Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[μ-*N*′-isobutyryl-1-oxidonaphthalene-2-carbohydrazidato(3-)]dipyridine-tricopper(II)

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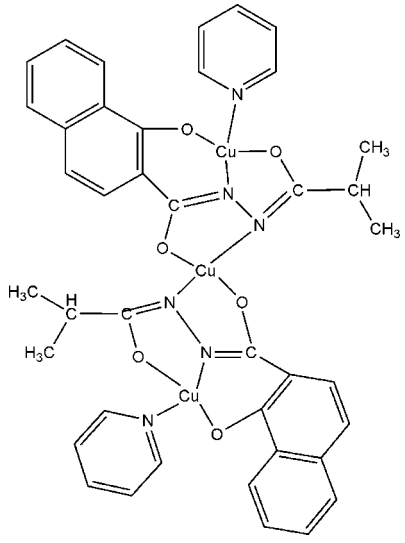
Received 20 February 2009; accepted 11 March 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.039; wR factor = 0.135; data-to-parameter ratio = 13.2.

The complete molecule of the title complex, $[Cu_3(C_{15}H_{13}N_2O_3)_2(C_5H_5N)_2]$, is generated by crystallographic twofold symmetry, with the central Cu atom lying on the rotation axis: it is coordinated by two *N*,*O*-bidentate ligands in a *trans*-CuN_2O_2 distorted square-planar arrangement. The other Cu atom is coordinated by an *N*,*O*,*O*′-tridentate ligand and a pyridine molecule in a distorted *trans*-CuN_2O_2 arrangement. In the crystal structure, a C—H$\cdots\pi$ interaction occurs.

Related literature

For related structures, see: Patole *et al.* (2003); Pouralimardan *et al.* (2007). For background on C—H$\cdots\pi$ interactions, see: Nishio (2004); Saalfrank & Bernt (1998).



Experimental

Crystal data

$[Cu_3(C_{15}H_{13}N_2O_3)_2(C_5H_5N)_2]$
M_r = 887.37
Monoclinic, $C2/c$
a = 23.661 (2) Å
b = 13.0521 (18) Å
c = 13.3142 (15) Å
β = 113.684 (2)°
V = 3765.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.74 mm^{-1}
T = 298 K
0.37 × 0.35 × 0.31 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.566, T_{max} = 0.615
(expected range = 0.537–0.584)
9477 measured reflections
3310 independent reflections
2319 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.135
S = 1.00
3310 reflections
251 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.920 (3)	Cu2—N1	1.884 (3)
Cu1—O1^{i}	1.920 (3)	Cu2—O2	1.890 (3)
Cu1—N2	1.946 (3)	Cu2—O3	1.953 (3)
Cu1—N2^{i}	1.946 (3)	Cu2—N3	1.975 (3)

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

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

*Cg*1 is the centroid of the C2–C7 ring.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C17—H17$\cdots$*Cg*1^{ii}	0.93	2.53	3.362 (4)	150

Symmetry code: (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

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*.

We acknowledge financial support from the National Natural Science Foundation of China (grant No. 20671048).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2917).

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supporting information

Acta Cryst. (2009). E**65**, m435 [doi:10.1107/S1600536809009003]

Bis[μ-*N*′-isobutyryl-1-oxidonaphthalene-2-carbohydrazidato(3-)]dipyridine-tricopper(II)

Xue-Feng Shi, Dacheng Li, Pi-Yong Li and Da-Qi Wang

S1. Comment

A large number of aroylhydrazine complexes have been prepared and studied due to their diverse molecular architectures and quite interesting chemical properties (Patole *et al.*, 2003; Pouralimardan *et al.*, 2007). However, researches on the copper(II) complexes with N-isobutyryl-1-hydroxy-2-naphthalenecarbohydrazide have not reported. So we have synthesized a new complex, (I), (Fig. 1), which has been characterized by X-ray diffraction and elemental analysis. The molecule of (I) contains three copper(II), two ligand molecules, and two pyridine molecules. Both copper centres adopt distorted square planar trans-CuN_2O_2 arrangements. The triple-deprotonated *N*-isobutyryl-1-hydroxy-2-naphthalene-carbohydrazide bridges the metal ions using a hydrazide N—N group and formed the trinuclear copper complex. In the crystal packing, the complex molecules are linked into two-dimensional network by intermolecular C—H···π interactions (Fig. 2) (Saalfrank & Bernt, 1998; Nishio, 2004).

S2. Experimental

Isobutyric anhydride (0.632 g, 4 mmol) and 1-hydroxy-2-naphthalenecarbohydrazide (0.808 g, 4 mmol) were added to 40 ml of chloroform at ice-water bath. The reaction mixture was slowly warmed to room temperature and stirred for 24 h. After overnight refrigeration, the resulting white precipitate was filtered and rinsed with chloroform and diethyl ether (1.02 g, 93.57% yield). A solution of $CuNO_3$(0.04 g,0.2 mmol) in methanol (10 ml) was added to a mixture of N-isobutyryl-1-hydroxy-2-naphthalenecarbohydrazide (0.055 g, 0.2 mmol) and sodium methylate (0.0324 g, 0.6 mmol) in pyridine (10 ml). A green solution was obtained after refluxing for 3 h. After being filtrated, dimethyl ether was slowly diffused into the filtrate, and green blocks of (I) were obtained after two weeks. Elemental analysis calculated for $C_{40}H_{36}N_6O_6Cu_3$: C, 54.09; H, 4.05; O, 10.78; N, 9.43. Found (%): C, 54.12; H, 4.06; O, 10.82; N, 9.47

S3. Refinement

The C-bound H atoms were positioned with idealized geometry (C—H = 0.93–0.98Å) and refined as riding with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5U_{eq}(methyl C).

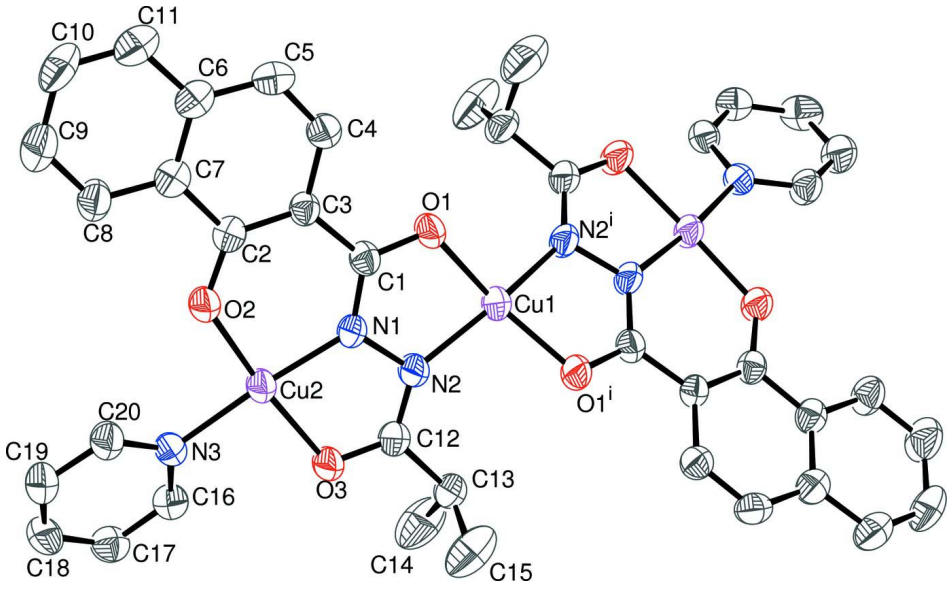

Figure 1

The molecular structure of (I) showing 40% probability displacement ellipsoids. H atoms have been omitted for clarity. Symmetry code: (i) 1–x, y, 1/2–z.

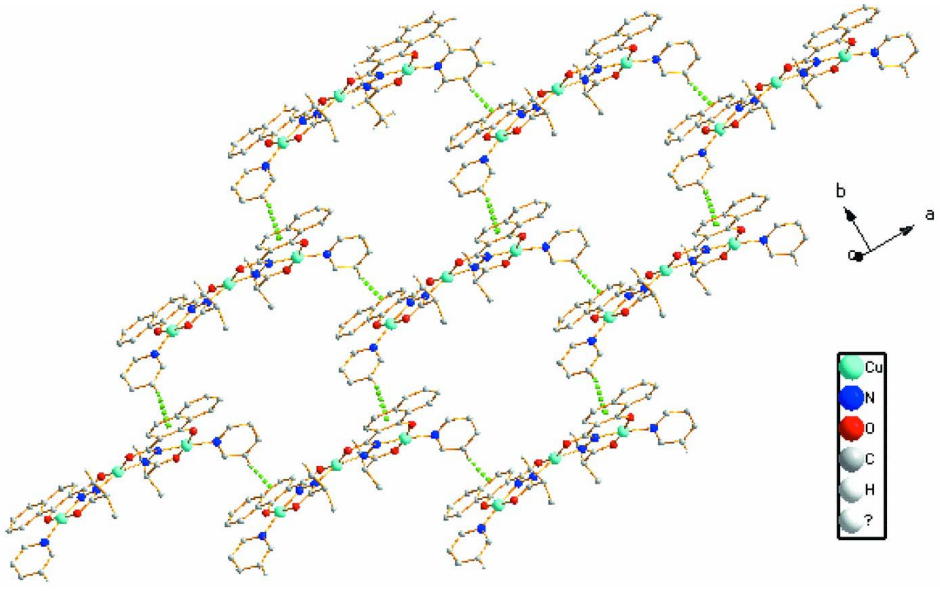

Figure 2

View of the two-dimensional network structure in (I). Intermolecular C—H···π are shown as dashed lines. Most of H atoms are omitted.

Bis[μ-*N*′-isobutyryl-1-oxidonaphthalene-2- carbohydrazidato(3-)]dipyridinetricopper(II)

Crystal data

$[Cu_3(C_{15}H_{13}N_2O_3)_2(C_5H_5N)_2]$
M_r = 887.37
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 23.661 (2) Å
b = 13.0521 (18) Å
c = 13.3142 (15) Å
β = 113.684 (2)°
V = 3765.5 (7) Å^3
Z = 4
F(000) = 1812
D_x = 1.565 Mg m^{-3}
D_m = 1.565 Mg m^{-3}
D_m measured by not measured
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 3140 reflections
θ = 2.7–26.3°
μ = 1.74 mm^{-1}
T = 298 K
Block, green
0.37 × 0.35 × 0.31 mm

Data collection

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.566, T_{max} = 0.615
9477 measured reflections
3310 independent reflections
2319 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −28→27
k = −14→15
l = −13→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.135
S = 1.00
3310 reflections
251 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
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 4.0071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.86302 (6)	0.2500	0.0410 (2)
Cu2	0.68569 (2)	0.80745 (4)	0.23216 (4)	0.0404 (2)
N1	0.62147 (15)	0.8496 (3)	0.2723 (3)	0.0401 (8)
N2	0.56137 (15)	0.8380 (3)	0.1900 (3)	0.0425 (9)
N3	0.74587 (15)	0.7504 (3)	0.1787 (3)	0.0386 (8)
O1	0.57183 (12)	0.8896 (2)	0.3816 (2)	0.0446 (7)
O2	0.74777 (12)	0.8431 (2)	0.3698 (2)	0.0442 (7)
O3	0.61596 (13)	0.7851 (3)	0.0920 (2)	0.0523 (8)
C1	0.62281 (18)	0.8758 (3)	0.3692 (3)	0.0363 (9)
C2	0.73934 (18)	0.8742 (3)	0.4567 (3)	0.0361 (9)
C3	0.68203 (18)	0.8912 (3)	0.4623 (3)	0.0341 (9)
C4	0.68036 (19)	0.9281 (3)	0.5618 (3)	0.0399 (10)

H4	0.6421	0.9386	0.5645	0.048*
C5	0.7314 (2)	0.9484 (3)	0.6518 (3)	0.0440 (11)
H5	0.7278	0.9733	0.7144	0.053*
C6	0.7909 (2)	0.9322 (3)	0.6522 (3)	0.0421 (10)
C7	0.79500 (19)	0.8936 (3)	0.5546 (3)	0.0398 (10)
C8	0.85377 (19)	0.8776 (4)	0.5545 (4)	0.0503 (11)
H8	0.8570	0.8522	0.4919	0.060*
C9	0.9059 (2)	0.8990 (5)	0.6448 (4)	0.0674 (15)
H9	0.9443	0.8885	0.6426	0.081*
C10	0.9026 (2)	0.9367 (4)	0.7415 (4)	0.0655 (15)
H10	0.9385	0.9507	0.8029	0.079*
C11	0.8464 (2)	0.9522 (4)	0.7439 (4)	0.0559 (13)
H11	0.8443	0.9767	0.8080	0.067*
C12	0.56432 (19)	0.8035 (4)	0.0990 (4)	0.0451 (11)
C13	0.5056 (2)	0.7872 (4)	−0.0027 (4)	0.0548 (13)
H13	0.4703	0.7944	0.0176	0.066*
C14	0.5046 (3)	0.6793 (5)	−0.0479 (5)	0.090 (2)
H14A	0.5318	0.6765	−0.0854	0.135*
H14B	0.4634	0.6627	−0.0982	0.135*
H14C	0.5180	0.6310	0.0114	0.135*
C15	0.5004 (3)	0.8681 (5)	−0.0879 (5)	0.0862 (19)
H15A	0.5084	0.9344	−0.0539	0.129*
H15B	0.4595	0.8668	−0.1449	0.129*
H15C	0.5299	0.8541	−0.1188	0.129*
C16	0.7284 (2)	0.6777 (3)	0.0995 (3)	0.0414 (10)
H16	0.6872	0.6577	0.0689	0.050*
C17	0.7684 (2)	0.6324 (3)	0.0624 (4)	0.0468 (11)
H17	0.7548	0.5822	0.0084	0.056*
C18	0.8288 (2)	0.6624 (4)	0.1064 (4)	0.0585 (13)
H18	0.8571	0.6324	0.0829	0.070*
C19	0.8476 (2)	0.7379 (5)	0.1861 (4)	0.0604 (13)
H19	0.8883	0.7605	0.2160	0.072*
C20	0.8046 (2)	0.7787 (4)	0.2200 (4)	0.0489 (11)
H20	0.8174	0.8285	0.2745	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0270 (4)	0.0562 (5)	0.0400 (4)	0.000	0.0138 (3)	0.000
Cu2	0.0282 (3)	0.0537 (4)	0.0391 (3)	−0.0004 (2)	0.0133 (2)	−0.0070 (2)
N1	0.0243 (17)	0.058 (2)	0.0350 (19)	−0.0019 (16)	0.0083 (15)	−0.0053 (17)
N2	0.0269 (18)	0.062 (2)	0.0371 (19)	−0.0036 (17)	0.0110 (16)	−0.0097 (18)
N3	0.0349 (19)	0.044 (2)	0.0392 (19)	0.0012 (16)	0.0175 (16)	−0.0024 (17)
O1	0.0286 (15)	0.0644 (19)	0.0435 (17)	−0.0017 (14)	0.0172 (13)	−0.0100 (15)
O2	0.0308 (15)	0.0602 (19)	0.0417 (17)	−0.0003 (14)	0.0146 (13)	−0.0083 (15)
O3	0.0291 (16)	0.088 (2)	0.0386 (17)	0.0002 (16)	0.0123 (13)	−0.0135 (16)
C1	0.031 (2)	0.039 (2)	0.041 (2)	−0.0013 (18)	0.0161 (18)	−0.0011 (19)
C2	0.034 (2)	0.032 (2)	0.040 (2)	−0.0022 (17)	0.0121 (18)	0.0006 (18)

C3	0.029 (2)	0.034 (2)	0.037 (2)	−0.0010 (17)	0.0120 (17)	−0.0024 (18)
C4	0.039 (2)	0.042 (2)	0.040 (2)	−0.0004 (19)	0.016 (2)	−0.0016 (19)
C5	0.057 (3)	0.041 (2)	0.034 (2)	−0.003 (2)	0.017 (2)	−0.0002 (19)
C6	0.046 (3)	0.032 (2)	0.041 (2)	−0.0017 (19)	0.011 (2)	0.0039 (19)
C7	0.040 (2)	0.032 (2)	0.043 (2)	−0.0017 (18)	0.013 (2)	0.0008 (19)
C8	0.034 (2)	0.059 (3)	0.053 (3)	0.002 (2)	0.012 (2)	−0.008 (2)
C9	0.037 (3)	0.089 (4)	0.066 (3)	0.001 (3)	0.009 (3)	−0.006 (3)
C10	0.041 (3)	0.072 (4)	0.058 (3)	−0.002 (3)	−0.007 (2)	−0.004 (3)
C11	0.057 (3)	0.054 (3)	0.043 (3)	−0.003 (2)	0.006 (2)	−0.002 (2)
C12	0.031 (2)	0.064 (3)	0.040 (2)	−0.001 (2)	0.0130 (19)	−0.001 (2)
C13	0.031 (2)	0.088 (4)	0.038 (2)	0.001 (2)	0.008 (2)	−0.009 (3)
C14	0.078 (4)	0.082 (4)	0.070 (4)	−0.011 (3)	−0.012 (3)	−0.016 (3)
C15	0.074 (4)	0.084 (4)	0.064 (4)	−0.006 (3)	−0.009 (3)	0.004 (3)
C16	0.042 (2)	0.038 (2)	0.044 (2)	−0.0023 (19)	0.018 (2)	0.001 (2)
C17	0.056 (3)	0.040 (3)	0.046 (3)	0.004 (2)	0.022 (2)	−0.002 (2)
C18	0.057 (3)	0.070 (3)	0.055 (3)	0.024 (3)	0.031 (3)	0.002 (3)
C19	0.035 (3)	0.089 (4)	0.056 (3)	0.005 (3)	0.017 (2)	−0.003 (3)
C20	0.035 (2)	0.062 (3)	0.047 (3)	0.000 (2)	0.014 (2)	−0.008 (2)

Geometric parameters (Å, º)

Cu1—O1	1.920 (3)	C8—C9	1.361 (6)
Cu1—O1^{i}	1.920 (3)	C8—H8	0.9300
Cu1—N2	1.946 (3)	C9—C10	1.409 (7)
Cu1—N2^{i}	1.946 (3)	C9—H9	0.9300
Cu2—N1	1.884 (3)	C10—C11	1.360 (7)
Cu2—O2	1.890 (3)	C10—H10	0.9300
Cu2—O3	1.953 (3)	C11—H11	0.9300
Cu2—N3	1.975 (3)	C12—C13	1.516 (6)
N1—C1	1.323 (5)	C13—C15	1.518 (8)
N1—N2	1.412 (5)	C13—C14	1.529 (8)
N2—C12	1.320 (5)	C13—H13	0.9800
N3—C20	1.326 (5)	C14—H14A	0.9600
N3—C16	1.354 (5)	C14—H14B	0.9600
O1—C1	1.294 (5)	C14—H14C	0.9600
O2—C2	1.315 (5)	C15—H15A	0.9600
O3—C12	1.285 (5)	C15—H15B	0.9600
C1—C3	1.465 (5)	C15—H15C	0.9600
C2—C3	1.405 (5)	C16—C17	1.365 (6)
C2—C7	1.455 (6)	C16—H16	0.9300
C3—C4	1.425 (6)	C17—C18	1.367 (7)
C4—C5	1.342 (6)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.384 (7)
C5—C6	1.423 (6)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.374 (6)
C6—C11	1.412 (6)	C19—H19	0.9300
C6—C7	1.433 (6)	C20—H20	0.9300
C7—C8	1.406 (6)		

O1—Cu1—O1^{i}	159.21 (19)	C7—C8—H8	119.5
O1—Cu1—N2	82.65 (13)	C8—C9—C10	121.0 (5)
O1^{i}—Cu1—N2	100.87 (13)	C8—C9—H9	119.5
O1—Cu1—N2^{i}	100.87 (13)	C10—C9—H9	119.5
O1^{i}—Cu1—N2^{i}	82.65 (13)	C11—C10—C9	119.2 (4)
N2—Cu1—N2^{i}	160.7 (2)	C11—C10—H10	120.4
N1—Cu2—O2	93.11 (13)	C9—C10—H10	120.4
N1—Cu2—O3	81.17 (13)	C10—C11—C6	122.0 (5)
O2—Cu2—O3	173.00 (13)	C10—C11—H11	119.0
N1—Cu2—N3	172.94 (14)	C6—C11—H11	119.0
O2—Cu2—N3	92.88 (13)	O3—C12—N2	122.2 (4)
O3—Cu2—N3	93.10 (13)	O3—C12—C13	117.8 (4)
C1—N1—N2	114.0 (3)	N2—C12—C13	120.0 (4)
C1—N1—Cu2	130.2 (3)	C12—C13—C15	109.9 (4)
N2—N1—Cu2	115.1 (3)	C12—C13—C14	110.1 (4)
C12—N2—N1	109.9 (3)	C15—C13—C14	111.2 (5)
C12—N2—Cu1	139.2 (3)	C12—C13—H13	108.5
N1—N2—Cu1	110.4 (2)	C15—C13—H13	108.5
C20—N3—C16	117.3 (4)	C14—C13—H13	108.5
C20—N3—Cu2	122.2 (3)	C13—C14—H14A	109.5
C16—N3—Cu2	120.4 (3)	C13—C14—H14B	109.5
C1—O1—Cu1	112.8 (3)	H14A—C14—H14B	109.5
C2—O2—Cu2	126.6 (3)	C13—C14—H14C	109.5
C12—O3—Cu2	111.4 (3)	H14A—C14—H14C	109.5
O1—C1—N1	120.1 (4)	H14B—C14—H14C	109.5
O1—C1—C3	119.8 (4)	C13—C15—H15A	109.5
N1—C1—C3	120.1 (3)	C13—C15—H15B	109.5
O2—C2—C3	125.9 (4)	H15A—C15—H15B	109.5
O2—C2—C7	116.0 (4)	C13—C15—H15C	109.5
C3—C2—C7	118.1 (4)	H15A—C15—H15C	109.5
C2—C3—C4	119.4 (4)	H15B—C15—H15C	109.5
C2—C3—C1	123.3 (4)	N3—C16—C17	123.1 (4)
C4—C3—C1	117.3 (3)	N3—C16—H16	118.5
C5—C4—C3	123.1 (4)	C17—C16—H16	118.5
C5—C4—H4	118.5	C16—C17—C18	118.6 (4)
C3—C4—H4	118.5	C16—C17—H17	120.7
C4—C5—C6	120.6 (4)	C18—C17—H17	120.7
C4—C5—H5	119.7	C17—C18—C19	119.4 (4)
C6—C5—H5	119.7	C17—C18—H18	120.3
C11—C6—C5	123.4 (4)	C19—C18—H18	120.3
C11—C6—C7	118.2 (4)	C20—C19—C18	118.4 (5)
C5—C6—C7	118.4 (4)	C20—C19—H19	120.8
C8—C7—C6	118.6 (4)	C18—C19—H19	120.8
C8—C7—C2	120.9 (4)	N3—C20—C19	123.2 (4)
C6—C7—C2	120.5 (4)	N3—C20—H20	118.4
C9—C8—C7	121.0 (5)	C19—C20—H20	118.4
C9—C8—H8	119.5		

O2—Cu2—N1—C1	−10.5 (4)	N1—C1—C3—C4	174.6 (4)
O3—Cu2—N1—C1	173.6 (4)	C2—C3—C4—C5	0.4 (6)
O2—Cu2—N1—N2	179.6 (3)	C1—C3—C4—C5	−177.8 (4)
O3—Cu2—N1—N2	3.6 (3)	C3—C4—C5—C6	−0.9 (7)
C1—N1—N2—C12	−174.6 (4)	C4—C5—C6—C11	179.9 (4)
Cu2—N1—N2—C12	−3.0 (5)	C4—C5—C6—C7	−0.1 (6)
C1—N1—N2—Cu1	−0.9 (5)	C11—C6—C7—C8	−0.1 (6)
Cu2—N1—N2—Cu1	170.69 (17)	C5—C6—C7—C8	179.8 (4)
O1—Cu1—N2—C12	172.5 (5)	C11—C6—C7—C2	−178.4 (4)
O1^{i}—Cu1—N2—C12	−28.3 (5)	C5—C6—C7—C2	1.6 (6)
N2^{i}—Cu1—N2—C12	70.6 (5)	O2—C2—C7—C8	−1.0 (6)
O1—Cu1—N2—N1	1.6 (3)	C3—C2—C7—C8	179.8 (4)
O1^{i}—Cu1—N2—N1	160.8 (3)	O2—C2—C7—C6	177.1 (4)
N2^{i}—Cu1—N2—N1	−100.4 (3)	C3—C2—C7—C6	−2.1 (6)
O2—Cu2—N3—C20	−23.5 (4)	C6—C7—C8—C9	−0.4 (7)
O3—Cu2—N3—C20	152.8 (4)	C2—C7—C8—C9	177.8 (5)
O2—Cu2—N3—C16	154.6 (3)	C7—C8—C9—C10	0.7 (8)
O3—Cu2—N3—C16	−29.1 (3)	C8—C9—C10—C11	−0.3 (9)
O1^{i}—Cu1—O1—C1	−103.3 (3)	C9—C10—C11—C6	−0.3 (8)
N2—Cu1—O1—C1	−2.0 (3)	C5—C6—C11—C10	−179.4 (5)
N2^{i}—Cu1—O1—C1	158.7 (3)	C7—C6—C11—C10	0.5 (7)
N1—Cu2—O2—C2	6.4 (3)	Cu2—O3—C12—N2	3.1 (6)
N3—Cu2—O2—C2	−169.9 (3)	Cu2—O3—C12—C13	−178.6 (3)
N1—Cu2—O3—C12	−3.6 (3)	N1—N2—C12—O3	−0.2 (6)
N3—Cu2—O3—C12	172.2 (3)	Cu1—N2—C12—O3	−171.2 (3)
Cu1—O1—C1—N1	2.2 (5)	N1—N2—C12—C13	−178.4 (4)
Cu1—O1—C1—C3	−179.0 (3)	Cu1—N2—C12—C13	10.7 (8)
N2—N1—C1—O1	−0.8 (6)	O3—C12—C13—C15	−69.6 (6)
Cu2—N1—C1—O1	−170.8 (3)	N2—C12—C13—C15	108.6 (5)
N2—N1—C1—C3	−179.6 (3)	O3—C12—C13—C14	53.2 (6)
Cu2—N1—C1—C3	10.4 (6)	N2—C12—C13—C14	−128.5 (5)
Cu2—O2—C2—C3	−3.0 (6)	C20—N3—C16—C17	0.9 (6)
Cu2—O2—C2—C7	177.9 (3)	Cu2—N3—C16—C17	−177.3 (3)
O2—C2—C3—C4	−178.1 (4)	N3—C16—C17—C18	−0.7 (7)
C7—C2—C3—C4	1.1 (6)	C16—C17—C18—C19	−0.5 (7)
O2—C2—C3—C1	0.1 (7)	C17—C18—C19—C20	1.4 (8)
C7—C2—C3—C1	179.2 (4)	C16—N3—C20—C19	0.0 (7)
O1—C1—C3—C2	177.6 (4)	Cu2—N3—C20—C19	178.2 (4)
N1—C1—C3—C2	−3.6 (6)	C18—C19—C20—N3	−1.2 (8)
O1—C1—C3—C4	−4.3 (6)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C17—H17···*Cg*1[ii]	0.93	2.53	3.362 (4)	150

Symmetry code: (ii) −*x*+3/2, *y*−1/2, −*z*+1/2.