Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-methyl-1*H*-imidazole-κN^3)bis[2-(naphthalen-2-yl)acetato-κO]copper(II)

Fu-Jun Yin,[a]* Li-Jun Han,[b] Shu-Ping Yang[c] and Xing You Xu[d]

[a]Jiangsu Marine Resources Development Research Institute, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [b]Department of Mathematics and Science, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [c]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, and [d]Huaiyin Insititute of Technology, Huaiyin 223003, People's Republic of China
Correspondence e-mail: yfj1999@126.com

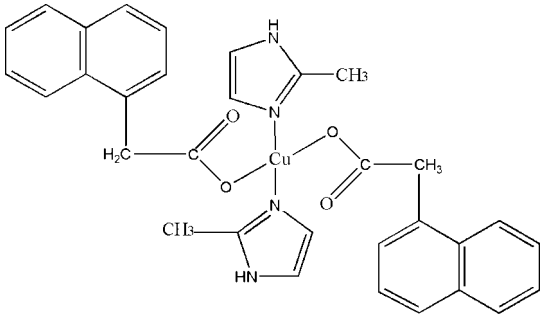
Received 8 November 2011; accepted 11 November 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.090; data-to-parameter ratio = 13.3.

In the crystal structure of the title compound, $[Cu(C_{12}H_9O_2)_2(C_4H_6N_2)_2]$, the Cu(II) cations are square-planar coordinated by two 1-naphthylacetate anions and two 2-methyl-imidazole ligands into discrete complexes that are located on centres of inversion. These complexes are linked into chains parallel to [010] by intermolecular N—H···O hydrogen bonding between the N—H H atom of the 2-methyl-imidazole ligands and the carboxylate O atoms that are not involved in metal coordination.

Related literature

For related structures, see: Liu *et al.* (2007); Chen *et al.* (2004); Yang *et al.* (2008); Tang *et al.* (2006); Ji *et al.* (2011).



Experimental

Crystal data

$[Cu(C_{12}H_9O_2)_2(C_4H_6N_2)_2]$
M_r = 598.14
Monoclinic, $C2/c$
a = 28.430 (4) Å
b = 7.5544 (10) Å
c = 13.9417 (19) Å
β = 108.216 (2)°
V = 2844.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 298 K
0.12 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.866, T_{max} = 0.903
10438 measured reflections
2507 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
S = 1.05
2507 reflections
188 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	1.97	2.775 (3)	155

Symmetry code: (i) $-x+1, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2255).

References

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, L.-F., Zhang, J., Song, L.-J., Wang, W.-G. & Ju, Z.-F. (2004). *Acta Cryst.* E**60**, m1032–m1034.
Ji, L.-L., Liu, J.-S. & Song, W.-D. (2011). *Acta Cryst.* E**67**, m606.
Liu, Y.-F., Xia, H.-T., Wang, D.-Q., Yang, S.-P. & Meng, Y.-L. (2007). *Acta Cryst.* E**63**, m2544.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tang, D.-X., Feng, L.-X. & Zhang, X.-Q. (2006). *Chin. J. Inorg. Chem.* **22**, 1891–1894.
Yang, Y.-Q., Li, C.-H. L. W. & Kuang, Y.-F. (2008). *Chin. J. Struct. Chem.* **30**, 4524–4530.

supporting information

Acta Cryst. (2011). E**67**, m1772 [https://doi.org/10.1107/S1600536811047969]

Bis(2-methyl-1*H*-imidazole-κN^3)bis[2-(naphthalen-2-yl)acetato-κO]copper(II)

Fu-Jun Yin, Li-Jun Han, Shu-Ping Yang and Xing You Xu

S1. Comment

The crystal structure of the title compound was determined as part of an ongoing study on the structural properties of copper complexes containing imidazole ligands. In this study 1-naphthylacetate was used as ligand, for which only a few metal complexes were reported (Liu *et al.*,2007; Chen *et al.*, 2004; Yang *et al.*, 2008; Tang *et al.*,2006 ; Ji *et al.*,2011).

In the crystal structure of the title compound $[Cu(C_{12}H_9O_2)_2(C_4H_6N_2)_2]$, each copper cation are coordinated by two N atoms of two symmetry equivalent 2-methyl-1*H*-imidazole ligands and by two carboxyl O atoms of two symmetry related 1-naphthylacetate anions within a square planar coordination (Fig. 1). The Cu—N and Cu—O bond lengths are 1.9750 (18) and 1.9791 (16) Å, respectively. The asymmetric unit consits of one Cu(II) cation that is located on a center of inversion as well of one neutral and one anionic ligand in general positions. The discrete complexes are linked into chains by N—H···O hydrogen bonding (Fig. 2 and Table 1).

S2. Experimental

The title compound was synthesized by the reaction of $Cu(NO_3)_2.3\ H_2O$ (72.3 mg, 0.3 mmol), 1-naphthylacetic acid (93 mg, 0.5 mmol), 2-methylimidazole (32.8 mg, 0.4 mmol) and NaOH (20 mg, 0.5 mmol) in 4 mL of a water-ethanol mixture (volume ratio = 1:1 of water:ethanol) under solvothermal conditions. The starting mixture was homogenized and transferred into a sealed teflon-lined solvothermal bomb (volume: 25 ml) and heated at 140° for three days. After cooling green crystals of the title compound were obtained, which were washed with distilled water and absolute ethyl alcohol (yield: 44.6% based on $Cu(NO_3)_2.3\ H_2O$).

S3. Refinement

The C-H H atoms were positioned with idealized geometry (methyl H atoms allowed to rotatae but not to tip) and were refined with U_{iso}(H) =1.2U_{eq}(C)] (1.5 for methyl H atoms) using a riding model.

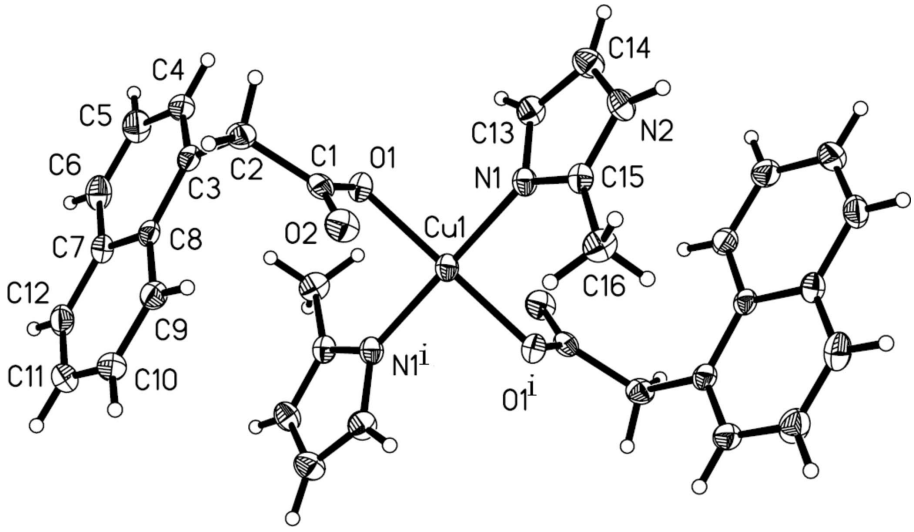


Figure 1

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 30% probability level. Symmetry code: i= -*x* + 1, -*y*, -*z* + 2)

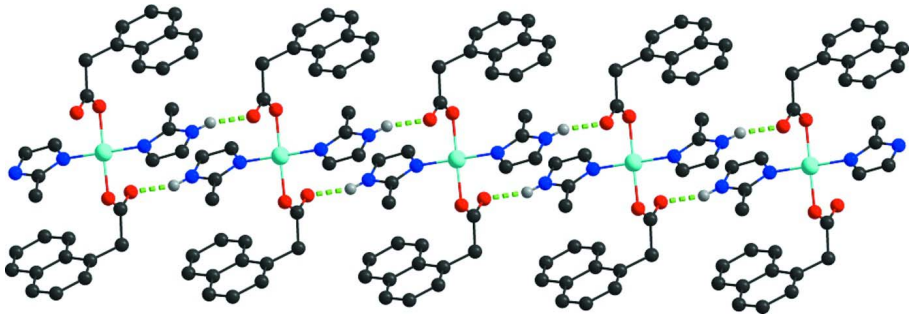


Figure 2

Part of the crystal structure of the title compound. Hydrogen bonding is shown as dashed lines and H atoms not involved in hydrogen bonding are omitted for clarity.

Bis(2-methyl-1*H*-imidazole-κN^3)bis[2-(naphthalen-1- yl)acetato-κO]copper(II)

Crystal data

$[Cu(C_{12}H_9O_2)_2(C_4H_6N_2)_2]$
M_r = 598.14
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 28.430 (4) Å
b = 7.5544 (10) Å
c = 13.9417 (19) Å
β = 108.216 (2)°
V = 2844.2 (7) Å^3
Z = 4
F(000) = 1244
D_x = 1.397 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2712 reflections
θ = 2.8–22.8°
μ = 0.81 mm^{-1}
T = 298 K
Block, green
0.12 × 0.10 × 0.10 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, 1996)
T_{min} = 0.866, T_{max} = 0.903
10438 measured reflections
2507 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.0°, θ_{min} = 2.8°
h = −33→33
k = −8→8
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
S = 1.05
2507 reflections
188 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
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 2.2367P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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	0.41432 (9)	0.1140 (3)	0.87770 (18)	0.0393 (5)
C2	0.36810 (9)	0.1271 (3)	0.78610 (19)	0.0444 (6)
H2A	0.3421	0.1850	0.8059	0.053*
H2B	0.3754	0.2004	0.7354	0.053*
C3	0.34946 (8)	−0.0505 (3)	0.74014 (17)	0.0387 (5)
C4	0.35305 (9)	−0.0972 (4)	0.64815 (18)	0.0488 (6)
H4	0.3677	−0.0190	0.6144	0.059*
C5	0.33521 (10)	−0.2605 (4)	0.6031 (2)	0.0586 (7)
H5	0.3384	−0.2895	0.5406	0.070*
C6	0.31340 (10)	−0.3760 (4)	0.6506 (2)	0.0553 (7)
H6	0.3011	−0.4829	0.6198	0.066*
C7	0.30908 (8)	−0.3357 (3)	0.74649 (18)	0.0414 (6)
C8	0.32775 (8)	−0.1709 (3)	0.79265 (16)	0.0356 (5)
C9	0.32324 (9)	−0.1349 (3)	0.88921 (18)	0.0442 (6)
H9	0.3357	−0.0293	0.9216	0.053*
C10	0.30110 (10)	−0.2521 (4)	0.9353 (2)	0.0561 (7)

H10	0.2985	−0.2253	0.9985	0.067*
C11	0.28210 (10)	−0.4129 (4)	0.8889 (2)	0.0587 (7)
H11	0.2666	−0.4911	0.9208	0.070*
C12	0.28645 (9)	−0.4541 (4)	0.7972 (2)	0.0521 (7)
H12	0.2743	−0.5618	0.7673	0.062*
C13	0.54765 (9)	0.2344 (3)	0.88513 (18)	0.0453 (6)
H13	0.5409	0.1555	0.8313	0.054*
C14	0.57019 (10)	0.3915 (3)	0.8895 (2)	0.0509 (7)
H14	0.5817	0.4416	0.8401	0.061*
C15	0.55191 (8)	0.3503 (3)	1.02945 (18)	0.0381 (5)
C16	0.54798 (10)	0.3857 (3)	1.13113 (19)	0.0500 (6)
H16A	0.5212	0.3179	1.1404	0.075*
H16B	0.5419	0.5095	1.1374	0.075*
H16C	0.5784	0.3527	1.1815	0.075*
N1	0.53589 (7)	0.2080 (2)	0.97253 (14)	0.0378 (5)
N2	0.57289 (8)	0.4629 (3)	0.98082 (16)	0.0453 (5)
H2	0.5859	0.5633	1.0036	0.054*
O1	0.44990 (6)	0.0258 (2)	0.86540 (12)	0.0421 (4)
O2	0.41557 (7)	0.1856 (2)	0.95858 (13)	0.0522 (5)
Cu1	0.5000	0.0000	1.0000	0.03683 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0456 (14)	0.0263 (11)	0.0454 (14)	−0.0092 (10)	0.0134 (11)	0.0017 (10)
C2	0.0460 (14)	0.0365 (13)	0.0504 (15)	0.0049 (11)	0.0146 (12)	0.0092 (11)
C3	0.0285 (12)	0.0464 (14)	0.0374 (13)	0.0043 (10)	0.0051 (10)	0.0046 (10)
C4	0.0409 (14)	0.0658 (17)	0.0397 (14)	−0.0029 (13)	0.0125 (11)	0.0072 (13)
C5	0.0520 (16)	0.082 (2)	0.0439 (15)	−0.0064 (15)	0.0177 (13)	−0.0145 (15)
C6	0.0461 (15)	0.0595 (17)	0.0565 (17)	−0.0061 (13)	0.0106 (13)	−0.0200 (14)
C7	0.0299 (12)	0.0470 (14)	0.0442 (14)	−0.0005 (10)	0.0072 (10)	−0.0022 (11)
C8	0.0250 (11)	0.0424 (13)	0.0361 (12)	0.0044 (9)	0.0045 (9)	0.0026 (10)
C9	0.0411 (14)	0.0503 (15)	0.0392 (13)	−0.0011 (11)	0.0098 (11)	−0.0009 (11)
C10	0.0477 (15)	0.080 (2)	0.0413 (15)	−0.0057 (14)	0.0151 (12)	0.0059 (14)
C11	0.0431 (15)	0.0704 (19)	0.0611 (18)	−0.0101 (14)	0.0143 (13)	0.0161 (16)
C12	0.0367 (14)	0.0507 (16)	0.0617 (18)	−0.0076 (11)	0.0052 (12)	0.0022 (13)
C13	0.0504 (15)	0.0453 (14)	0.0417 (14)	−0.0035 (12)	0.0167 (12)	−0.0097 (11)
C14	0.0587 (17)	0.0489 (15)	0.0517 (16)	−0.0046 (13)	0.0266 (13)	−0.0030 (12)
C15	0.0334 (12)	0.0346 (12)	0.0441 (13)	0.0019 (10)	0.0090 (10)	−0.0045 (10)
C16	0.0597 (16)	0.0451 (15)	0.0454 (15)	0.0053 (12)	0.0169 (13)	−0.0084 (12)
N1	0.0364 (11)	0.0340 (10)	0.0414 (11)	−0.0033 (8)	0.0098 (9)	−0.0055 (9)
N2	0.0486 (12)	0.0337 (11)	0.0555 (13)	−0.0086 (9)	0.0190 (10)	−0.0074 (9)
O1	0.0368 (9)	0.0444 (10)	0.0412 (9)	−0.0025 (7)	0.0065 (7)	−0.0054 (7)
O2	0.0678 (12)	0.0392 (9)	0.0518 (11)	−0.0075 (8)	0.0219 (9)	−0.0115 (8)
Cu1	0.0348 (2)	0.0341 (2)	0.0391 (2)	−0.00479 (17)	0.00786 (17)	−0.00590 (17)

Geometric parameters (Å, º)

C1—O2	1.241 (3)	C10—H10	0.9300
C1—O1	1.267 (3)	C11—C12	1.358 (4)
C1—C2	1.523 (3)	C11—H11	0.9300
C2—C3	1.510 (3)	C12—H12	0.9300
C2—H2A	0.9700	C13—C14	1.341 (3)
C2—H2B	0.9700	C13—N1	1.375 (3)
C3—C4	1.364 (3)	C13—H13	0.9300
C3—C8	1.424 (3)	C14—N2	1.363 (3)
C4—C5	1.405 (4)	C14—H14	0.9300
C4—H4	0.9300	C15—N1	1.329 (3)
C5—C6	1.358 (4)	C15—N2	1.339 (3)
C5—H5	0.9300	C15—C16	1.481 (3)
C6—C7	1.413 (3)	C16—H16A	0.9600
C6—H6	0.9300	C16—H16B	0.9600
C7—C12	1.413 (3)	C16—H16C	0.9600
C7—C8	1.425 (3)	N1—Cu1	1.9750 (18)
C8—C9	1.418 (3)	N2—H2	0.8600
C9—C10	1.358 (3)	O1—Cu1	1.9791 (16)
C9—H9	0.9300	Cu1—N1^{i}	1.9750 (18)
C10—C11	1.402 (4)	Cu1—O1^{i}	1.9791 (16)
O2—C1—O1	123.7 (2)	C12—C11—H11	120.1
O2—C1—C2	120.4 (2)	C10—C11—H11	120.1
O1—C1—C2	115.9 (2)	C11—C12—C7	121.0 (3)
C3—C2—C1	113.22 (18)	C11—C12—H12	119.5
C3—C2—H2A	108.9	C7—C12—H12	119.5
C1—C2—H2A	108.9	C14—C13—N1	109.5 (2)
C3—C2—H2B	108.9	C14—C13—H13	125.3
C1—C2—H2B	108.9	N1—C13—H13	125.2
H2A—C2—H2B	107.7	C13—C14—N2	106.2 (2)
C4—C3—C8	119.3 (2)	C13—C14—H14	126.9
C4—C3—C2	120.6 (2)	N2—C14—H14	126.9
C8—C3—C2	120.1 (2)	N1—C15—N2	109.6 (2)
C3—C4—C5	121.6 (2)	N1—C15—C16	127.1 (2)
C3—C4—H4	119.2	N2—C15—C16	123.3 (2)
C5—C4—H4	119.2	C15—C16—H16A	109.5
C6—C5—C4	120.2 (2)	C15—C16—H16B	109.5
C6—C5—H5	119.9	H16A—C16—H16B	109.5
C4—C5—H5	119.9	C15—C16—H16C	109.5
C5—C6—C7	120.8 (2)	H16A—C16—H16C	109.5
C5—C6—H6	119.6	H16B—C16—H16C	109.5
C7—C6—H6	119.6	C15—N1—C13	106.20 (19)
C6—C7—C12	121.6 (2)	C15—N1—Cu1	128.97 (16)
C6—C7—C8	119.0 (2)	C13—N1—Cu1	124.80 (15)
C12—C7—C8	119.3 (2)	C15—N2—C14	108.5 (2)
C9—C8—C3	123.2 (2)	C15—N2—H2	125.6

C9—C8—C7	117.7 (2)	C14—N2—H2	125.9
C3—C8—C7	119.1 (2)	C1—O1—Cu1	106.96 (15)
C10—C9—C8	121.1 (2)	N1—Cu1—N1^{i}	180.00 (11)
C10—C9—H9	119.4	N1—Cu1—O1^{i}	89.99 (7)
C8—C9—H9	119.4	N1^{i}—Cu1—O1^{i}	90.01 (7)
C9—C10—C11	121.0 (3)	N1—Cu1—O1	90.01 (7)
C9—C10—H10	119.5	N1^{i}—Cu1—O1	89.99 (7)
C11—C10—H10	119.5	O1^{i}—Cu1—O1	180.000 (1)
C12—C11—C10	119.8 (3)		

O2—C1—C2—C3	−127.3 (2)	C10—C11—C12—C7	−1.2 (4)
O1—C1—C2—C3	52.1 (3)	C6—C7—C12—C11	−179.3 (3)
C1—C2—C3—C4	−110.1 (3)	C8—C7—C12—C11	0.2 (4)
C1—C2—C3—C8	70.1 (3)	N1—C13—C14—N2	0.5 (3)
C8—C3—C4—C5	0.9 (4)	N2—C15—N1—C13	0.1 (3)
C2—C3—C4—C5	−178.9 (2)	C16—C15—N1—C13	179.9 (2)
C3—C4—C5—C6	0.5 (4)	N2—C15—N1—Cu1	−177.75 (15)
C4—C5—C6—C7	−1.2 (4)	C16—C15—N1—Cu1	2.1 (4)
C5—C6—C7—C12	179.9 (3)	C14—C13—N1—C15	−0.4 (3)
C5—C6—C7—C8	0.4 (4)	C14—C13—N1—Cu1	177.56 (17)
C4—C3—C8—C9	178.9 (2)	N1—C15—N2—C14	0.2 (3)
C2—C3—C8—C9	−1.3 (3)	C16—C15—N2—C14	−179.6 (2)
C4—C3—C8—C7	−1.6 (3)	C13—C14—N2—C15	−0.5 (3)
C2—C3—C8—C7	178.2 (2)	O2—C1—O1—Cu1	7.9 (3)
C6—C7—C8—C9	−179.5 (2)	C2—C1—O1—Cu1	−171.46 (15)
C12—C7—C8—C9	1.0 (3)	C15—N1—Cu1—O1^{i}	−50.3 (2)
C6—C7—C8—C3	1.0 (3)	C13—N1—Cu1—O1^{i}	132.28 (19)
C12—C7—C8—C3	−178.5 (2)	C15—N1—Cu1—O1	129.7 (2)
C3—C8—C9—C10	178.3 (2)	C13—N1—Cu1—O1	−47.72 (19)
C7—C8—C9—C10	−1.2 (3)	C1—O1—Cu1—N1	−95.44 (14)
C8—C9—C10—C11	0.2 (4)	C1—O1—Cu1—N1^{i}	84.56 (14)
C9—C10—C11—C12	1.0 (4)		

Symmetry code: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{ii}	0.86	1.97	2.775 (3)	155

Symmetry code: (ii) −*x*+1, −*y*+1, −*z*+2.