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Bis(μ-biphenyl-2,2′-dicarboxylato)-bis[(2,2′-bipyridine)copper(II)] tetrahydrate

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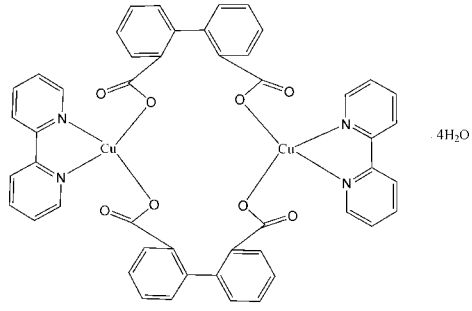
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.058; wR factor = 0.132; data-to-parameter ratio = 11.9.

The title compound, $[Cu_2(C_{14}H_8O_4)_2(C_{10}H_8N_2)_2]\cdot 4H_2O$, contains a centrosymmetric binuclear copper(II) complex, with Cu···Cu = 5.6865 (16) Å. The Cu atom displays a *cis*-CuN_2O_2 square-planar geometry, although two long (>2.6 Å) Cu···O contacts complete a distorted *cis*-CuN_2O_4 octahedron. The crystal packing is consolidated by O—H···O hydrogen bonds to form infinite chains. One water molecule is disordered over two sites, with occupancy factors of *ca* 0.7 and 0.3.

Related literature

For related literature, see: He & Zhu (2003); Wang *et al.* (2006); Zhu *et al.* (2001).



Experimental

Crystal data

$[Cu_2(C_{14}H_8O_4)_2(C_{10}H_8N_2)_2]\cdot 4H_2O$
M_r = 991.92
Monoclinic, $P2_1/n$
a = 11.428 (3) Å
b = 9.816 (2) Å
c = 19.774 (4) Å
β = 97.098 (4)°
V = 2201.2 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 293 (2) K
0.19 × 0.12 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.827, T_{max} = 0.980
15487 measured reflections
3875 independent reflections
2635 reflections with $I > 2\sigma(I)$
R_{int} = 0.091

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.132
S = 1.02
3875 reflections
326 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O4^{i}	1.953 (3)	Cu1—N2	1.984 (3)
Cu1—O1	1.955 (3)	Cu1—N1	1.989 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O2^{ii}	0.85 (5)	2.29 (7)	3.009 (5)	144 (6)
O5—H5B···O1	0.86 (3)	2.11 (3)	2.932 (4)	160 (8)
O6—H6A···O5^{iii}	0.85 (6)	2.06 (5)	2.903 (8)	171 (7)
O6—H6B···O3	0.86 (5)	2.01 (5)	2.849 (7)	167 (9)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2407).

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supplementary materials

Acta Cryst. (2007). E**63**, m2007 [**doi:10.1107/S1600536807030747**]

Bis(μ-biphenyl-2,2'-dicarboxylato)bis[(2,2'-bipyridine)copper(II)] tetrahydrate

H.-Y. He, Y.-L. Zhou and J. Gao

Comment

Binuclear copper(II) complexes have been intensely investigated owing to their potential application as magnetic materials and catalysts (Zhu *et al.*, 2001). Here we present the synthesis and crystal structure of the title compound, (I), $[Cu_2(dpa)_2(bipy)_2]\cdot 4H_2O$ (dpa = the diphenyl-2,2'dicarboxylato dianion and bipy = 2,2'-bipyridine), which contains a centrosymmetric binuclear complex. The copper(II) atom adopts a distorted square geometry (Table 1, Fig. 1). The bipy ligand shows its classical bidentate coordination mode, albeit with a shorter mean Cu—N bond length than in the related complex $[Cu_2(C_2O_4)(C_{12}H_8N_2)_2(C_3H_7NO)_2](ClO_4)_2$ (Wang *et al.*, 2006). The dpa ligand adopts a μ_2-bridged coordination and the dihedral angle between its aromatic rings is 86.7 (2)°. As well as the short Cu—O bonds, two long (> 2.60 Å) Cu—O contacts that might be regarded as secondary bonds (He & Zhu, 2003) complete a distorted octahedron. The Cu···Cu^{i} (i = $1-x$, $1-y$, $1-z$) distance bridged by the dpa ligands is 5.6865 (16) Å.

The complex (I) is extended into one dimensional framework by O—H···O hydrogen bonds (Table 2, Fig.2).

Experimental

0.0705 g (0.3 mmol) $Cu(NO_3)_2\cdot 6H_2O$, 0.0734 g diphenyl-2,2'-dicarboxyl acid) and 0.0473 g 2,2'-bipyridine were dissolved in 20 ml water, to obtain a blue solution. After about two weeks at room temperature, blue plates of (I) were obtained and filtered off.

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 map and refined with a distance restraint of O—H = 0.85 (1) Å and the constraint $U_{iso}(H) = 1.5U_{eq}(O)$. Due to the disorder of the water molecules the location of their H atoms should be regarded as less certain.

Figures

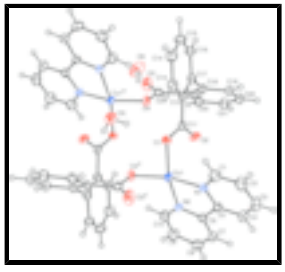

Fig. 1. View of the molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms).

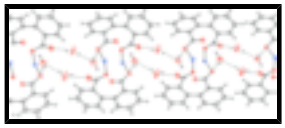

Fig. 2. The one dimensional chain in (I) formed by O—H···O hydrogen bongs. Displacement ellipsoids are drawn at the 30% probability level. The bipy ligands are omitted for clarity.

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Crystal data

$[Cu_2(C_{14}H_8O_4)_2(C_{10}H_8N_2)_2]\cdot 4H_2O$	$F_{000} = 1020$
$M_r = 991.92$	$D_x = 1.496$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 15487 reflections
$a = 11.428$ (3) Å	$\theta = 2.0$–25º
$b = 9.816$ (2) Å	$\mu = 1.04$ mm^{-1}
$c = 19.774$ (4) Å	$T = 293$ (2) K
$\beta = 97.098$ (4)º	Plate, blue
$V = 2201.2$ (9) Å^3	0.19 × 0.12 × 0.02 mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	3875 independent reflections
Radiation source: fine-focus sealed tube	2635 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.091$
$T = 293(2)$ K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -13\rightarrow13$
$T_{min} = 0.827$, $T_{max} = 0.980$	$k = -11\rightarrow11$
15487 measured reflections	$l = -23\rightarrow23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.058$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.132$	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
3875 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
326 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
O3	−0.1297 (3)	−0.3198 (3)	−0.11357 (19)	0.0617 (10)	
C24	−0.0584 (4)	−0.2244 (4)	−0.1138 (2)	0.0349 (11)	
O4	−0.0740 (2)	−0.1116 (3)	−0.08590 (14)	0.0358 (7)	
O5	−0.1362 (3)	0.2058 (4)	−0.02708 (18)	0.0670 (11)	
O6	−0.2335 (5)	−0.5841 (6)	−0.1210 (4)	0.095 (3)	0.703 (7)
O6'	−0.1884 (17)	−0.515 (2)	−0.0306 (11)	0.192 (11)	0.297 (7)
H6A	−0.201 (8)	−0.639 (4)	−0.091 (3)	0.288*	0.703 (7)
H6B	−0.204 (8)	−0.505 (3)	−0.112 (5)	0.288*	0.703 (7)
H6B'	−0.202 (6)	−0.53 (3)	−0.073 (3)	0.288*	0.297 (7)
H6A'	−0.114 (3)	−0.51 (3)	−0.020 (5)	0.288*	0.297 (7)
H5B	−0.066 (2)	0.223 (9)	−0.036 (3)	0.288*	
H5A	−0.132 (6)	0.170 (8)	0.012 (2)	0.288*	
Cu1	0.21213 (4)	0.14650 (5)	0.03932 (2)	0.03214 (16)	
O2	0.2010 (2)	0.0042 (3)	−0.07275 (14)	0.0422 (8)	
O1	0.1142 (2)	0.1934 (3)	−0.04561 (14)	0.0377 (7)	
N2	0.3250 (3)	0.0462 (3)	0.10571 (16)	0.0343 (9)	
N1	0.3617 (3)	0.2201 (3)	0.01224 (16)	0.0332 (9)	
C18	0.1004 (3)	−0.1420 (4)	−0.1838 (2)	0.0314 (10)	
C11	0.1296 (3)	0.0982 (4)	−0.0884 (2)	0.0290 (10)	
C5	0.4607 (3)	0.1641 (4)	0.0449 (2)	0.0334 (10)	
C12	0.0576 (3)	0.1050 (4)	−0.15634 (19)	0.0305 (10)	
C17	0.0412 (3)	−0.0076 (4)	−0.1992 (2)	0.0329 (10)	
C23	0.0521 (3)	−0.2448 (4)	−0.1464 (2)	0.0308 (10)	
C6	0.4389 (3)	0.0638 (4)	0.0973 (2)	0.0322 (10)	
C8	0.4958 (4)	−0.0963 (5)	0.1854 (2)	0.0536 (14)	
H8	0.5538	−0.1442	0.2127	0.064*	
C16	−0.0338 (4)	0.0043 (5)	−0.2599 (2)	0.0385 (11)	
H16	−0.0467	−0.0713	−0.2882	0.046*	
C22	0.1106 (4)	−0.3689 (5)	−0.1356 (2)	0.0427 (12)	
H22	0.0785	−0.4369	−0.1107	0.051*	
C13	0.0006 (4)	0.2268 (4)	−0.1761 (2)	0.0375 (11)	
H13	0.0111	0.3026	−0.1479	0.045*	
C15	−0.0894 (4)	0.1248 (5)	−0.2792 (2)	0.0487 (13)	

H15	−0.1387	0.1307	−0.3202	0.058*
C7	0.5268 (4)	−0.0085 (5)	0.1364 (2)	0.0441 (12)
H7	0.6054	0.0023	0.1297	0.053*
C19	0.2051 (4)	−0.1712 (4)	−0.2100 (2)	0.0408 (12)
H19	0.2373	−0.1056	−0.2362	0.049*
C2	0.4777 (4)	0.3556 (5)	−0.0524 (3)	0.0559 (14)
H2	0.4817	0.4218	−0.0857	0.067*
C20	0.2626 (4)	−0.2930 (5)	−0.1986 (2)	0.0496 (13)
H20	0.3333	−0.3082	−0.2162	0.060*
C10	0.2967 (4)	−0.0408 (4)	0.1524 (2)	0.0430 (12)
H10	0.2174	−0.0530	0.1572	0.052*
C4	0.5699 (4)	0.2020 (5)	0.0290 (2)	0.0472 (13)
H4	0.6378	0.1623	0.0515	0.057*
C14	−0.0716 (4)	0.2355 (5)	−0.2377 (2)	0.0460 (13)
H14	−0.1082	0.3176	−0.2508	0.055*
C1	0.3707 (4)	0.3143 (5)	−0.0355 (2)	0.0507 (13)
H1	0.3024	0.3529	−0.0579	0.061*
C21	0.2161 (4)	−0.3922 (5)	−0.1615 (2)	0.0492 (13)
H21	0.2550	−0.4750	−0.1536	0.059*
C3	0.5780 (4)	0.2990 (5)	−0.0201 (3)	0.0576 (15)
H3	0.6513	0.3257	−0.0313	0.069*
C9	0.3793 (4)	−0.1136 (5)	0.1939 (2)	0.0520 (14)
H9	0.3571	−0.1728	0.2267	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.057 (2)	0.043 (2)	0.090 (3)	−0.0187 (17)	0.0289 (19)	−0.0131 (18)
C24	0.036 (2)	0.038 (3)	0.029 (2)	−0.002 (2)	−0.0003 (19)	0.008 (2)
O4	0.0300 (15)	0.0339 (17)	0.0458 (18)	−0.0023 (13)	0.0140 (14)	−0.0038 (14)
O5	0.050 (2)	0.088 (3)	0.063 (2)	0.015 (2)	0.0054 (18)	0.009 (2)
O6	0.071 (4)	0.060 (4)	0.151 (7)	−0.010 (3)	−0.005 (4)	0.038 (4)
O6'	0.24 (2)	0.095 (15)	0.28 (3)	0.015 (15)	0.16 (2)	0.057 (16)
Cu1	0.0225 (3)	0.0413 (3)	0.0322 (3)	0.0016 (2)	0.0020 (2)	0.0023 (3)
O2	0.0353 (17)	0.0431 (18)	0.0443 (19)	0.0077 (14)	−0.0101 (14)	−0.0023 (15)
O1	0.0327 (16)	0.0478 (19)	0.0311 (16)	0.0110 (14)	−0.0023 (13)	−0.0057 (14)
N2	0.0287 (19)	0.044 (2)	0.030 (2)	−0.0011 (16)	0.0006 (15)	0.0037 (17)
N1	0.034 (2)	0.036 (2)	0.029 (2)	−0.0029 (16)	0.0020 (16)	0.0042 (16)
C18	0.031 (2)	0.034 (2)	0.029 (2)	−0.0021 (19)	0.0016 (18)	−0.004 (2)
C11	0.021 (2)	0.032 (2)	0.034 (2)	−0.0012 (18)	0.0039 (18)	0.003 (2)
C5	0.026 (2)	0.036 (3)	0.038 (3)	0.0020 (19)	0.0039 (19)	−0.010 (2)
C12	0.027 (2)	0.038 (3)	0.026 (2)	−0.0052 (18)	0.0019 (17)	0.0020 (19)
C17	0.029 (2)	0.038 (3)	0.033 (2)	−0.0057 (19)	0.0098 (19)	0.004 (2)
C23	0.030 (2)	0.036 (3)	0.027 (2)	−0.0016 (19)	0.0031 (19)	−0.0040 (19)
C6	0.028 (2)	0.036 (2)	0.032 (2)	0.0040 (19)	0.0007 (18)	−0.006 (2)
C8	0.051 (3)	0.058 (3)	0.047 (3)	0.010 (2)	−0.011 (2)	0.011 (3)
C16	0.037 (3)	0.045 (3)	0.033 (3)	−0.002 (2)	−0.001 (2)	0.002 (2)
C22	0.047 (3)	0.041 (3)	0.040 (3)	0.003 (2)	0.006 (2)	−0.003 (2)

C13	0.040 (3)	0.035 (3)	0.038 (3)	−0.001 (2)	0.007 (2)	0.007 (2)
C15	0.042 (3)	0.064 (3)	0.036 (3)	−0.002 (2)	−0.008 (2)	0.012 (2)
C7	0.033 (3)	0.058 (3)	0.040 (3)	0.003 (2)	−0.001 (2)	0.000 (2)
C19	0.035 (2)	0.047 (3)	0.041 (3)	0.000 (2)	0.008 (2)	0.000 (2)
C2	0.061 (3)	0.051 (3)	0.058 (3)	−0.011 (3)	0.019 (3)	0.016 (3)
C20	0.036 (3)	0.066 (3)	0.049 (3)	0.009 (2)	0.012 (2)	−0.007 (3)
C10	0.038 (3)	0.043 (3)	0.048 (3)	−0.002 (2)	0.008 (2)	0.003 (2)
C4	0.032 (3)	0.052 (3)	0.057 (3)	0.000 (2)	0.007 (2)	0.000 (3)
C14	0.045 (3)	0.045 (3)	0.048 (3)	0.008 (2)	0.002 (2)	0.015 (2)
C1	0.048 (3)	0.053 (3)	0.051 (3)	−0.003 (2)	0.008 (2)	0.014 (3)
C21	0.050 (3)	0.046 (3)	0.051 (3)	0.018 (2)	0.003 (2)	−0.006 (2)
C3	0.045 (3)	0.062 (3)	0.069 (4)	−0.005 (3)	0.023 (3)	0.002 (3)
C9	0.054 (3)	0.051 (3)	0.049 (3)	−0.001 (2)	0.000 (2)	0.019 (2)

Geometric parameters (Å, °)

O3—C24	1.242 (5)	C23—C22	1.394 (6)
C24—O4	1.260 (5)	C6—C7	1.385 (5)
C24—C23	1.500 (6)	C8—C9	1.372 (6)
C24—Cu1^{i}	2.545 (4)	C8—C7	1.375 (6)
O4—Cu1^{i}	1.953 (3)	C8—H8	0.9300
O5—H5B	0.855 (18)	C16—C15	1.375 (6)
O5—H5A	0.86 (2)	C16—H16	0.9300
O6—H6A	0.85 (2)	C22—C21	1.386 (6)
O6—H6B	0.86 (2)	C22—H22	0.9300
O6—H6B'	1.09 (8)	C13—C14	1.387 (6)
O6'—H6B'	0.85 (2)	C13—H13	0.9300
O6'—H6A'	0.85 (2)	C15—C14	1.361 (6)
Cu1—O4^{i}	1.953 (3)	C15—H15	0.9300
Cu1—O1	1.955 (3)	C7—H7	0.9300
Cu1—N2	1.984 (3)	C19—C20	1.369 (6)
Cu1—N1	1.989 (3)	C19—H19	0.9300
O2—C11	1.245 (4)	C2—C3	1.360 (6)
O1—C11	1.287 (5)	C2—C1	1.368 (6)
N2—C10	1.326 (5)	C2—H2	0.9300
N2—C6	1.343 (5)	C20—C21	1.366 (6)
N1—C1	1.334 (5)	C20—H20	0.9300
N1—C5	1.348 (5)	C10—C9	1.373 (6)
C18—C19	1.392 (5)	C10—H10	0.9300
C18—C23	1.404 (6)	C4—C3	1.371 (6)
C18—C17	1.496 (5)	C4—H4	0.9300
C11—C12	1.488 (5)	C14—H14	0.9300
C5—C4	1.376 (6)	C1—H1	0.9300
C5—C6	1.474 (6)	C21—H21	0.9300
C12—C17	1.391 (5)	C3—H3	0.9300
C12—C13	1.394 (6)	C9—H9	0.9300
C17—C16	1.392 (5)		
O3—C24—O4	122.2 (4)	C7—C6—C5	124.1 (4)

O3—C24—C23	119.2 (4)	C9—C8—C7	120.2 (4)
O4—C24—C23	118.5 (4)	C9—C8—H8	119.9
O3—C24—Cu1^{i}	74.0 (3)	C7—C8—H8	119.9
O4—C24—Cu1^{i}	48.49 (19)	C15—C16—C17	121.8 (4)
C23—C24—Cu1^{i}	165.1 (3)	C15—C16—H16	119.1
C24—O4—Cu1^{i}	102.6 (2)	C17—C16—H16	119.1
H5B—O5—H5A	109 (3)	C21—C22—C23	120.7 (4)
H6A—O6—H6B	108 (3)	C21—C22—H22	119.7
H6A—O6—H6B'	68 (10)	C23—C22—H22	119.7
H6B—O6—H6B'	48 (10)	C14—C13—C12	120.4 (4)
H6B'—O6'—H6A'	109 (4)	C14—C13—H13	119.8
O4^{i}—Cu1—O1	92.09 (12)	C12—C13—H13	119.8
O4^{i}—Cu1—N2	95.61 (13)	C14—C15—C16	119.3 (4)
O1—Cu1—N2	160.33 (13)	C14—C15—H15	120.3
O4^{i}—Cu1—N1	164.13 (13)	C16—C15—H15	120.3
O1—Cu1—N1	95.89 (12)	C8—C7—C6	118.8 (4)
N2—Cu1—N1	81.29 (13)	C8—C7—H7	120.6
O4^{i}—Cu1—C24^{i}	28.88 (12)	C6—C7—H7	120.6
O1—Cu1—C24^{i}	93.65 (12)	C20—C19—C18	122.4 (4)
N2—Cu1—C24^{i}	101.82 (13)	C20—C19—H19	118.8
N1—Cu1—C24^{i}	136.39 (14)	C18—C19—H19	118.8
C11—O1—Cu1	106.5 (2)	C3—C2—C1	119.4 (5)
C10—N2—C6	119.5 (4)	C3—C2—H2	120.3
C10—N2—Cu1	125.8 (3)	C1—C2—H2	120.3
C6—N2—Cu1	114.5 (3)	C21—C20—C19	120.0 (4)
C1—N1—C5	119.2 (4)	C21—C20—H20	120.0
C1—N1—Cu1	125.9 (3)	C19—C20—H20	120.0
C5—N1—Cu1	114.9 (3)	N2—C10—C9	122.8 (4)
C19—C18—C23	117.4 (4)	N2—C10—H10	118.6
C19—C18—C17	119.6 (4)	C9—C10—H10	118.6
C23—C18—C17	122.9 (4)	C3—C4—C5	119.4 (4)
O2—C11—O1	120.9 (4)	C3—C4—H4	120.3
O2—C11—C12	122.0 (4)	C5—C4—H4	120.3
O1—C11—C12	117.1 (3)	C15—C14—C13	120.6 (4)
N1—C5—C4	120.8 (4)	C15—C14—H14	119.7
N1—C5—C6	113.9 (3)	C13—C14—H14	119.7
C4—C5—C6	125.3 (4)	N1—C1—C2	121.9 (5)
C17—C12—C13	119.2 (4)	N1—C1—H1	119.1
C17—C12—C11	122.1 (4)	C2—C1—H1	119.1
C13—C12—C11	118.6 (4)	C20—C21—C22	119.7 (4)
C12—C17—C16	118.7 (4)	C20—C21—H21	120.2
C12—C17—C18	123.6 (4)	C22—C21—H21	120.2
C16—C17—C18	117.7 (4)	C2—C3—C4	119.3 (5)
C22—C23—C18	119.8 (4)	C2—C3—H3	120.3
C22—C23—C24	117.7 (4)	C4—C3—H3	120.3
C18—C23—C24	122.5 (4)	C8—C9—C10	117.9 (4)
N2—C6—C7	120.8 (4)	C8—C9—H9	121.1

N2—C6—C5	115.1 (3)	C10—C9—H9	121.1
O3—C24—O4—Cu1^{i}	7.1 (5)	C17—C18—C23—C24	−5.0 (6)
C23—C24—O4—Cu1^{i}	−170.9 (3)	O3—C24—C23—C22	−40.9 (6)
O4^{i}—Cu1—O1—C11	−111.8 (2)	O4—C24—C23—C22	137.2 (4)
N2—Cu1—O1—C11	1.4 (5)	Cu1^{i}—C24—C23—C22	109.9 (11)
N1—Cu1—O1—C11	81.9 (3)	O3—C24—C23—C18	142.3 (4)
C24^{i}—Cu1—O1—C11	−140.7 (3)	O4—C24—C23—C18	−39.6 (6)
O4^{i}—Cu1—N2—C10	15.1 (4)	Cu1^{i}—C24—C23—C18	−66.9 (12)
O1—Cu1—N2—C10	−97.5 (5)	C10—N2—C6—C7	0.5 (6)
N1—Cu1—N2—C10	179.4 (4)	Cu1—N2—C6—C7	−174.8 (3)
C24^{i}—Cu1—N2—C10	43.7 (4)	C10—N2—C6—C5	−179.2 (4)
O4^{i}—Cu1—N2—C6	−170.0 (3)	Cu1—N2—C6—C5	5.6 (5)
O1—Cu1—N2—C6	77.4 (5)	N1—C5—C6—N2	−1.6 (5)
N1—Cu1—N2—C6	−5.7 (3)	C4—C5—C6—N2	177.8 (4)
C24^{i}—Cu1—N2—C6	−141.4 (3)	N1—C5—C6—C7	178.8 (4)
O4^{i}—Cu1—N1—C1	−97.5 (6)	C4—C5—C6—C7	−1.8 (7)
O1—Cu1—N1—C1	22.3 (4)	C12—C17—C16—C15	1.6 (6)
N2—Cu1—N1—C1	−177.3 (4)	C18—C17—C16—C15	−178.2 (4)
C24^{i}—Cu1—N1—C1	−79.3 (4)	C18—C23—C22—C21	−0.1 (6)
O4^{i}—Cu1—N1—C5	84.6 (6)	C24—C23—C22—C21	−177.0 (4)
O1—Cu1—N1—C5	−155.6 (3)	C17—C12—C13—C14	0.1 (6)
N2—Cu1—N1—C5	4.8 (3)	C11—C12—C13—C14	−177.1 (4)
C24^{i}—Cu1—N1—C5	102.8 (3)	C17—C16—C15—C14	−0.5 (7)
Cu1—O1—C11—O2	−3.4 (4)	C9—C8—C7—C6	1.4 (7)
Cu1—O1—C11—C12	175.8 (3)	N2—C6—C7—C8	−1.6 (7)
C1—N1—C5—C4	−0.6 (6)	C5—C6—C7—C8	178.0 (4)
Cu1—N1—C5—C4	177.4 (3)	C23—C18—C19—C20	−2.0 (6)
C1—N1—C5—C6	178.8 (4)	C17—C18—C19—C20	−179.0 (4)
Cu1—N1—C5—C6	−3.2 (4)	C18—C19—C20—C21	1.3 (7)
O2—C11—C12—C17	17.5 (6)	C6—N2—C10—C9	0.9 (7)
O1—C11—C12—C17	−161.7 (4)	Cu1—N2—C10—C9	175.6 (3)
O2—C11—C12—C13	−165.4 (4)	N1—C5—C4—C3	0.6 (7)
O1—C11—C12—C13	15.3 (5)	C6—C5—C4—C3	−178.7 (4)
C13—C12—C17—C16	−1.4 (6)	C16—C15—C14—C13	−0.8 (7)
C11—C12—C17—C16	175.7 (4)	C12—C13—C14—C15	1.1 (7)
C13—C12—C17—C18	178.4 (4)	C5—N1—C1—C2	0.1 (7)
C11—C12—C17—C18	−4.5 (6)	Cu1—N1—C1—C2	−177.7 (4)
C19—C18—C17—C12	−94.7 (5)	C3—C2—C1—N1	0.4 (8)
C23—C18—C17—C12	88.5 (5)	C19—C20—C21—C22	0.1 (7)
C19—C18—C17—C16	85.1 (5)	C23—C22—C21—C20	−0.7 (7)
C23—C18—C17—C16	−91.8 (5)	C1—C2—C3—C4	−0.4 (8)
C19—C18—C23—C22	1.4 (6)	C5—C4—C3—C2	−0.1 (8)
C17—C18—C23—C22	178.3 (4)	C7—C8—C9—C10	−0.1 (7)
C19—C18—C23—C24	178.1 (4)	N2—C10—C9—C8	−1.1 (7)

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O2^{ii}	0.85 (5)	2.29 (7)	3.009 (5)	144 (6)
O5—H5B···O1	0.86 (3)	2.11 (3)	2.932 (4)	160 (8)
O6—H6A···O5^{iii}	0.85 (6)	2.06 (5)	2.903 (8)	171 (7)
O6—H6B···O3	0.86 (5)	2.01 (5)	2.849 (7)	167 (9)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) *x*, *y*−1, *z*.

Fig. 1

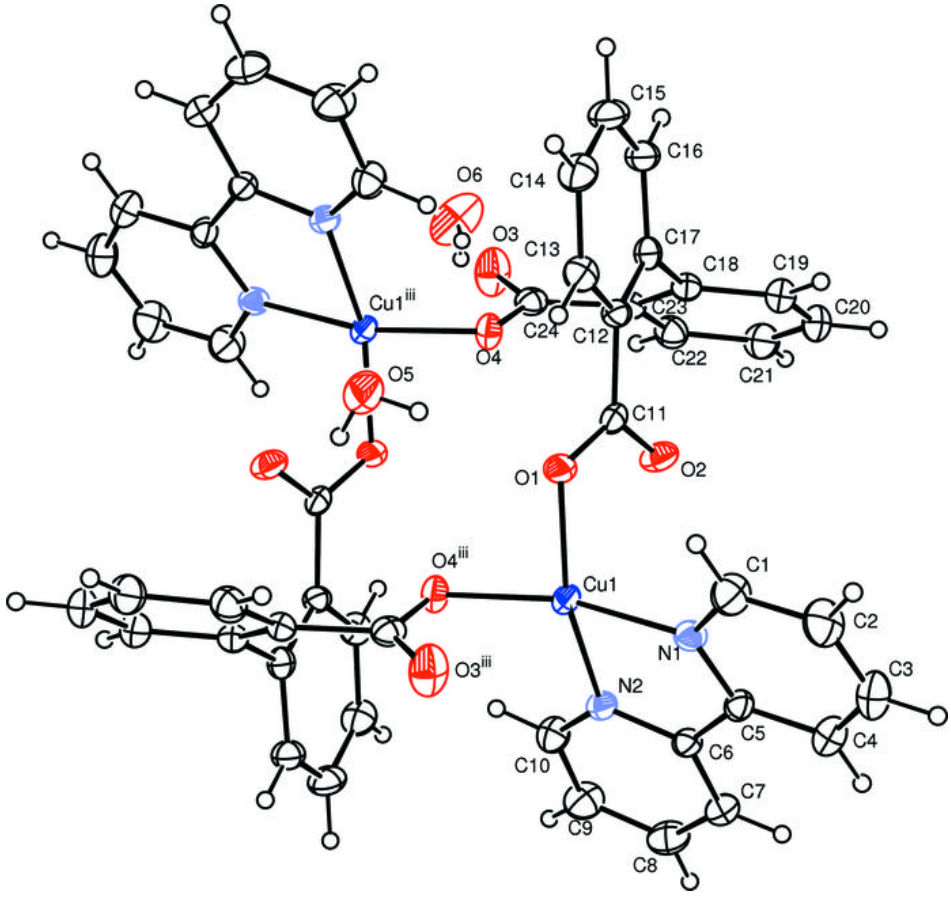
C15
C16
C14
O6
O3
C13
C17
C18
C19
Cu1iii
C23
C20
C24
C12
O4
C22
C21
O5
C11
O1
O2
O4iii
Cu1
C1
C2
N1
O3iii
N2
C3
C5
C4
C6
C10
C7
C9
C8

Fig. 2