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[5,5′-Dihydroxy-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato}-copper(II) methanol disolvate

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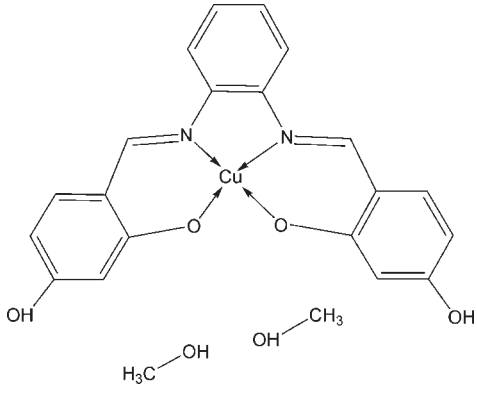
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 12.8.

In the title compound, $[Cu(C_{20}H_{14}N_2O_4)]\cdot 2CH_3OH$, the Cu^{II} ion is coordinated by two N [Cu—N = 1.933 (2) and 1.941 (2) Å] and two O [Cu—O = 1.890 (2) and 1.9038 (19) Å] atoms from the tetradentate Schiff base ligand 5,5′-dihydroxy-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenolate (*L*) in a distorted square-planar geometry. In the crystal, intermolecular O—H···O hydrogen bonds link two Cu*L* molecules and four solvent molecules into a centrosymmetric cluster. The crystal packing exhibits short intermolecular C···C contacts of 3.185 (4) and 3.232 (4) Å.

Related literature

For related structures, see: Amirnasr *et al.* (2006); Arola-Arnal *et al.* (2008); Sundaravel *et al.* (2009); Lu *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{20}H_{14}N_2O_4)]\cdot 2CH_4O$
M_r = 473.96
Triclinic, $P\overline{1}$
a = 7.9520 (17) Å
b = 11.066 (2) Å
c = 11.870 (2) Å
α = 91.796 (2)°
β = 94.604 (3)°
γ = 94.241 (3)°
V = 1037.6 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 293 K
0.53 × 0.48 × 0.21 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.595, T_{max} = 0.803
5360 measured reflections
3592 independent reflections
2873 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.00
3592 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O5^{i}	0.82	1.91	2.704 (3)	163
O4—H4···O6^{ii}	0.82	1.82	2.602 (4)	159
O5—H5···O4^{iii}	0.82	1.97	2.788 (3)	176
O6—H6···O1	0.82	2.18	2.777 (3)	130
O6—H6···O3	0.82	2.34	3.037 (4)	144

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+2, -y+2, -z+1$; (iii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2670).

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supplementary materials

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[5,5'-Dihydroxy-2,2'-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato}copper(II) methanol disolvate

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Comment

Copper complexes have attracted intensive interest in the past decade because they play important roles on the fields of coordination chemistry, bioinorganic chemistry, redox enzyme systems and others (Amirnasr *et al.*, 2006). In a continuation of a study of Schiff base ligands and their copper(II) complexes, we report here the title complex, (I).

In (I) (Fig. 1),the main plane being formed by the three phenyl and the N_2O_2. The angles O1—Cu1—N2 (178.64 (9)°) and O3—Cu1—N1 (178.39 (9)°) indicate that the coordination geometry of the copper atom is four-coordinate in an approximately square planar, which acts as a tetradentate ligand through its *o*-phenylenediamine N atoms and its deprotonated phenol O atoms. This square planar geometry is the most usual for Cu^{II} complexes (Arola-Arnal *et al.*, 2008) in the N_20_2 donor set with Schiff base ligands. The Cu—O distances of 1.9022 (19)Å and 1.889 (2)Å are very close to the corresponding values in related structures (1.904 (2)Å and 1.884 (3) Å; Sundaravel *et al.*, 2009). The Cu—N distances of 1.932 (2)Å and 1.942 (2)Å are very close to the corresponding values in related structures(1.946 (2) Å; Lu *et al.*, 2006). Intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into a centrosymmetric cluster.

Experimental

o-Phenylenediamine(1 mmol, 108.22 mg) was dissolved in hot ethanol (20 ml) and added dropwise to a ethanol solution (10 ml) of 2,4-dihydroxybenzaldehyde (2 mmol, 276.2 mg). The mixture was then stirred at 323 K for 4 h. The triethylamine solution (3 ml) of Copper (II) acetate (1.5 mmol, 299.5 mg) was then added dropwise and the mixture stirred for another 5 h, at which point a red precipitate collected by suction filtration and washed with ethanol and ether. Crystals of the title compound suitable for X-ray analysis were from the methanol and dimethylformamide solution after about two weeks.

Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms with C—H = 0.96 Å (methylene) or 0.93 Å (aromatic), 0.82 Å (hydroxyl) and U_{iso}(H) = 1.2-1.5U_{eq} of the parent atom.

Figures

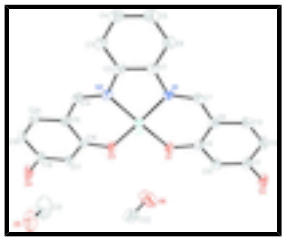


Fig. 1. The molecular structure of the title compound showing the atomic labels and 30% probability displacement ellipsoids.

[5,5'-Dihydroxy-2,2'-[*o*- phenylenebis(nitrilomethylidyne)]diphenolato}copper(II) methanol disolvate

Crystal data

$[Cu(C_{20}H_{14}N_2O_4)]\cdot 2CH_4O$	$Z = 2$
$M_r = 473.96$	$F(000) = 490$
Triclinic, $P\overline{1}$	$D_x = 1.517$ Mg m^{-3}
$a = 7.9520$ (17) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.066$ (2) Å	Cell parameters from 2490 reflections
$c = 11.870$ (2) Å	$\theta = 2.5$–$26.4°$
$\alpha = 91.796$ (2)°	$\mu = 1.10$ mm^{-1}
$\beta = 94.604$ (3)°	$T = 293$ K
$\gamma = 94.241$ (3)°	Block, red
$V = 1037.6$ (4) Å^3	0.53 × 0.48 × 0.21 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	3592 independent reflections
Radiation source: fine-focus sealed tube	2873 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.027$
phi and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -9\rightarrow9$
$T_{min} = 0.595$, $T_{max} = 0.803$	$k = -12\rightarrow13$
5360 measured reflections	$l = -14\rightarrow10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.099$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.5623P]$ where $P = (F_o^2 + 2F_c^2)/3$
3592 reflections	$(\Delta/\sigma)_{max} < 0.001$
280 parameters	$\Delta\rho_{max} = 0.46$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.36$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.84950 (4)	0.91865 (3)	0.07516 (3)	0.03348 (14)
N1	0.7711 (3)	0.9467 (2)	−0.07955 (19)	0.0322 (5)

N2	0.9482 (3)	0.7807 (2)	0.00880 (19)	0.0317 (5)
O1	0.7530 (2)	1.05584 (16)	0.13697 (16)	0.0356 (5)
O2	0.4653 (3)	1.41526 (18)	0.14493 (19)	0.0522 (6)
H2	0.4991	1.4142	0.2120	0.078*
O3	0.9320 (3)	0.89012 (18)	0.22501 (16)	0.0433 (5)
O4	1.2805 (4)	0.7377 (2)	0.52128 (19)	0.0724 (8)
H4	1.2474	0.7960	0.5551	0.109*
O5	0.6076 (4)	0.4576 (2)	0.3584 (2)	0.0780 (8)
H5	0.6454	0.4010	0.3927	0.117*
O6	0.7454 (6)	1.0573 (3)	0.3705 (3)	0.1286 (17)
H6	0.8050	1.0433	0.3191	0.193*
C1	0.8192 (4)	0.8588 (3)	−0.1582 (2)	0.0374 (7)
C2	0.9139 (4)	0.7681 (3)	−0.1106 (3)	0.0373 (7)
C3	0.9676 (4)	0.6789 (3)	−0.1807 (3)	0.0455 (8)
H3	1.0314	0.6191	−0.1498	0.055*
C4	0.9275 (5)	0.6780 (3)	−0.2961 (3)	0.0581 (9)
H4A	0.9624	0.6170	−0.3425	0.070*
C5	0.8358 (6)	0.7674 (3)	−0.3423 (3)	0.0670 (11)
H5A	0.8101	0.7672	−0.4201	0.080*
C6	0.7815 (5)	0.8574 (3)	−0.2742 (3)	0.0561 (9)
H6A	0.7193	0.9174	−0.3063	0.067*
C7	0.6728 (4)	1.0312 (3)	−0.1095 (2)	0.0351 (7)
H7	0.6340	1.0315	−0.1855	0.042*
C8	0.6194 (3)	1.1225 (2)	−0.0376 (2)	0.0318 (6)
C9	0.6652 (3)	1.1344 (2)	0.0815 (2)	0.0314 (6)
C10	0.6127 (4)	1.2337 (2)	0.1415 (3)	0.0366 (7)
H10	0.6430	1.2431	0.2188	0.044*
C11	0.5170 (4)	1.3183 (3)	0.0890 (3)	0.0378 (7)
C12	0.4682 (4)	1.3056 (3)	−0.0271 (3)	0.0436 (8)
H12	0.4022	1.3618	−0.0624	0.052*
C13	0.5181 (4)	1.2108 (3)	−0.0873 (3)	0.0395 (7)
H13	0.4849	1.2029	−0.1643	0.047*
C14	1.0398 (4)	0.7072 (2)	0.0662 (2)	0.0357 (7)
H14	1.0792	0.6432	0.0259	0.043*
C15	1.0849 (4)	0.7158 (2)	0.1845 (2)	0.0361 (7)
C16	1.0355 (4)	0.8091 (2)	0.2577 (2)	0.0356 (7)
C17	1.1031 (4)	0.8149 (3)	0.3713 (3)	0.0444 (8)
H17	1.0741	0.8761	0.4198	0.053*
C18	1.2108 (4)	0.7320 (3)	0.4118 (3)	0.0487 (8)
C19	1.2564 (4)	0.6381 (3)	0.3410 (3)	0.0500 (8)
H19	1.3279	0.5813	0.3690	0.060*
C20	1.1945 (4)	0.6318 (3)	0.2312 (3)	0.0438 (8)
H20	1.2253	0.5696	0.1844	0.053*
C21	0.7229 (7)	0.5589 (4)	0.3737 (5)	0.1056 (17)
H21A	0.7013	0.6045	0.4404	0.158*
H21B	0.7110	0.6087	0.3092	0.158*
H21C	0.8358	0.5332	0.3820	0.158*
C22	0.6689 (6)	0.9506 (5)	0.4033 (4)	0.0857 (14)
H22A	0.6713	0.9513	0.4843	0.129*

H22B	0.7282	0.8840	0.3772	0.129*
H22C	0.5537	0.9418	0.3714	0.129*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0365 (2)	0.0294 (2)	0.0349 (2)	0.00663 (14)	0.00252 (14)	−0.00080 (14)
N1	0.0339 (13)	0.0275 (12)	0.0353 (13)	0.0012 (10)	0.0054 (10)	−0.0027 (10)
N2	0.0280 (12)	0.0304 (12)	0.0360 (13)	−0.0005 (10)	0.0034 (10)	−0.0040 (10)
O1	0.0411 (11)	0.0303 (10)	0.0356 (11)	0.0106 (9)	−0.0022 (9)	0.0002 (8)
O2	0.0675 (15)	0.0326 (12)	0.0578 (14)	0.0219 (11)	−0.0016 (11)	−0.0014 (10)
O3	0.0554 (14)	0.0415 (12)	0.0356 (11)	0.0245 (10)	0.0028 (10)	−0.0013 (9)
O4	0.111 (2)	0.0646 (17)	0.0450 (14)	0.0490 (16)	−0.0096 (14)	0.0024 (12)
O5	0.113 (2)	0.0505 (16)	0.0681 (17)	0.0266 (16)	−0.0249 (16)	−0.0026 (13)
O6	0.272 (5)	0.072 (2)	0.0547 (19)	0.053 (3)	0.061 (3)	−0.0016 (16)
C1	0.0372 (16)	0.0361 (16)	0.0380 (17)	−0.0040 (13)	0.0053 (13)	−0.0033 (13)
C2	0.0354 (16)	0.0331 (15)	0.0423 (17)	−0.0042 (13)	0.0070 (13)	−0.0082 (13)
C3	0.0447 (19)	0.0407 (18)	0.050 (2)	0.0028 (14)	0.0047 (15)	−0.0109 (15)
C4	0.073 (3)	0.051 (2)	0.051 (2)	0.0060 (18)	0.0110 (18)	−0.0194 (17)
C5	0.101 (3)	0.065 (2)	0.0360 (19)	0.018 (2)	0.0022 (19)	−0.0094 (17)
C6	0.080 (3)	0.050 (2)	0.0397 (19)	0.0174 (18)	0.0036 (17)	−0.0033 (16)
C7	0.0366 (16)	0.0346 (16)	0.0330 (16)	−0.0040 (13)	0.0020 (13)	0.0027 (13)
C8	0.0290 (15)	0.0286 (14)	0.0373 (16)	−0.0023 (12)	0.0026 (12)	0.0047 (12)
C9	0.0265 (14)	0.0266 (14)	0.0402 (16)	−0.0030 (11)	0.0006 (12)	0.0020 (12)
C10	0.0374 (17)	0.0301 (15)	0.0416 (17)	0.0024 (12)	−0.0008 (13)	0.0009 (13)
C11	0.0348 (16)	0.0283 (15)	0.0498 (18)	0.0011 (12)	0.0006 (14)	0.0046 (13)
C12	0.0433 (18)	0.0337 (16)	0.055 (2)	0.0091 (14)	0.0009 (15)	0.0154 (15)
C13	0.0403 (17)	0.0387 (17)	0.0388 (16)	−0.0007 (14)	−0.0011 (13)	0.0100 (14)
C14	0.0351 (16)	0.0257 (14)	0.0468 (18)	0.0017 (12)	0.0097 (13)	−0.0053 (13)
C15	0.0395 (17)	0.0271 (15)	0.0429 (17)	0.0043 (12)	0.0090 (13)	0.0015 (13)
C16	0.0384 (17)	0.0306 (15)	0.0394 (16)	0.0071 (13)	0.0079 (13)	0.0042 (13)
C17	0.058 (2)	0.0395 (17)	0.0384 (17)	0.0193 (15)	0.0086 (15)	0.0000 (14)
C18	0.060 (2)	0.0445 (18)	0.0445 (19)	0.0187 (16)	0.0029 (16)	0.0093 (15)
C19	0.062 (2)	0.0371 (17)	0.055 (2)	0.0244 (16)	0.0060 (17)	0.0118 (15)
C20	0.052 (2)	0.0307 (16)	0.0510 (19)	0.0140 (14)	0.0117 (16)	0.0022 (14)
C21	0.113 (4)	0.073 (3)	0.125 (4)	0.007 (3)	−0.021 (3)	−0.008 (3)
C22	0.093 (3)	0.116 (4)	0.055 (3)	0.039 (3)	0.016 (2)	0.007 (3)

Geometric parameters (Å, °)

Cu1—O3	1.890 (2)	C7—C8	1.412 (4)
Cu1—O1	1.9038 (19)	C7—H7	0.9300
Cu1—N1	1.933 (2)	C8—C13	1.425 (4)
Cu1—N2	1.941 (2)	C8—C9	1.430 (4)
N1—C7	1.303 (4)	C9—C10	1.398 (4)
N1—C1	1.421 (4)	C10—C11	1.382 (4)
N2—C14	1.303 (3)	C10—H10	0.9300
N2—C2	1.422 (4)	C11—C12	1.401 (4)
O1—C9	1.315 (3)	C12—C13	1.352 (4)

O2—C11	1.351 (4)	C12—H12	0.9300
O2—H2	0.8200	C13—H13	0.9300
O3—C16	1.308 (3)	C14—C15	1.420 (4)
O4—C18	1.368 (4)	C14—H14	0.9300
O4—H4	0.8200	C15—C20	1.416 (4)
O5—C21	1.392 (5)	C15—C16	1.426 (4)
O5—H5	0.8200	C16—C17	1.408 (4)
O6—C22	1.369 (6)	C17—C18	1.373 (4)
O6—H6	0.8200	C17—H17	0.9300
C1—C6	1.385 (4)	C18—C19	1.402 (4)
C1—C2	1.405 (4)	C19—C20	1.354 (5)
C2—C3	1.385 (4)	C19—H19	0.9300
C3—C4	1.381 (5)	C20—H20	0.9300
C3—H3	0.9300	C21—H21A	0.9600
C4—C5	1.374 (5)	C21—H21B	0.9600
C4—H4A	0.9300	C21—H21C	0.9600
C5—C6	1.378 (5)	C22—H22A	0.9600
C5—H5A	0.9300	C22—H22B	0.9600
C6—H6A	0.9300	C22—H22C	0.9600
C7···C9^{i}	3.185 (4)	C8···C14^{ii}	3.232 (4)
O3—Cu1—O1	86.42 (8)	C11—C10—C9	121.7 (3)
O3—Cu1—N1	178.39 (9)	C11—C10—H10	119.2
O1—Cu1—N1	94.78 (9)	C9—C10—H10	119.2
O3—Cu1—N2	94.77 (9)	O2—C11—C10	122.8 (3)
O1—Cu1—N2	178.65 (9)	O2—C11—C12	116.9 (3)
N1—Cu1—N2	84.02 (9)	C10—C11—C12	120.3 (3)
C7—N1—C1	122.4 (2)	C13—C12—C11	119.2 (3)
C7—N1—Cu1	124.2 (2)	C13—C12—H12	120.4
C1—N1—Cu1	113.23 (18)	C11—C12—H12	120.4
C14—N2—C2	122.5 (2)	C12—C13—C8	122.7 (3)
C14—N2—Cu1	124.2 (2)	C12—C13—H13	118.7
C2—N2—Cu1	113.32 (18)	C8—C13—H13	118.7
C9—O1—Cu1	127.17 (18)	N2—C14—C15	126.1 (3)
C11—O2—H2	109.5	N2—C14—H14	117.0
C16—O3—Cu1	127.11 (18)	C15—C14—H14	117.0
C18—O4—H4	109.5	C20—C15—C14	118.0 (3)
C21—O5—H5	109.5	C20—C15—C16	118.1 (3)
C22—O6—H6	109.5	C14—C15—C16	123.7 (3)
C6—C1—C2	119.5 (3)	O3—C16—C17	118.3 (3)
C6—C1—N1	125.5 (3)	O3—C16—C15	123.7 (3)
C2—C1—N1	115.1 (2)	C17—C16—C15	118.1 (3)
C3—C2—C1	119.2 (3)	C18—C17—C16	121.4 (3)
C3—C2—N2	126.4 (3)	C18—C17—H17	119.3
C1—C2—N2	114.4 (2)	C16—C17—H17	119.3
C4—C3—C2	120.7 (3)	O4—C18—C17	122.2 (3)
C4—C3—H3	119.7	O4—C18—C19	117.1 (3)
C2—C3—H3	119.7	C17—C18—C19	120.7 (3)
C5—C4—C3	119.8 (3)	C20—C19—C18	118.8 (3)

C5—C4—H4A	120.1	C20—C19—H19	120.6
C3—C4—H4A	120.1	C18—C19—H19	120.6
C4—C5—C6	120.5 (3)	C19—C20—C15	122.8 (3)
C4—C5—H5A	119.7	C19—C20—H20	118.6
C6—C5—H5A	119.7	C15—C20—H20	118.6
C5—C6—C1	120.3 (3)	O5—C21—H21A	109.5
C5—C6—H6A	119.9	O5—C21—H21B	109.5
C1—C6—H6A	119.9	H21A—C21—H21B	109.5
N1—C7—C8	126.3 (3)	O5—C21—H21C	109.5
N1—C7—H7	116.9	H21A—C21—H21C	109.5
C8—C7—H7	116.9	H21B—C21—H21C	109.5
C7—C8—C13	118.0 (3)	O6—C22—H22A	109.5
C7—C8—C9	124.3 (3)	O6—C22—H22B	109.5
C13—C8—C9	117.7 (3)	H22A—C22—H22B	109.5
O1—C9—C10	118.7 (3)	O6—C22—H22C	109.5
O1—C9—C8	123.0 (3)	H22A—C22—H22C	109.5
C10—C9—C8	118.4 (2)	H22B—C22—H22C	109.5
O3—Cu1—N1—C7	−144 (3)	Cu1—N1—C7—C8	6.1 (4)
O1—Cu1—N1—C7	−5.2 (2)	N1—C7—C8—C13	177.0 (3)
N2—Cu1—N1—C7	175.4 (2)	N1—C7—C8—C9	−0.8 (4)
O3—Cu1—N1—C1	42 (3)	Cu1—O1—C9—C10	−176.41 (18)
O1—Cu1—N1—C1	−179.98 (18)	Cu1—O1—C9—C8	4.1 (4)
N2—Cu1—N1—C1	0.65 (18)	C7—C8—C9—O1	−4.7 (4)
O3—Cu1—N2—C14	−1.3 (2)	C13—C8—C9—O1	177.5 (2)
O1—Cu1—N2—C14	150 (4)	C7—C8—C9—C10	175.8 (3)
N1—Cu1—N2—C14	177.7 (2)	C13—C8—C9—C10	−2.0 (4)
O3—Cu1—N2—C2	179.91 (18)	O1—C9—C10—C11	−178.6 (2)
O1—Cu1—N2—C2	−28 (4)	C8—C9—C10—C11	0.9 (4)
N1—Cu1—N2—C2	−1.15 (18)	C9—C10—C11—O2	−179.7 (3)
O3—Cu1—O1—C9	179.2 (2)	C9—C10—C11—C12	0.7 (4)
N1—Cu1—O1—C9	0.3 (2)	O2—C11—C12—C13	179.3 (3)
N2—Cu1—O1—C9	27 (4)	C10—C11—C12—C13	−1.0 (4)
O1—Cu1—O3—C16	−172.9 (2)	C11—C12—C13—C8	−0.2 (5)
N1—Cu1—O3—C16	−34 (3)	C7—C8—C13—C12	−176.3 (3)
N2—Cu1—O3—C16	6.5 (2)	C9—C8—C13—C12	1.7 (4)
C7—N1—C1—C6	5.7 (5)	C2—N2—C14—C15	177.7 (3)
Cu1—N1—C1—C6	−179.4 (3)	Cu1—N2—C14—C15	−1.1 (4)
C7—N1—C1—C2	−174.9 (2)	N2—C14—C15—C20	−176.1 (3)
Cu1—N1—C1—C2	0.0 (3)	N2—C14—C15—C16	−0.5 (5)
C6—C1—C2—C3	−0.1 (4)	Cu1—O3—C16—C17	170.0 (2)
N1—C1—C2—C3	−179.5 (2)	Cu1—O3—C16—C15	−9.4 (4)
C6—C1—C2—N2	178.5 (3)	C20—C15—C16—O3	−178.4 (3)
N1—C1—C2—N2	−0.9 (4)	C14—C15—C16—O3	6.0 (5)
C14—N2—C2—C3	1.0 (4)	C20—C15—C16—C17	2.1 (4)
Cu1—N2—C2—C3	179.9 (2)	C14—C15—C16—C17	−173.5 (3)
C14—N2—C2—C1	−177.4 (2)	O3—C16—C17—C18	179.2 (3)
Cu1—N2—C2—C1	1.4 (3)	C15—C16—C17—C18	−1.3 (5)
C1—C2—C3—C4	−0.7 (5)	C16—C17—C18—O4	178.6 (3)
N2—C2—C3—C4	−179.0 (3)	C16—C17—C18—C19	−0.3 (5)

C2—C3—C4—C5	1.1 (5)	O4—C18—C19—C20	−177.8 (3)
C3—C4—C5—C6	−0.9 (6)	C17—C18—C19—C20	1.1 (5)
C4—C5—C6—C1	0.1 (6)	C18—C19—C20—C15	−0.2 (5)
C2—C1—C6—C5	0.3 (5)	C14—C15—C20—C19	174.4 (3)
N1—C1—C6—C5	179.7 (3)	C16—C15—C20—C19	−1.4 (5)
C1—N1—C7—C8	−179.6 (2)		

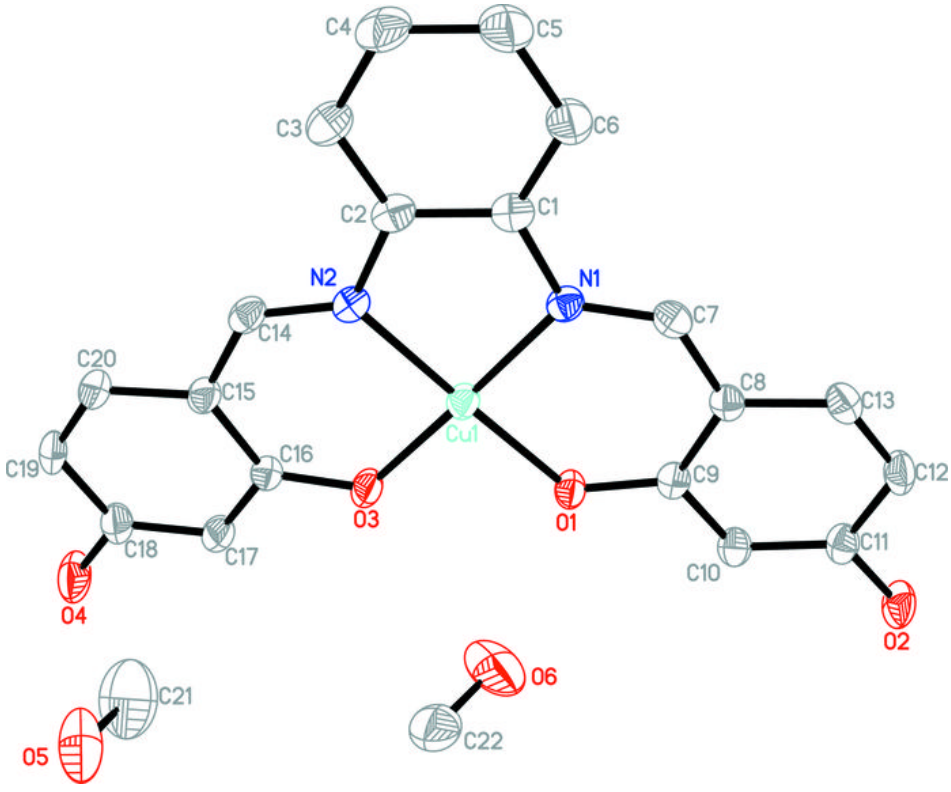
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*; (ii) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O5^{iii}	0.82	1.91	2.704 (3)	163
O4—H4···O6^{iv}	0.82	1.82	2.602 (4)	159
O5—H5···O4^{v}	0.82	1.97	2.788 (3)	176
O6—H6···O1	0.82	2.18	2.777 (3)	130
O6—H6···O3	0.82	2.34	3.037 (4)	144

Symmetry codes: (iii) *x*, *y*+1, *z*; (iv) −*x*+2, −*y*+2, −*z*+1; (v) −*x*+2, −*y*+1, −*z*+1.

Fig. 1


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