

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

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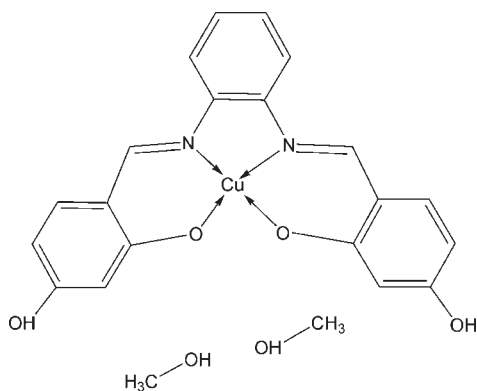
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 12.8.

In the title compound, $[\text{Cu}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_4)] \cdot 2\text{CH}_3\text{OH}$, the Cu^{II} ion is coordinated by two N [$\text{Cu}-\text{N} = 1.933(2)$ and $1.941(2)$ Å] and two O [$\text{Cu}-\text{O} = 1.890(2)$ 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 $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds link two CuL molecules and four solvent molecules into a centrosymmetric cluster. The crystal packing exhibits short intermolecular $\text{C} \cdots \text{C}$ 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

$[\text{Cu}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_4)] \cdot 2\text{CH}_4\text{O}$	$\gamma = 94.241(3)^\circ$
$M_r = 473.96$	$V = 1037.6(4)$ Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.9520(17)$ Å	Mo $K\alpha$ radiation
$b = 11.066(2)$ Å	$\mu = 1.10$ mm ⁻¹
$c = 11.870(2)$ Å	$T = 293$ K
$\alpha = 91.796(2)^\circ$	$0.53 \times 0.48 \times 0.21$ mm
$\beta = 94.604(3)^\circ$	

Data collection

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

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O}2-\text{H}2 \cdots \text{O}5^{\text{i}}$	0.82	1.91	2.704 (3)	163
$\text{O}4-\text{H}4 \cdots \text{O}6^{\text{ii}}$	0.82	1.82	2.602 (4)	159
$\text{O}5-\text{H}5 \cdots \text{O}4^{\text{iii}}$	0.82	1.97	2.788 (3)	176
$\text{O}6-\text{H}6 \cdots \text{O}1$	0.82	2.18	2.777 (3)	130
$\text{O}6-\text{H}6 \cdots \text{O}3$	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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supporting information

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S1. 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 N₂O₂. 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 N₂O₂ 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.

S2. 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.

S3. 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 $U_{\text{iso}}(\text{H}) = 1.2-1.5U_{\text{eq}}$ of the parent atom.

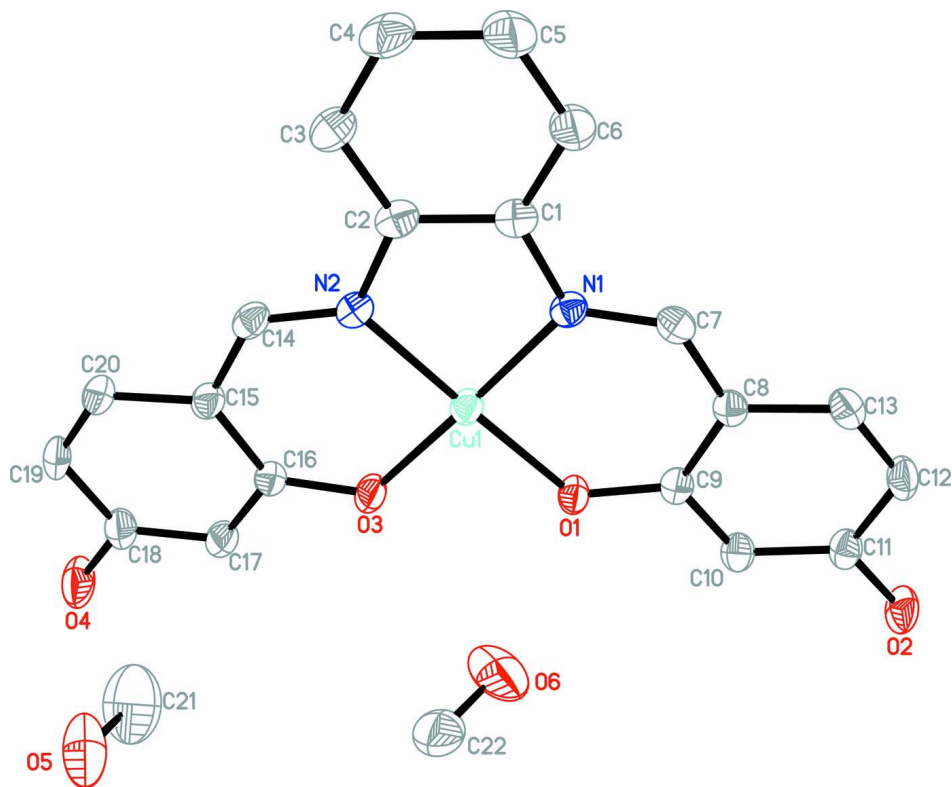


Figure 1

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(C₂₀H₁₄N₂O₄)]·2CH₄O

M_r = 473.96

Triclinic, *P*1̄

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) Å³

Z = 2

F(000) = 490

D_x = 1.517 Mg m⁻³

Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 2490 reflections

θ = 2.5–26.4°

μ = 1.10 mm⁻¹

T = 293 K

Block, red

0.53 × 0.48 × 0.21 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and *ω* scans

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* > 2σ(*I*)

R_{int} = 0.027

θ_{max} = 25.0°, *θ_{min}* = 1.7°

h = -9→9

k = -12→13

l = -14→10

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.099$

$S = 1.00$

3592 reflections

280 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.5623P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (Å²)

	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 ($\text{\AA}, ^\circ$)

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

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