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

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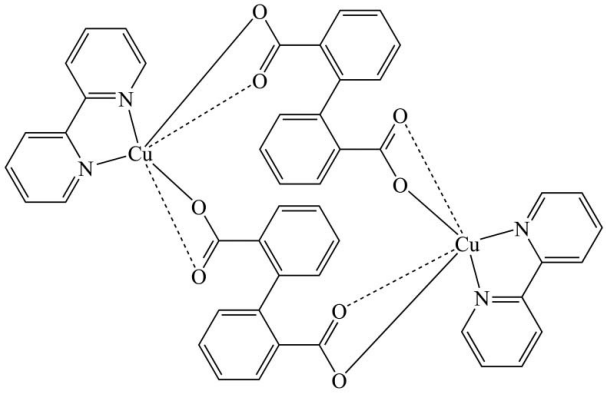
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.088; data-to-parameter ratio = 13.0.

The title compound, $[Cu_2(C_{14}H_8O_4)_2(C_{10}H_8N_2)_2]$, was obtained by solvothermal synthesis. The Cu^{II} atom is coordinated by one chelating 2,2′-bipyridine ligand and two carboxyl groups from different biphenyl-2,2′-dicarboxylate ligands, leading to a distorted octahedral environment. Each carboxylate group makes one short Cu—O bond [1.9608 (14) and 1.9701 (14) Å] and one longer Cu—O contact [2.4338 (17) and 2.5541 (17) Å] to each Cu^{II} atom. The biphenyl-2,2′-dicarboxylate ligands bridge between Cu^{II} atoms, forming a dinuclear complex around a crystallographic inversion centre.

Related literature

For complexes of biphenyl-2,2′-dicarboxylic acid, a good candidate for the construction of metal–organic frameworks, see: Rueff *et al.* (2003); Xu *et al.* (2006); An & Niu (2008).



Experimental

Crystal data

$[Cu_2(C_{14}H_8O_4)_2(C_{10}H_8N_2)_2]$
M_r = 919.86
Monoclinic, $P2_1/n$
a = 11.220 (2) Å
b = 13.350 (3) Å
c = 13.400 (3) Å
β = 103.02 (3)°
V = 1955.5 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 296 K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.874, T_{max} = 0.913
10453 measured reflections
3644 independent reflections
3099 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.088
S = 1.00
3644 reflections
280 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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: BI2358).

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supporting information

Acta Cryst. (2009). E**65**, m412 [doi:10.1107/S1600536809008976]

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

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S1. Comment

Biphenyl-2,2′-dicarboxylic acid (H_2dpa) has been demonstrated to be a good candidate for the construction of metal-organic frameworks, and some complexes based on 2,2′-dpa have been reported (Rueff *et al.*, 2003; Xu *et al.*, 2006; An & Niu, 2008). In this paper, we report a new metal complex constructed from dpa, 2,2-bipyridine and copper(II) (Figure 1).

S2. Experimental

A mixture of $Cu(CH_3COO)_2.H_2O$ (1 mmol), biphenyl-2,2′-dicarboxylic acid (1 mmol), and 2,2′-bipyridine (1 mmol) in 20 ml methanol/water (1:1) were placed in a 25 ml Teflon-lined stainless steel autoclave and kept at 453 K for five days. Blue crystals were obtained after cooling to room temperature.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

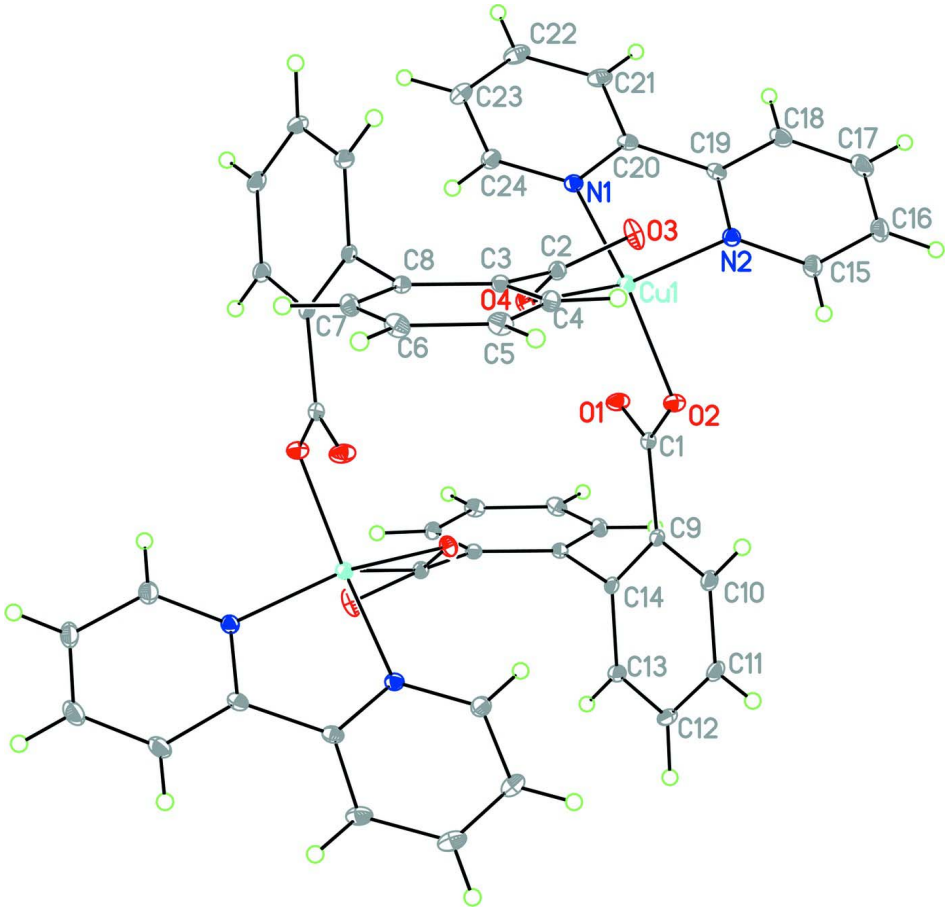

Figure 1

Molecular structure drawn with 30% probability displacement ellipsoids for the non-H atoms. Unlabelled atoms are related to labelled atoms by the symmetry code 1 - *x*, 1 - *y*, 1 - *z*.

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$[Cu_2(C_{14}H_8O_4)_2(C_{10}H_8N_2)_2]$
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Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.220$ (2) Å
$b = 13.350$ (3) Å
$c = 13.400$ (3) Å
$\beta = 103.02$ (3)°
$V = 1955.5$ (7) Å^3
$Z = 2$
$F(000) = 940$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3644 reflections
$\theta = 2.1$–25.5°
$\mu = 1.15$ mm^{-1}
$T = 296$ K
Block, blue
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.874$, $T_{max} = 0.913$
10453 measured reflections
3644 independent reflections

3099 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.1°$
$h = -13 \rightarrow 13$
$k = -16 \rightarrow 10$
$l = -16 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.088$
$S = 1.00$
3644 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 not refined
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.1P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.031$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.52301 (18)	0.68894 (15)	0.42300 (15)	0.0295 (4)
C2	0.28746 (17)	0.57752 (15)	0.60591 (15)	0.0293 (4)
C3	0.30695 (16)	0.51522 (15)	0.70154 (14)	0.0270 (4)
C4	0.33117 (18)	0.56634 (16)	0.79532 (15)	0.0341 (5)
H4	0.3274	0.6359	0.7960	0.041*
C5	0.36046 (19)	0.51453 (18)	0.88649 (15)	0.0393 (5)
H5	0.3786	0.5489	0.9484	0.047*
C6	0.3627 (2)	0.41049 (18)	0.88508 (16)	0.0404 (5)
H6	0.3821	0.3752	0.9464	0.048*
C7	0.33624 (19)	0.35926 (16)	0.79356 (16)	0.0344 (5)
H7	0.3370	0.2896	0.7939	0.041*
C8	0.30828 (16)	0.41025 (15)	0.70031 (14)	0.0268 (4)
C9	0.66065 (16)	0.69929 (14)	0.45025 (14)	0.0270 (4)
C10	0.71452 (18)	0.75479 (16)	0.53682 (16)	0.0358 (5)
H10	0.6646	0.7884	0.5725	0.043*
C11	0.83990 (19)	0.76120 (16)	0.57103 (17)	0.0388 (5)
H11	0.8741	0.7992	0.6285	0.047*
C12	0.91368 (18)	0.71022 (17)	0.51856 (17)	0.0393 (5)
H12	0.9983	0.7130	0.5410	0.047*
C13	0.86141 (19)	0.65506 (15)	0.43273 (17)	0.0339 (5)
H13	0.9120	0.6208	0.3982	0.041*
C14	0.73499 (18)	0.64916 (13)	0.39621 (15)	0.0270 (4)

C15	0.2751 (2)	0.87802 (18)	0.39294 (19)	0.0426 (5)
H15	0.3426	0.8868	0.4470	0.051*
C16	0.2221 (2)	0.96089 (18)	0.3405 (2)	0.0522 (7)
H16	0.2509	1.0248	0.3605	0.063*
C17	0.1257 (2)	0.9477 (2)	0.2579 (2)	0.0557 (7)
H17	0.0896	1.0026	0.2202	0.067*
C18	0.0830 (2)	0.85266 (19)	0.2316 (2)	0.0463 (6)
H18	0.0188	0.8425	0.1751	0.056*
C19	0.13647 (18)	0.77206 (16)	0.29011 (15)	0.0320 (5)
C20	0.09346 (18)	0.66758 (16)	0.27505 (16)	0.0322 (5)
C21	−0.0050 (2)	0.6365 (2)	0.19990 (18)	0.0442 (6)
H21	−0.0477	0.6818	0.1522	0.053*
C22	−0.0390 (2)	0.5368 (2)	0.19696 (18)	0.0511 (7)
H22	−0.1050	0.5145	0.1468	0.061*
C23	0.0242 (2)	0.4706 (2)	0.26769 (19)	0.0481 (6)
H23	0.0014	0.4036	0.2664	0.058*
C24	0.1223 (2)	0.50567 (17)	0.34091 (17)	0.0390 (5)
H24	0.1658	0.4612	0.3890	0.047*
Cu1	0.30127 (2)	0.660694 (17)	0.440302 (17)	0.033 (2)
N1	0.15643 (14)	0.60194 (13)	0.34444 (12)	0.0304 (4)
N2	0.23357 (15)	0.78535 (13)	0.36946 (12)	0.0309 (4)
O1	0.46909 (13)	0.65650 (12)	0.33944 (13)	0.0462 (4)
O2	0.46709 (12)	0.71453 (11)	0.49257 (10)	0.0356 (3)
O3	0.23951 (18)	0.66102 (11)	0.60315 (13)	0.0510 (5)
O4	0.32843 (13)	0.54377 (10)	0.53117 (10)	0.0336 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0289 (10)	0.0228 (10)	0.0359 (11)	−0.0009 (8)	0.0052 (9)	−0.0015 (8)
C2	0.0303 (10)	0.0261 (11)	0.0293 (10)	−0.0008 (9)	0.0020 (8)	−0.0012 (8)
C3	0.0237 (9)	0.0287 (11)	0.0276 (10)	0.0006 (8)	0.0037 (8)	−0.0014 (8)
C4	0.0347 (11)	0.0317 (11)	0.0353 (11)	−0.0009 (9)	0.0066 (9)	−0.0056 (9)
C5	0.0389 (12)	0.0508 (14)	0.0255 (11)	0.0029 (10)	0.0017 (9)	−0.0075 (9)
C6	0.0429 (12)	0.0495 (14)	0.0281 (11)	0.0081 (11)	0.0064 (9)	0.0077 (10)
C7	0.0384 (12)	0.0307 (11)	0.0345 (12)	0.0044 (9)	0.0092 (9)	0.0057 (9)
C8	0.0242 (9)	0.0282 (11)	0.0285 (10)	0.0001 (8)	0.0070 (8)	0.0000 (8)
C9	0.0272 (10)	0.0219 (10)	0.0306 (10)	−0.0026 (8)	0.0037 (8)	−0.0006 (8)
C10	0.0384 (12)	0.0289 (11)	0.0410 (12)	−0.0041 (9)	0.0112 (10)	−0.0089 (9)
C11	0.0411 (12)	0.0324 (12)	0.0389 (12)	−0.0111 (10)	0.0006 (10)	−0.0098 (9)
C12	0.0273 (10)	0.0399 (13)	0.0474 (13)	−0.0093 (9)	0.0017 (9)	−0.0005 (10)
C13	0.0294 (11)	0.0344 (12)	0.0386 (12)	−0.0011 (9)	0.0094 (9)	−0.0025 (9)
C14	0.0285 (10)	0.0207 (10)	0.0302 (11)	−0.0030 (8)	0.0035 (8)	0.0037 (8)
C15	0.0469 (13)	0.0349 (13)	0.0462 (13)	0.0000 (11)	0.0107 (11)	0.0032 (10)
C16	0.0572 (16)	0.0295 (13)	0.0745 (18)	0.0032 (11)	0.0246 (14)	0.0086 (12)
C17	0.0516 (15)	0.0475 (16)	0.0698 (18)	0.0163 (12)	0.0177 (13)	0.0268 (13)
C18	0.0385 (13)	0.0495 (16)	0.0488 (15)	0.0134 (11)	0.0053 (11)	0.0158 (11)
C19	0.0284 (10)	0.0400 (12)	0.0292 (10)	0.0078 (9)	0.0095 (8)	0.0072 (9)

C20	0.0260 (10)	0.0433 (13)	0.0281 (11)	0.0036 (9)	0.0077 (8)	0.0052 (9)
C21	0.0310 (11)	0.0635 (17)	0.0344 (12)	−0.0044 (11)	−0.0006 (9)	0.0078 (11)
C22	0.0376 (13)	0.0725 (19)	0.0395 (14)	−0.0156 (12)	0.0010 (11)	−0.0042 (12)
C23	0.0442 (13)	0.0493 (15)	0.0501 (15)	−0.0174 (11)	0.0089 (11)	−0.0039 (12)
C24	0.0381 (11)	0.0380 (13)	0.0391 (12)	−0.0041 (10)	0.0051 (10)	0.0015 (10)
Cu1	0.045 (5)	0.025 (4)	0.028 (4)	−0.004 (4)	0.002 (4)	0.002 (3)
N1	0.0279 (8)	0.0338 (10)	0.0284 (9)	−0.0003 (7)	0.0042 (7)	0.0018 (7)
N2	0.0308 (9)	0.0305 (10)	0.0315 (9)	0.0017 (7)	0.0069 (7)	0.0038 (7)
O1	0.0303 (8)	0.0595 (11)	0.0457 (10)	−0.0038 (7)	0.0022 (7)	−0.0248 (8)
O2	0.0284 (7)	0.0461 (10)	0.0318 (8)	−0.0007 (6)	0.0058 (6)	−0.0052 (6)
O3	0.0790 (13)	0.0343 (10)	0.0429 (10)	0.0232 (8)	0.0207 (9)	0.0070 (7)
O4	0.0423 (8)	0.0315 (8)	0.0269 (7)	0.0067 (6)	0.0078 (6)	0.0043 (6)

Geometric parameters (Å, º)

Cu1—O1	2.5541 (17)	C11—H11	0.930
Cu1—O2	1.9701 (14)	C12—C13	1.380 (3)
Cu1—O3	2.4338 (17)	C12—H12	0.930
Cu1—O4	1.9608 (14)	C13—C14	1.395 (3)
Cu1—N1	1.9914 (17)	C13—H13	0.930
Cu1—N2	1.9806 (17)	C14—C8^{i}	1.502 (3)
C1—O1	1.226 (2)	C15—N2	1.334 (3)
C1—O2	1.282 (2)	C15—C16	1.372 (3)
C1—C9	1.511 (3)	C15—H15	0.930
C2—O3	1.235 (2)	C16—C17	1.373 (4)
C2—O4	1.275 (2)	C16—H16	0.930
C2—C3	1.502 (3)	C17—C18	1.374 (4)
C3—C8	1.402 (3)	C17—H17	0.930
C3—C4	1.402 (3)	C18—C19	1.386 (3)
C4—C5	1.378 (3)	C18—H18	0.930
C4—H4	0.930	C19—N2	1.352 (3)
C5—C6	1.389 (3)	C19—C20	1.475 (3)
C5—H5	0.930	C20—N1	1.355 (3)
C6—C7	1.377 (3)	C20—C21	1.381 (3)
C6—H6	0.930	C21—C22	1.383 (4)
C7—C8	1.395 (3)	C21—H21	0.930
C7—H7	0.930	C22—C23	1.370 (4)
C8—C14^{i}	1.502 (3)	C22—H22	0.930
C9—C14	1.393 (3)	C23—C24	1.381 (3)
C9—C10	1.394 (3)	C23—H23	0.9300
C10—C11	1.381 (3)	C24—N1	1.339 (3)
C10—H10	0.930	C24—H24	0.930
C11—C12	1.380 (3)		
O1—C1—O2	122.48 (18)	C17—C16—H16	120.6
O1—C1—C9	121.35 (18)	C15—C16—H16	120.6
O2—C1—C9	116.17 (17)	C16—C17—C18	119.4 (2)
O3—C2—O4	121.83 (18)	C16—C17—H17	120.3

O3—C2—C3	120.29 (18)	C18—C17—H17	120.3
O4—C2—C3	117.75 (17)	C19—C18—C17	119.4 (2)
C8—C3—C4	119.79 (18)	C19—C18—H18	120.3
C8—C3—C2	122.93 (17)	C17—C18—H18	120.3
C4—C3—C2	117.19 (18)	N2—C19—C18	120.8 (2)
C5—C4—C3	120.7 (2)	N2—C19—C20	114.37 (17)
C5—C4—H4	119.7	C18—C19—C20	124.8 (2)
C3—C4—H4	119.7	N1—C20—C21	121.0 (2)
C4—C5—C6	119.4 (2)	N1—C20—C19	114.45 (18)
C4—C5—H5	120.3	C21—C20—C19	124.6 (2)
C6—C5—H5	120.3	C20—C21—C22	118.7 (2)
C7—C6—C5	120.52 (19)	C20—C21—H21	120.7
C7—C6—H6	119.7	C22—C21—H21	120.7
C5—C6—H6	119.7	C23—C22—C21	120.3 (2)
C6—C7—C8	121.0 (2)	C23—C22—H22	119.9
C6—C7—H7	119.5	C21—C22—H22	119.9
C8—C7—H7	119.5	C22—C23—C24	118.6 (2)
C7—C8—C3	118.56 (18)	C22—C23—H23	120.7
C7—C8—C14^{i}	118.53 (18)	C24—C23—H23	120.7
C3—C8—C14^{i}	122.41 (17)	N1—C24—C23	121.8 (2)
C14—C9—C10	119.32 (18)	N1—C24—H24	119.1
C14—C9—C1	121.98 (17)	C23—C24—H24	119.1
C10—C9—C1	118.52 (17)	O4—Cu1—O2	93.87 (6)
C11—C10—C9	121.83 (19)	O4—Cu1—N2	162.88 (6)
C11—C10—H10	119.1	O2—Cu1—N2	95.36 (7)
C9—C10—H10	119.1	O4—Cu1—N1	94.42 (7)
C12—C11—C10	118.92 (19)	O2—Cu1—N1	160.23 (6)
C12—C11—H11	120.5	N2—Cu1—N1	81.52 (7)
C10—C11—H11	120.5	O4—Cu1—O3	58.70 (5)
C11—C12—C13	119.77 (19)	O2—Cu1—O3	96.74 (7)
C11—C12—H12	120.1	N2—Cu1—O3	105.80 (6)
C13—C12—H12	120.1	N1—Cu1—O3	102.90 (7)
C14—C13—C12	122.0 (2)	C24—N1—C20	119.72 (18)
C14—C13—H13	119.0	C24—N1—Cu1	125.89 (14)
C12—C13—H13	119.0	C20—N1—Cu1	114.30 (14)
C13—C14—C9	118.12 (18)	C15—N2—C19	118.94 (18)
C13—C14—C8^{i}	115.98 (17)	C15—N2—Cu1	126.17 (15)
C9—C14—C8^{i}	125.89 (17)	C19—N2—Cu1	114.89 (14)
N2—C15—C16	122.6 (2)	C1—O2—Cu1	102.82 (12)
N2—C15—H15	118.7	C2—O3—Cu1	79.35 (12)
C16—C15—H15	118.7	C2—O4—Cu1	99.98 (12)
C17—C16—C15	118.8 (2)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.