenzoato] monohydrate]

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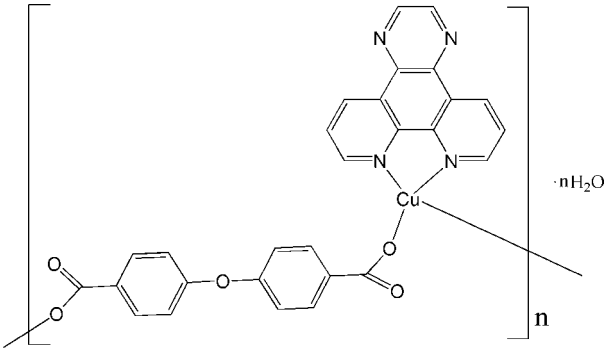
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 14.9.

In the title compound, $\{[Cu(C_{14}H_8O_5)(C_{14}H_8N_4)]\cdot H_2O\}_n$, the Cu^{II} atom adopts a distorted *cis*-CuN_2O_2 square-planar coordination geometry. 4,4′-Oxydibenzoate (L) ligands link the Cu^{II} atoms, generating a helical chain. Neighbouring chains are linked through π–π interactions between pyrazino[2,3-*f*][1,10]phenanthroline ligands with a centroid–centroid distance of *ca* 3.44 Å, resulting in a two-dimensional supramolecular structure. The structure is completed by O—H···O hydrogen bonds.

Related literature

For the crystal structure of the zinc 4,4′-oxydibenzoate adduct with bis(3-pyridylmethylene)-*p*-phenylenediamine, see Kim *et al.* (2005). For the crystal structure of the acid itself, see Dey & Desiraju (2005). For background, see: Chen & Liu (2002).



Experimental

Crystal data

$[Cu(C_{14}H_8O_5)(C_{14}H_8N_4)]\cdot H_2O$
M_r = 570.00
Monoclinic, $P2_1/n$
a = 5.8092 (12) Å
b = 14.635 (3) Å
c = 27.600 (6) Å
β = 91.87 (3)°
V = 2345.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 293 (2) K
0.22 × 0.19 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.801, T_{max} = 0.837
21478 measured reflections
5350 independent reflections
4136 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 0.93
5350 reflections
358 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	2.0052 (18)	Cu1—O1	1.9279 (17)
Cu1—N2	2.0038 (18)	Cu1—O5^{i}	1.9165 (17)

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
O1W—HW11···O2	0.81 (3)	2.22 (5)	2.808 (3)	129 (4)

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2595).

References

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supplementary materials

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catena-Poly[[[(pyrazino[2,3-*f*][1,10]phenanthroline)copper(II)]-μ-4,4'-oxydibenzoato] monohydrate]

C.-B. Liu, Y. Liu, L. Lu and J. Sun

Comment

Studies on metal dicarboxylato complexes with heteroaromatic N-donor chelating ligands are of current interest (Chen & Liu, 2002). Pyrazino[2,3-*f*][1,10]phenanthroline (Pyphen) as a new phen derivative possesses an extended aromatic system. We selected 4,4'-oxybis(benzoic acid) (H_2L) as a linker and Pyphen as a secondary chelating ligand, and in combination with Cu^{2+} ions, generaed the new coordination polymer, $[Cu(L)(Pyphen)]\cdot H_2O$, (I), which is reported here.

In compound (I) the Cu^{II} atom is four-coordinated by two Pyphen N atoms and two carboxylate O atoms, and exhibits a distorted square-planar coordination sphere (Table 1, Fig. 1). The *L* ligands link the Cu^{II} atoms to generate a distinctive helical chain structure (Fig. 2). The Pyphen ligands are attached on both sides of the chains. The neighbouring chains are linked through π-π interactions between Pyphen ligands with a π-π stacking distance of *ca* 3.44 Å, resulting in a two-dimensional supramolecular structure (Fig. 3). Finally, O—H···O hydrogen bonds involving the water molecule and carboxylate O atom acceptors (Table 2) complete the structure of (I).

Experimental

A mixture of $CuCl_2\cdot 2H_2O$ (0.5 mmol), H_2L (0.5 mmol), Pyphen (0.5 mmol), and H_2O (500 mmol) was adjusted to pH = 5.5 by addition of aqueous NaOH solution, and heated at 453 K for six days. After the mixture was slowly cooled to room temperature, blue blocks of (I) resulted.

Refinement

The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H-atoms were located in a difference Fourier map, and their positions were freely refined with $U_{iso}(H) = 1.2U_{eq}(O)$.

Figures

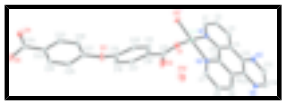

Fig. 1. The structure of (I), showing displacement ellipsoids at the 30% probability level (H atoms have been omitted). Symmetry code: (i) −1/2 − *x*, *y* − 1/2, 1/2 − *z*.

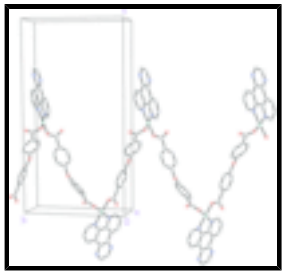

Fig. 2. View of the helical chain structure of (I).

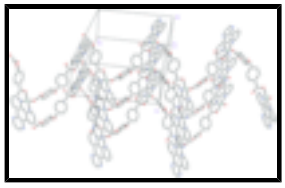

Fig. 3. View of the two-dimensional supramolecular structure of (1).

catena-Poly[[[(pyrazino[2,3-_f_][1,10]phenanthroline)copper(II)]-μ-4,4'- oxydibenzoato] monohydrate]

Crystal data

$[Cu(C_{14}H_8O_5)(C_{14}H_8N_4)]\cdot H_2O$	F_{000} = 1164
M_r = 570.00	D_x = 1.614 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 16143 reflections
a = 5.8092 (12) Å	θ = 3.0–27.5º
b = 14.635 (3) Å	μ = 0.99 mm^{-1}
c = 27.600 (6) Å	T = 293 (2) K
β = 91.87 (3)º	Block, blue
V = 2345.2 (8) Å^3	0.22 × 0.19 × 0.18 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	5350 independent reflections
Radiation source: rotor target	4136 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.2º
ω scans	h = −6→7
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −18→18
T_{min} = 0.801, T_{max} = 0.837	l = −35→35
21478 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.093$

$S = 0.93$

5350 reflections

358 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 1.748P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.38$ e Å^{-3}

$\Delta\rho_{min} = -0.28$ e Å^{-3}

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}
C1	0.4790 (4)	0.12450 (17)	−0.00903 (8)	0.0361 (5)
H1	0.4997	0.1093	0.0235	0.043*
C2	0.6371 (4)	0.09219 (17)	−0.04221 (9)	0.0388 (5)
H2	0.7596	0.0554	−0.0318	0.047*
C3	0.6096 (4)	0.11542 (17)	−0.09034 (9)	0.0388 (5)
H3	0.7119	0.0938	−0.1129	0.047*
C4	0.4259 (4)	0.17202 (15)	−0.10503 (7)	0.0315 (5)
C5	0.2744 (4)	0.20030 (15)	−0.06972 (7)	0.0283 (4)
C6	0.0836 (4)	0.25939 (15)	−0.08175 (7)	0.0281 (4)
C7	−0.2261 (4)	0.33950 (17)	−0.05277 (8)	0.0370 (5)
H7	−0.3182	0.3559	−0.0272	0.044*
C8	−0.2754 (4)	0.37489 (18)	−0.09876 (9)	0.0423 (6)
H8	−0.3974	0.4154	−0.1035	0.051*
C9	−0.1446 (4)	0.35019 (17)	−0.13711 (8)	0.0394 (5)
H9	−0.1790	0.3726	−0.1680	0.047*
C10	0.0412 (4)	0.29078 (15)	−0.12899 (7)	0.0321 (5)
C11	0.1980 (4)	0.26118 (16)	−0.16618 (7)	0.0359 (5)
C12	0.3847 (4)	0.20461 (16)	−0.15441 (7)	0.0357 (5)
C13	0.4951 (6)	0.2109 (2)	−0.23221 (10)	0.0637 (9)
H13	0.5960	0.1955	−0.2564	0.076*

C14	0.3086 (6)	0.2657 (2)	−0.24421 (9)	0.0639 (9)
H14	0.2875	0.2849	−0.2762	0.077*
C15	−0.1443 (4)	0.3508 (2)	0.07387 (8)	0.0434 (6)
C16	−0.2925 (4)	0.38171 (17)	0.11430 (7)	0.0349 (5)
C17	−0.2267 (4)	0.45479 (18)	0.14310 (9)	0.0425 (6)
H17	−0.0891	0.4848	0.1374	0.051*
C18	−0.3623 (4)	0.48415 (17)	0.18046 (8)	0.0421 (6)
H18	−0.3158	0.5330	0.2000	0.051*
C19	−0.5678 (4)	0.43965 (17)	0.18814 (7)	0.0348 (5)
C20	−0.6358 (4)	0.36678 (18)	0.15973 (8)	0.0399 (6)
H20	−0.7745	0.3374	0.1652	0.048*
C21	−0.4979 (4)	0.33725 (18)	0.12300 (8)	0.0397 (5)
H21	−0.5429	0.2874	0.1041	0.048*
C22	−0.4232 (4)	0.51097 (18)	0.33805 (8)	0.0385 (5)
H22	−0.2904	0.4936	0.3554	0.046*
C23	−0.5780 (4)	0.56945 (16)	0.35915 (7)	0.0320 (5)
C24	−0.5366 (4)	0.60147 (17)	0.41048 (7)	0.0363 (5)
C25	−0.7731 (4)	0.59633 (18)	0.33245 (8)	0.0407 (6)
H25	−0.8773	0.6364	0.3460	0.049*
C26	−0.8138 (4)	0.5641 (2)	0.28603 (8)	0.0431 (6)
H26	−0.9448	0.5823	0.2683	0.052*
C27	−0.6593 (4)	0.50457 (17)	0.26594 (7)	0.0356 (5)
C28	−0.4628 (4)	0.47786 (18)	0.29149 (8)	0.0414 (6)
H28	−0.3584	0.4382	0.2777	0.050*
N1	0.3008 (3)	0.17603 (13)	−0.02252 (6)	0.0306 (4)
N2	−0.0514 (3)	0.28303 (13)	−0.04452 (6)	0.0303 (4)
N3	0.5371 (4)	0.17933 (17)	−0.18796 (7)	0.0514 (6)
N4	0.1586 (4)	0.29205 (16)	−0.21202 (7)	0.0508 (6)
O1	−0.2016 (3)	0.27603 (14)	0.05340 (6)	0.0499 (5)
O2	0.0231 (4)	0.3962 (2)	0.06309 (8)	0.0843 (9)
O1W	0.3162 (5)	0.4364 (2)	−0.01300 (11)	0.0905 (9)
HW11	0.314 (9)	0.413 (3)	0.0136 (15)	0.136*
HW12	0.198 (6)	0.474 (3)	−0.0176 (17)	0.136*
O3	−0.7268 (3)	0.47003 (14)	0.22092 (6)	0.0481 (5)
O4	−0.3897 (3)	0.56465 (15)	0.43667 (6)	0.0551 (5)
O5	−0.6671 (3)	0.66682 (14)	0.42371 (6)	0.0467 (4)
Cu1	0.05118 (5)	0.22577 (2)	0.018498 (8)	0.03191 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0395 (12)	0.0371 (13)	0.0316 (11)	−0.0004 (10)	−0.0021 (9)	0.0035 (9)
C2	0.0370 (12)	0.0345 (13)	0.0449 (13)	0.0059 (10)	−0.0003 (10)	0.0003 (10)
C3	0.0383 (12)	0.0361 (13)	0.0425 (12)	0.0002 (10)	0.0084 (10)	−0.0072 (10)
C4	0.0376 (11)	0.0308 (11)	0.0263 (10)	−0.0045 (9)	0.0038 (9)	−0.0050 (8)
C5	0.0339 (11)	0.0278 (11)	0.0233 (9)	−0.0033 (8)	0.0025 (8)	−0.0007 (8)
C6	0.0341 (11)	0.0287 (11)	0.0216 (9)	−0.0035 (9)	0.0021 (8)	−0.0007 (8)
C7	0.0380 (12)	0.0388 (13)	0.0343 (11)	0.0037 (10)	0.0056 (9)	−0.0010 (10)

C8	0.0442 (13)	0.0402 (14)	0.0421 (13)	0.0059 (11)	−0.0026 (11)	0.0051 (11)
C9	0.0471 (13)	0.0400 (14)	0.0308 (11)	−0.0028 (11)	−0.0044 (10)	0.0074 (10)
C10	0.0395 (12)	0.0312 (12)	0.0255 (10)	−0.0032 (9)	−0.0003 (9)	0.0012 (8)
C11	0.0532 (14)	0.0329 (12)	0.0217 (9)	−0.0064 (11)	0.0049 (9)	0.0001 (9)
C12	0.0494 (14)	0.0339 (13)	0.0243 (10)	−0.0074 (10)	0.0096 (9)	−0.0057 (8)
C13	0.097 (2)	0.064 (2)	0.0325 (13)	0.0064 (18)	0.0293 (15)	−0.0031 (13)
C14	0.108 (3)	0.0623 (19)	0.0226 (11)	0.0064 (19)	0.0156 (14)	0.0029 (12)
C15	0.0414 (13)	0.0634 (18)	0.0258 (11)	0.0038 (12)	0.0059 (10)	0.0018 (11)
C16	0.0395 (12)	0.0404 (13)	0.0250 (10)	−0.0003 (10)	0.0050 (9)	−0.0009 (9)
C17	0.0419 (13)	0.0452 (15)	0.0407 (12)	−0.0099 (11)	0.0058 (10)	−0.0019 (11)
C18	0.0521 (14)	0.0376 (14)	0.0364 (12)	−0.0048 (11)	−0.0015 (11)	−0.0111 (10)
C19	0.0397 (12)	0.0425 (13)	0.0222 (9)	0.0065 (10)	−0.0001 (9)	−0.0056 (9)
C20	0.0406 (13)	0.0511 (15)	0.0284 (10)	−0.0091 (11)	0.0066 (9)	−0.0080 (10)
C21	0.0456 (13)	0.0446 (14)	0.0292 (11)	−0.0083 (11)	0.0061 (10)	−0.0109 (10)
C22	0.0406 (12)	0.0445 (14)	0.0299 (10)	0.0088 (11)	−0.0048 (9)	−0.0011 (10)
C23	0.0386 (12)	0.0343 (12)	0.0231 (9)	−0.0011 (9)	−0.0001 (8)	−0.0001 (8)
C24	0.0416 (12)	0.0445 (14)	0.0227 (10)	−0.0087 (11)	0.0007 (9)	−0.0023 (9)
C25	0.0433 (13)	0.0492 (15)	0.0296 (11)	0.0140 (11)	−0.0002 (10)	−0.0095 (10)
C26	0.0400 (13)	0.0599 (17)	0.0291 (11)	0.0158 (12)	−0.0051 (10)	−0.0094 (11)
C27	0.0388 (12)	0.0439 (14)	0.0240 (9)	0.0037 (10)	−0.0005 (9)	−0.0085 (9)
C28	0.0439 (13)	0.0462 (15)	0.0338 (11)	0.0140 (11)	−0.0010 (10)	−0.0083 (10)
N1	0.0348 (9)	0.0332 (10)	0.0237 (8)	0.0000 (8)	−0.0002 (7)	0.0025 (7)
N2	0.0350 (9)	0.0322 (10)	0.0240 (8)	0.0004 (8)	0.0041 (7)	0.0006 (7)
N3	0.0666 (15)	0.0540 (14)	0.0349 (11)	0.0030 (12)	0.0217 (10)	−0.0061 (10)
N4	0.0791 (17)	0.0493 (14)	0.0242 (9)	0.0031 (12)	0.0051 (10)	0.0051 (9)
O1	0.0619 (12)	0.0558 (12)	0.0328 (8)	0.0094 (10)	0.0170 (8)	−0.0032 (8)
O2	0.0653 (14)	0.134 (2)	0.0556 (12)	−0.0439 (15)	0.0313 (11)	−0.0251 (14)
O1W	0.0792 (18)	0.097 (2)	0.098 (2)	−0.0191 (15)	0.0410 (16)	−0.0156 (16)
O3	0.0406 (9)	0.0732 (13)	0.0304 (8)	0.0079 (9)	0.0001 (7)	−0.0229 (8)
O4	0.0686 (12)	0.0633 (13)	0.0323 (9)	0.0052 (10)	−0.0163 (9)	−0.0004 (9)
O5	0.0503 (10)	0.0640 (12)	0.0260 (8)	0.0021 (9)	0.0041 (7)	−0.0141 (8)
Cu1	0.03902 (16)	0.03777 (16)	0.01924 (12)	0.00211 (12)	0.00540 (10)	0.00198 (11)

Geometric parameters (Å, °)

C1—N1	1.324 (3)	C16—C17	1.379 (3)
C1—C2	1.401 (3)	C16—C21	1.387 (3)
C1—H1	0.9300	C17—C18	1.386 (3)
C2—C3	1.375 (3)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.382 (3)
C3—C4	1.401 (3)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.374 (3)
C4—C5	1.397 (3)	C19—O3	1.387 (3)
C4—C12	1.456 (3)	C20—C21	1.382 (3)
C5—N1	1.354 (3)	C20—H20	0.9300
C5—C6	1.437 (3)	C21—H21	0.9300
C6—N2	1.357 (3)	C22—C28	1.386 (3)
C6—C10	1.397 (3)	C22—C23	1.384 (3)
C7—N2	1.323 (3)	C22—H22	0.9300

C7—C8	1.392 (3)	C23—C25	1.389 (3)
C7—H7	0.9300	C23—C24	1.504 (3)
C8—C9	1.371 (3)	C24—O4	1.225 (3)
C8—H8	0.9300	C24—O5	1.281 (3)
C9—C10	1.399 (3)	C25—C26	1.379 (3)
C9—H9	0.9300	C25—H25	0.9300
C10—C11	1.460 (3)	C26—C27	1.380 (3)
C11—N4	1.356 (3)	C26—H26	0.9300
C11—C12	1.394 (4)	C27—C28	1.379 (3)
C12—N3	1.353 (3)	C27—O3	1.386 (2)
C13—N3	1.321 (4)	C28—H28	0.9300
C13—C14	1.380 (5)	Cu1—N1	2.0052 (18)
C13—H13	0.9300	Cu1—N2	2.0038 (18)
C14—N4	1.322 (4)	Cu1—O1	1.9279 (17)
C14—H14	0.9300	O1W—HW11	0.81 (3)
C15—O2	1.222 (3)	O1W—HW12	0.89 (4)
C15—O1	1.271 (3)	Cu1—O5^{i}	1.9165 (17)
C15—C16	1.501 (3)		
N1—C1—C2	122.1 (2)	C19—C18—C17	118.8 (2)
N1—C1—H1	118.9	C19—C18—H18	120.6
C2—C1—H1	118.9	C17—C18—H18	120.6
C3—C2—C1	119.3 (2)	C20—C19—C18	120.8 (2)
C3—C2—H2	120.3	C20—C19—O3	115.8 (2)
C1—C2—H2	120.3	C18—C19—O3	123.1 (2)
C2—C3—C4	119.3 (2)	C19—C20—C21	119.9 (2)
C2—C3—H3	120.3	C19—C20—H20	120.1
C4—C3—H3	120.3	C21—C20—H20	120.1
C5—C4—C3	117.7 (2)	C20—C21—C16	120.2 (2)
C5—C4—C12	117.9 (2)	C20—C21—H21	119.9
C3—C4—C12	124.4 (2)	C16—C21—H21	119.9
N1—C5—C4	122.7 (2)	C28—C22—C23	121.1 (2)
N1—C5—C6	116.26 (18)	C28—C22—H22	119.5
C4—C5—C6	121.07 (19)	C23—C22—H22	119.5
N2—C6—C10	122.3 (2)	C22—C23—C25	118.9 (2)
N2—C6—C5	116.04 (18)	C22—C23—C24	120.2 (2)
C10—C6—C5	121.66 (19)	C25—C23—C24	120.9 (2)
N2—C7—C8	121.5 (2)	O4—C24—O5	124.6 (2)
N2—C7—H7	119.2	O4—C24—C23	120.4 (2)
C8—C7—H7	119.2	O5—C24—C23	115.0 (2)
C9—C8—C7	120.2 (2)	C26—C25—C23	120.5 (2)
C9—C8—H8	119.9	C26—C25—H25	119.7
C7—C8—H8	119.9	C23—C25—H25	119.7
C8—C9—C10	119.0 (2)	C25—C26—C27	119.7 (2)
C8—C9—H9	120.5	C25—C26—H26	120.1
C10—C9—H9	120.5	C27—C26—H26	120.1
C6—C10—C9	117.7 (2)	C28—C27—C26	120.8 (2)
C6—C10—C11	117.6 (2)	C28—C27—O3	124.1 (2)
C9—C10—C11	124.6 (2)	C26—C27—O3	114.9 (2)

N4—C11—C12	121.4 (2)	C27—C28—C22	119.0 (2)
N4—C11—C10	117.8 (2)	C27—C28—H28	120.5
C12—C11—C10	120.71 (19)	C22—C28—H28	120.5
N3—C12—C11	121.6 (2)	C1—N1—C5	118.86 (18)
N3—C12—C4	117.4 (2)	C1—N1—Cu1	128.39 (15)
C11—C12—C4	121.01 (19)	C5—N1—Cu1	112.75 (14)
N3—C13—C14	123.1 (2)	C7—N2—C6	119.19 (18)
N3—C13—H13	118.5	C7—N2—Cu1	127.99 (15)
C14—C13—H13	118.5	C6—N2—Cu1	112.81 (14)
N4—C14—C13	122.5 (2)	C13—N3—C12	115.6 (3)
N4—C14—H14	118.7	C14—N4—C11	115.8 (3)
C13—C14—H14	118.7	C15—O1—Cu1	110.98 (16)
O2—C15—O1	124.0 (2)	HW11—O1W—HW12	111 (3)
O2—C15—C16	119.8 (3)	C27—O3—C19	121.76 (18)
O1—C15—C16	116.2 (2)	C24—O5—Cu1^{ii}	112.20 (15)
C17—C16—C21	119.2 (2)	O5^{i}—Cu1—O1	90.49 (8)
C17—C16—C15	120.5 (2)	O5^{i}—Cu1—N2	175.81 (7)
C21—C16—C15	120.3 (2)	O1—Cu1—N2	93.69 (8)
C16—C17—C18	121.0 (2)	O5^{i}—Cu1—N1	93.75 (8)
C16—C17—H17	119.5	O1—Cu1—N1	175.61 (7)
C18—C17—H17	119.5	N2—Cu1—N1	82.06 (7)

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*
O1W—HW11···O2	0.81 (3)	2.22 (5)	2.808 (3)	129 (4)

Fig. 1

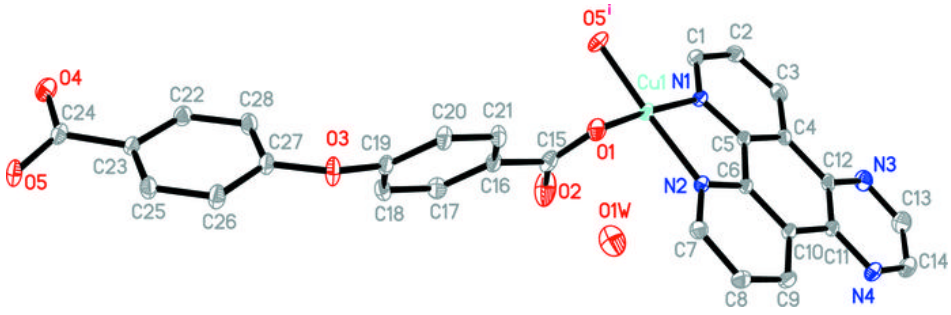
O5i
C1
C2
O4
C22
C28
Cu1
N1
C3
C24
C20
C21
C4
C27
O3
C19
C15
O1
C5
C12
N3
O5
C23
C6
N2
C13
C25
C26
C18
C17
C16
O2
O1W
C7
C10
C11
C14
C8
C9
N4

Fig. 2

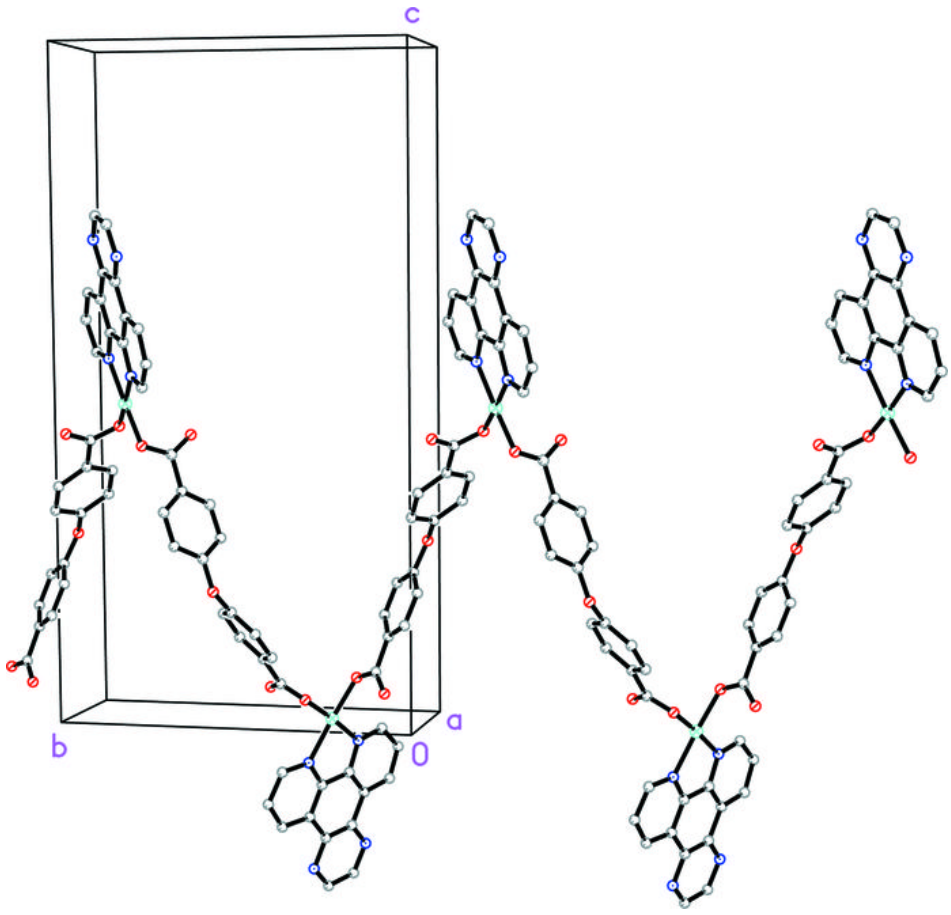

Fig. 3