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Poly[[(μ_4-naphthalene-1,4-dicarboxylato-$\kappa^4O:O:O:O'$)(μ_2-naphthalene-1,4-dicarboxylato-$\kappa^2O:O'$)bis(pyrazino[2,3-*f*][1,10]phenanthroline-κ^2N,N')dicopper(II)] tetrahydrate]

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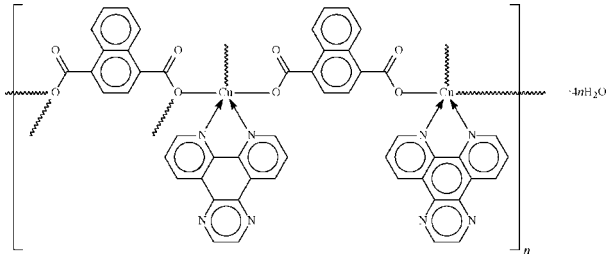
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; H-atom completeness 78%; R factor = 0.055; wR factor = 0.190; data-to-parameter ratio = 15.8.

One naphthalene-1,4-dicarboxylate dianion in the title compound, $[Cu_2(C_{12}H_6O_4)_2(C_{14}H_8N_4)_2]\cdot 4H_2O$, bridges two *N*-heterocycle-chelated Cu atoms whereas the other one bridges four *N*-heterocycle-chelated Cu atoms, linking them into a flat carboxylate-bridged layer. The two independent Cu atoms show square-pyramidal coordination. Water molecules occupy the space between adjacent layers; they are possibly disordered, and their H atoms were not located.

Related literature

The Cambridge Structural Database [Version 5.28, November 2006; Allen (2002)] lists several examples of metal(II) naphthalene-1,4-dicarboxylates. For hydrated diaqua(4,4′-bipyridine)-cobalt, -nickel and -copper compounds, see: Maji *et al.* (2005); Zheng *et al.* (2004). For the hydrated 1,2-bis(4-pyridyl)ethanecopper compound, see: Maji *et al.* (2005). For the crystal structure of naphthalene-1,4-dicarboxylic acid, see: Derissen *et al.* (1979). For the copper terephthalate complex of the *N*-heterocycle, see: Wang *et al.* (2006).



Experimental

Crystal data

$[Cu_2(C_{12}H_6O_4)_2(C_{14}H_8N_4)_2]\cdot 4H_2O$
M_r = 1091.97
Triclinic, $P\overline{1}$
a = 12.679 (5) Å
b = 14.690 (6) Å
c = 14.833 (7) Å
α = 69.37 (2)°
β = 82.05 (2)°
γ = 65.13 (2)°
V = 2346 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 295 (2) K
0.38 × 0.27 × 0.16 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.618, T_{max} = 0.859
22789 measured reflections
10535 independent reflections
6887 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.190
S = 1.09
10535 reflections
667 parameters
436 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.924 (3)	Cu1—N4	2.037 (3)
Cu1—O5	1.965 (2)	Cu2—O3	1.916 (3)
Cu1—O5^{i}	2.440 (3)	Cu2—O7^{ii}	1.964 (2)
Cu1—N1	2.012 (3)	Cu2—O7^{iii}	2.348 (3)

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2581).

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supplementary materials

Acta Cryst. (2007). E**63**, m2984-m2985 [**doi:10.1107/S1600536807056310**]

Poly[[(μ_4-naphthalene-1,4-dicarboxylato-κ^4O:O:O:O')(μ_2-naphthalene-1,4-dicarboxylato-κ^2O:O')bis(pyrazino[2,3-*f*][1,10]phenanthroline-κ^2N,N')dicopper(II)] tetrahydrate\]

G.-B. Che, C.-B. Liu and S. W. Ng

Comment

The Cambridge Structural Database (Version 5.28, November 2006) lists several examples of metal(II) naphthalene-1,4-dicarboxylates (Maji *et al.*, 2005; Zheng *et al.*, 2004). The dicarboxylate group is rigid, like terephthalic acid. The copper terephthalate complex of the title heterocycle (Wang *et al.*, 2006) has water in the coordination enviroment of the cadmium atom; the compound exists as a linear chain; one carboxyl end is chelating whereas the other is unidentate.

Experimental

Copper chloride dihydrate (0.1 mmol), naphthalene-1,4-dicarboxylic acid (0.1 mmol), pyrazino[2,3-*f*][1,10]phenanthroline and water (12 ml) were sealed in a 23-ml Teflon-lined Parr bomb, which was heated at 423 K for two days. Blue block crystals were picked from the cool solution by hand in about 30% yield.

Refinement

As all C–, N– and O-atoms showed somewhat elongated ellipsoids, their anisotropic temperature factors were restrained to be nearly isotropic. The O2, O4, O6 and O8 atoms, which are not involved in coordination, showed large displacement parameters. An attempt was made to refine each atom as two atoms of half site-occupancy each, with the pairs of C–O double-bond distances restrained to within 0.01 Å of each other. However, this treatment required the carboxyl $–CO_2$ group to be approximately planar, so that the O1, O3, O5 and O7 atoms that are involved in coordination would have to be split into two. As the treatment led to only a minor separation between the disorder components, the structure was refined without disorder.

Carbon-bound H atoms were placed in calculated positions [C—H 0.93–0.97 Å and U_{iso}(H) 1.2–1.5U_{eq}(C)], and were included in the refinement in the riding-model approximation. The water H-atoms could not be placed in chemically sensible positions on the basis of hydrogen bonding, and were not included.

The final difference Fourier map had a large peak near O3*w*.

Figures

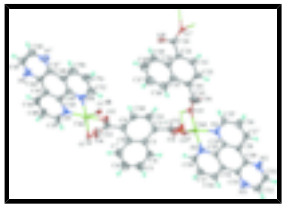


Fig. 1. **Figure 1**. Thermal ellipsoid plot of a portion of the chain structure; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. (Symmetry codes are given in Table 1.)

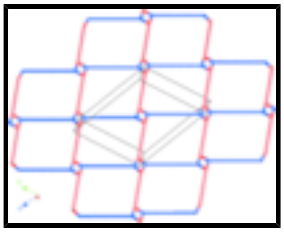


Fig. 2. *OLEX* (Dolomanov *et al.*, 2003) representation of the layer network.

Poly[[(μ$_4$-naphthalene-1,4-dicarboxylato- κ^4*O*:*O*:*O*:*O*')(μ$_2$-naphthalene-1,4- dicarboxylato-κ^2*O*:*O*')bis(pyrazino[2,3-*f*][1,10]phenanthroline-κ^2*N*,*N*')dicopper(II)] tetrahydrate]

Crystal data

$[Cu_2(C_{12}H_6O_4)_2(C_{14}H_8N_4)_2]\cdot 4H_2O$	$Z = 2$
$M_r = 1091.97$	$F_{000} = 1116$
Triclinic, $P\bar{1}$	$D_x = 1.546$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.679$ (5) Å	Cell parameters from 15645 reflections
$b = 14.690$ (6) Å	$\theta = 3.0$–27.5º
$c = 14.833$ (7) Å	$\mu = 0.98$ mm^{-1}
$\alpha = 69.37$ (2)º	$T = 295$ (2) K
$\beta = 82.05$ (2)º	Block, blue
$\gamma = 65.13$ (2)º	0.38 × 0.27 × 0.16 mm
$V = 2346$ (2) Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	10535 independent reflections
Radiation source: fine-focus sealed tube	6887 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295(2)$ K	$\theta_{min} = 3.0$º
ω–scans	$h = -16\rightarrow16$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -18\rightarrow19$
$T_{min} = 0.618$, $T_{max} = 0.859$	$l = -19\rightarrow19$
22789 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.190$	$w = 1/[\sigma^2(F_o^2) + (0.1132P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
10535 reflections	$\Delta\rho_{max} = 1.03$ e Å^{-3}
667 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
436 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.40502 (3)	0.45832 (4)	0.46309 (3)	0.03280 (15)
Cu2	1.08859 (3)	0.04876 (3)	0.02766 (3)	0.03177 (15)
O1	0.5140 (2)	0.4239 (2)	0.3639 (2)	0.0448 (7)
O2	0.4999 (3)	0.2724 (3)	0.3878 (3)	0.0798 (12)
O3	0.9640 (2)	0.1145 (3)	0.1032 (2)	0.0484 (7)
O4	0.9801 (3)	0.2685 (3)	0.0434 (3)	0.0950 (14)
O5	0.5321 (2)	0.4001 (2)	0.55622 (19)	0.0403 (6)
O6	0.5128 (5)	0.2520 (4)	0.6161 (4)	0.166 (3)
O7	0.9755 (2)	0.0895 (2)	0.92765 (18)	0.0358 (6)
O8	1.0457 (3)	0.1950 (3)	0.8171 (3)	0.0884 (14)
O1W	0.4320 (7)	0.1517 (6)	0.3165 (6)	0.172 (3)
O2W	0.4226 (10)	−0.0548 (8)	0.4733 (8)	0.264 (5)
O3W	0.2273 (10)	0.2971 (9)	0.1769 (10)	0.269 (5)
O4W	0.0234 (8)	0.4201 (7)	0.0950 (7)	0.199 (3)
N1	0.2756 (3)	0.5119 (3)	0.5508 (2)	0.0365 (7)
N2	−0.1416 (3)	0.6969 (3)	0.5521 (3)	0.0618 (11)
N3	−0.1518 (3)	0.6744 (3)	0.3731 (3)	0.0564 (11)
N4	0.2664 (3)	0.5018 (3)	0.3791 (2)	0.0374 (7)
N5	1.2335 (3)	−0.0271 (3)	−0.0366 (2)	0.0370 (7)
N6	1.6504 (3)	−0.2026 (4)	0.0081 (4)	0.0778 (15)
N7	1.6236 (4)	−0.1483 (4)	0.1776 (4)	0.0813 (16)
N8	1.2092 (3)	0.0200 (3)	0.1218 (2)	0.0419 (8)
C1	0.5436 (3)	0.3354 (4)	0.3488 (3)	0.0456 (10)
C2	0.6396 (4)	0.3128 (3)	0.2770 (3)	0.0410 (9)
C3	0.6428 (3)	0.3867 (3)	0.1860 (3)	0.0412 (9)
C4	0.5545 (4)	0.4905 (4)	0.1521 (3)	0.0542 (11)
H4	0.4929	0.5122	0.1924	0.065*
C5	0.5566 (5)	0.5586 (5)	0.0639 (4)	0.0773 (17)
H5	0.4963	0.6256	0.0439	0.093*
C6	0.6494 (5)	0.5291 (5)	0.0019 (4)	0.0838 (18)
H6	0.6509	0.5767	−0.0589	0.101*
C7	0.7375 (5)	0.4303 (5)	0.0309 (4)	0.0701 (15)
H7	0.7980	0.4115	−0.0111	0.084*
C8	0.7392 (4)	0.3555 (4)	0.1236 (3)	0.0448 (10)
C9	0.8284 (4)	0.2514 (4)	0.1551 (3)	0.0446 (10)
C10	0.8216 (4)	0.1838 (4)	0.2438 (3)	0.0497 (11)
H10	0.8805	0.1161	0.2646	0.060*

C11	0.7283 (4)	0.2133 (4)	0.3046 (3)	0.0475 (10)
H11	0.7261	0.1648	0.3647	0.057*
C12	0.9324 (3)	0.2109 (4)	0.0949 (3)	0.0519 (11)
C13	0.5642 (3)	0.3075 (4)	0.6105 (3)	0.0597 (14)
C14	0.6719 (4)	0.2660 (3)	0.6709 (3)	0.0467 (11)
C15	0.7829 (4)	0.2141 (4)	0.6364 (3)	0.0525 (12)
C16	0.7986 (5)	0.1958 (5)	0.5469 (4)	0.0658 (14)
H16	0.7337	0.2181	0.5094	0.079*
C17	0.9053 (6)	0.1467 (5)	0.5149 (4)	0.0778 (17)
H17	0.9133	0.1356	0.4559	0.093*
C18	1.0043 (5)	0.1124 (5)	0.5705 (5)	0.0752 (16)
H18	1.0777	0.0779	0.5485	0.090*
C19	0.9937 (4)	0.1291 (4)	0.6554 (4)	0.0594 (13)
H19	1.0604	0.1067	0.6907	0.071*
C20	0.8835 (4)	0.1799 (3)	0.6927 (3)	0.0458 (10)
C21	0.8679 (3)	0.1958 (3)	0.7835 (3)	0.0451 (11)
C22	0.7598 (4)	0.2426 (4)	0.8150 (3)	0.0497 (11)
H22	0.7507	0.2500	0.8756	0.060*
C23	0.6608 (4)	0.2801 (4)	0.7583 (4)	0.0533 (12)
H23	0.5875	0.3146	0.7804	0.064*
C24	0.9719 (3)	0.1584 (3)	0.8466 (3)	0.0448 (10)
C25	0.2843 (4)	0.5114 (4)	0.6399 (3)	0.0494 (11)
H25	0.3574	0.4808	0.6686	0.059*
C26	0.1866 (4)	0.5557 (4)	0.6905 (3)	0.0559 (12)
H26	0.1953	0.5534	0.7526	0.067*
C27	0.0786 (4)	0.6022 (4)	0.6508 (4)	0.0523 (11)
H27	0.0135	0.6327	0.6846	0.063*
C28	0.0674 (3)	0.6034 (3)	0.5569 (3)	0.0418 (9)
C29	0.1678 (3)	0.5570 (3)	0.5106 (3)	0.0341 (8)
C30	−0.0446 (3)	0.6484 (3)	0.5075 (3)	0.0437 (10)
C31	−0.2407 (4)	0.7337 (4)	0.5027 (5)	0.0748 (17)
H31	−0.3103	0.7697	0.5288	0.090*
C32	−0.2450 (4)	0.7213 (4)	0.4169 (5)	0.0688 (16)
H32	−0.3171	0.7471	0.3881	0.083*
C33	−0.0489 (3)	0.6382 (3)	0.4184 (3)	0.0431 (10)
C34	0.0568 (3)	0.5868 (3)	0.3719 (3)	0.0372 (9)
C35	0.1630 (3)	0.5495 (3)	0.4170 (3)	0.0344 (8)
C36	0.0581 (4)	0.5722 (4)	0.2839 (3)	0.0485 (11)
H36	−0.0110	0.5966	0.2510	0.058*
C37	0.1624 (4)	0.5215 (4)	0.2462 (3)	0.0545 (12)
H37	0.1647	0.5098	0.1882	0.065*
C38	0.2649 (4)	0.4877 (4)	0.2954 (3)	0.0461 (10)
H38	0.3352	0.4539	0.2688	0.055*
C39	1.2428 (4)	−0.0517 (4)	−0.1160 (3)	0.0507 (11)
H39	1.1752	−0.0320	−0.1490	0.061*
C40	1.3496 (4)	−0.1059 (5)	−0.1521 (4)	0.0703 (16)
H40	1.3522	−0.1187	−0.2097	0.084*
C41	1.4494 (4)	−0.1399 (4)	−0.1038 (4)	0.0653 (14)
H41	1.5206	−0.1774	−0.1268	0.078*

C42	1.4433 (3)	−0.1176 (4)	−0.0183 (4)	0.0500 (11)
C43	1.3335 (3)	−0.0605 (3)	0.0128 (3)	0.0413 (9)
C44	1.5449 (4)	−0.1491 (4)	0.0385 (4)	0.0564 (13)
C45	1.7391 (5)	−0.2288 (5)	0.0639 (6)	0.092 (2)
H45	1.8138	−0.2663	0.0461	0.110*
C46	1.7261 (5)	−0.2040 (5)	0.1441 (5)	0.083 (2)
H46	1.7928	−0.2268	0.1797	0.100*
C47	1.5308 (4)	−0.1213 (4)	0.1220 (4)	0.0596 (14)
C48	1.4168 (4)	−0.0613 (4)	0.1527 (3)	0.0505 (12)
C49	1.3201 (3)	−0.0329 (3)	0.0982 (3)	0.0400 (9)
C50	1.3978 (5)	−0.0324 (4)	0.2340 (4)	0.0670 (16)
H50	1.4603	−0.0486	0.2715	0.080*
C51	1.2862 (5)	0.0203 (5)	0.2597 (4)	0.0687 (15)
H51	1.2724	0.0392	0.3152	0.082*
C52	1.1935 (4)	0.0454 (4)	0.2016 (3)	0.0564 (12)
H52	1.1181	0.0811	0.2195	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0200 (2)	0.0465 (3)	0.0297 (2)	−0.00772 (19)	−0.00046 (17)	−0.0166 (2)
Cu2	0.0223 (2)	0.0404 (3)	0.0325 (3)	−0.00717 (19)	−0.00198 (18)	−0.0176 (2)
O1	0.0337 (14)	0.064 (2)	0.0453 (16)	−0.0163 (13)	0.0082 (12)	−0.0347 (15)
O2	0.083 (3)	0.069 (3)	0.095 (3)	−0.041 (2)	0.049 (2)	−0.039 (2)
O3	0.0386 (15)	0.059 (2)	0.0553 (18)	−0.0118 (14)	0.0079 (13)	−0.0397 (15)
O4	0.080 (3)	0.075 (3)	0.131 (4)	−0.035 (2)	0.065 (3)	−0.053 (3)
O5	0.0303 (13)	0.0463 (17)	0.0372 (14)	−0.0089 (12)	−0.0103 (11)	−0.0097 (12)
O6	0.147 (4)	0.117 (4)	0.211 (5)	−0.098 (4)	−0.135 (4)	0.081 (4)
O7	0.0293 (13)	0.0411 (15)	0.0345 (13)	−0.0118 (11)	−0.0063 (11)	−0.0097 (11)
O8	0.066 (2)	0.099 (3)	0.084 (3)	−0.057 (2)	−0.035 (2)	0.032 (2)
O1W	0.197 (6)	0.211 (6)	0.183 (6)	−0.103 (5)	0.048 (5)	−0.141 (5)
O2W	0.328 (9)	0.227 (8)	0.238 (8)	−0.108 (7)	−0.058 (7)	−0.058 (7)
O3W	0.299 (9)	0.204 (7)	0.322 (10)	−0.126 (7)	0.007 (7)	−0.078 (7)
O4W	0.228 (7)	0.191 (7)	0.233 (7)	−0.109 (6)	−0.009 (6)	−0.096 (5)
N1	0.0255 (15)	0.052 (2)	0.0351 (16)	−0.0147 (14)	0.0023 (13)	−0.0198 (15)
N2	0.0331 (19)	0.062 (3)	0.081 (3)	−0.0132 (17)	0.0146 (19)	−0.025 (2)
N3	0.0281 (18)	0.054 (2)	0.075 (3)	−0.0136 (16)	−0.0103 (18)	−0.006 (2)
N4	0.0279 (16)	0.049 (2)	0.0358 (16)	−0.0146 (14)	−0.0005 (13)	−0.0153 (15)
N5	0.0241 (15)	0.0434 (19)	0.0405 (17)	−0.0082 (13)	−0.0024 (13)	−0.0160 (14)
N6	0.0276 (19)	0.069 (3)	0.107 (4)	−0.0112 (19)	−0.006 (2)	−0.002 (3)
N7	0.049 (2)	0.093 (3)	0.081 (3)	−0.039 (2)	−0.029 (2)	0.019 (3)
N8	0.0455 (19)	0.047 (2)	0.0385 (17)	−0.0212 (16)	−0.0095 (15)	−0.0123 (15)
C1	0.037 (2)	0.060 (3)	0.042 (2)	−0.017 (2)	0.0058 (18)	−0.024 (2)
C2	0.039 (2)	0.050 (2)	0.041 (2)	−0.0161 (18)	0.0030 (17)	−0.0263 (18)
C3	0.038 (2)	0.048 (2)	0.039 (2)	−0.0114 (17)	0.0058 (17)	−0.0254 (18)
C4	0.043 (2)	0.051 (3)	0.055 (3)	−0.008 (2)	0.010 (2)	−0.019 (2)
C5	0.075 (4)	0.055 (3)	0.067 (3)	−0.004 (3)	0.005 (3)	−0.010 (3)
C6	0.087 (4)	0.073 (4)	0.059 (3)	−0.021 (3)	0.015 (3)	−0.006 (3)

C7	0.072 (3)	0.075 (4)	0.051 (3)	−0.024 (3)	0.020 (2)	−0.022 (3)
C8	0.043 (2)	0.053 (3)	0.043 (2)	−0.0166 (19)	0.0082 (18)	−0.0264 (19)
C9	0.039 (2)	0.051 (3)	0.049 (2)	−0.0126 (18)	0.0089 (18)	−0.032 (2)
C10	0.050 (2)	0.043 (2)	0.051 (2)	−0.0058 (19)	0.006 (2)	−0.027 (2)
C11	0.050 (2)	0.052 (3)	0.038 (2)	−0.013 (2)	0.0053 (18)	−0.0219 (19)
C12	0.042 (2)	0.059 (3)	0.056 (3)	−0.016 (2)	0.015 (2)	−0.031 (2)
C13	0.045 (2)	0.055 (3)	0.069 (3)	−0.026 (2)	−0.033 (2)	0.012 (2)
C14	0.038 (2)	0.038 (2)	0.052 (2)	−0.0141 (18)	−0.0200 (19)	0.0060 (18)
C15	0.051 (3)	0.054 (3)	0.048 (2)	−0.030 (2)	−0.019 (2)	0.005 (2)
C16	0.064 (3)	0.084 (4)	0.053 (3)	−0.034 (3)	−0.012 (2)	−0.016 (3)
C17	0.090 (4)	0.088 (4)	0.062 (3)	−0.041 (3)	−0.007 (3)	−0.022 (3)
C18	0.067 (3)	0.072 (4)	0.080 (4)	−0.023 (3)	0.007 (3)	−0.027 (3)
C19	0.052 (3)	0.057 (3)	0.062 (3)	−0.023 (2)	−0.011 (2)	−0.005 (2)
C20	0.038 (2)	0.045 (2)	0.047 (2)	−0.0190 (18)	−0.0133 (19)	0.0008 (18)
C21	0.032 (2)	0.042 (2)	0.049 (2)	−0.0174 (17)	−0.0159 (18)	0.0078 (18)
C22	0.040 (2)	0.053 (3)	0.050 (2)	−0.0193 (19)	−0.0116 (19)	−0.004 (2)
C23	0.033 (2)	0.047 (3)	0.068 (3)	−0.0118 (18)	−0.015 (2)	−0.005 (2)
C24	0.031 (2)	0.048 (2)	0.045 (2)	−0.0144 (18)	−0.0130 (18)	−0.0004 (18)
C25	0.033 (2)	0.083 (3)	0.043 (2)	−0.026 (2)	0.0028 (17)	−0.030 (2)
C26	0.048 (3)	0.093 (4)	0.048 (2)	−0.034 (2)	0.011 (2)	−0.043 (2)
C27	0.042 (2)	0.067 (3)	0.064 (3)	−0.026 (2)	0.021 (2)	−0.041 (2)
C28	0.0299 (19)	0.047 (2)	0.051 (2)	−0.0175 (17)	0.0084 (17)	−0.0198 (19)
C29	0.0256 (17)	0.041 (2)	0.0377 (19)	−0.0150 (15)	0.0030 (15)	−0.0147 (16)
C30	0.0262 (18)	0.039 (2)	0.061 (3)	−0.0124 (16)	0.0056 (18)	−0.0135 (19)
C31	0.021 (2)	0.073 (4)	0.104 (4)	−0.005 (2)	0.008 (3)	−0.019 (3)
C32	0.030 (2)	0.064 (3)	0.093 (4)	−0.014 (2)	−0.011 (3)	−0.006 (3)
C33	0.0269 (19)	0.038 (2)	0.057 (2)	−0.0139 (16)	−0.0053 (18)	−0.0034 (18)
C34	0.0268 (18)	0.040 (2)	0.0400 (19)	−0.0135 (16)	−0.0072 (16)	−0.0044 (16)
C35	0.0279 (18)	0.037 (2)	0.0366 (19)	−0.0146 (15)	0.0003 (15)	−0.0075 (16)
C36	0.044 (2)	0.059 (3)	0.042 (2)	−0.026 (2)	−0.0122 (19)	−0.0059 (19)
C37	0.057 (3)	0.077 (3)	0.036 (2)	−0.031 (2)	−0.007 (2)	−0.017 (2)
C38	0.036 (2)	0.070 (3)	0.035 (2)	−0.021 (2)	0.0015 (17)	−0.0209 (19)
C39	0.035 (2)	0.068 (3)	0.058 (3)	−0.017 (2)	0.0049 (19)	−0.036 (2)
C40	0.042 (3)	0.099 (4)	0.085 (4)	−0.024 (3)	0.018 (3)	−0.060 (3)
C41	0.034 (2)	0.068 (3)	0.095 (4)	−0.012 (2)	0.016 (2)	−0.045 (3)
C42	0.0228 (19)	0.046 (2)	0.071 (3)	−0.0091 (17)	−0.0041 (19)	−0.012 (2)
C43	0.0266 (18)	0.040 (2)	0.052 (2)	−0.0137 (16)	−0.0056 (17)	−0.0069 (18)
C44	0.029 (2)	0.044 (3)	0.078 (3)	−0.0104 (18)	−0.012 (2)	0.000 (2)
C45	0.033 (3)	0.083 (4)	0.117 (5)	−0.015 (3)	−0.013 (3)	0.009 (4)
C46	0.037 (3)	0.088 (4)	0.107 (5)	−0.028 (3)	−0.031 (3)	0.005 (3)
C47	0.033 (2)	0.053 (3)	0.077 (3)	−0.023 (2)	−0.027 (2)	0.013 (2)
C48	0.048 (2)	0.048 (3)	0.052 (2)	−0.025 (2)	−0.021 (2)	0.002 (2)
C49	0.035 (2)	0.038 (2)	0.045 (2)	−0.0155 (17)	−0.0133 (18)	−0.0042 (17)
C50	0.071 (3)	0.071 (3)	0.067 (3)	−0.040 (3)	−0.029 (3)	−0.006 (3)
C51	0.087 (4)	0.085 (4)	0.049 (3)	−0.039 (3)	−0.015 (3)	−0.028 (3)
C52	0.061 (3)	0.067 (3)	0.050 (2)	−0.026 (2)	−0.006 (2)	−0.025 (2)

Geometric parameters (Å, °)

Cu1—O1	1.924 (3)	C15—C16	1.416 (7)
Cu1—O5	1.965 (2)	C15—C20	1.427 (5)
Cu1—O5^{i}	2.440 (3)	C16—C17	1.349 (8)
Cu1—N1	2.012 (3)	C16—H16	0.9300
Cu1—N4	2.037 (3)	C17—C18	1.404 (8)
Cu2—O3	1.916 (3)	C17—H17	0.9300
Cu2—O7^{ii}	1.964 (2)	C18—C19	1.345 (8)
Cu2—O7^{iii}	2.348 (3)	C18—H18	0.9300
Cu2—N5	2.017 (3)	C19—C20	1.419 (7)
Cu2—N8	2.024 (3)	C19—H19	0.9300
O1—C1	1.287 (5)	C20—C21	1.421 (6)
O2—C1	1.209 (5)	C21—C22	1.352 (6)
O3—C12	1.262 (6)	C21—C24	1.511 (5)
O4—C12	1.230 (6)	C22—C23	1.404 (6)
O5—C13	1.232 (5)	C22—H22	0.9300
O5—Cu1^{i}	2.440 (3)	C23—H23	0.9300
O6—C13	1.216 (6)	C25—C26	1.390 (6)
O7—C24	1.262 (5)	C25—H25	0.9300
O7—Cu2^{iv}	1.964 (2)	C26—C27	1.357 (6)
O7—Cu2^{iii}	2.348 (3)	C26—H26	0.9300
O8—C24	1.224 (5)	C27—C28	1.414 (6)
N1—C25	1.339 (5)	C27—H27	0.9300
N1—C29	1.360 (5)	C28—C29	1.384 (6)
N2—C31	1.347 (6)	C28—C30	1.464 (6)
N2—C30	1.353 (6)	C29—C35	1.441 (5)
N3—C32	1.308 (7)	C30—C33	1.393 (6)
N3—C33	1.357 (5)	C31—C32	1.359 (8)
N4—C38	1.332 (5)	C31—H31	0.9300
N4—C35	1.352 (5)	C32—H32	0.9300
N5—C39	1.325 (5)	C33—C34	1.449 (6)
N5—C43	1.367 (5)	C34—C36	1.393 (6)
N6—C45	1.329 (7)	C34—C35	1.391 (5)
N6—C44	1.344 (7)	C36—C37	1.370 (7)
N7—C46	1.349 (9)	C36—H36	0.9300
N7—C47	1.366 (5)	C37—C38	1.389 (6)
N8—C52	1.329 (6)	C37—H37	0.9300
N8—C49	1.357 (5)	C38—H38	0.9300
C1—C2	1.508 (6)	C39—C40	1.396 (6)
C2—C11	1.376 (6)	C39—H39	0.9300
C2—C3	1.412 (6)	C40—C41	1.354 (7)
C3—C4	1.418 (6)	C40—H40	0.9300
C3—C8	1.441 (6)	C41—C42	1.402 (7)
C4—C5	1.342 (7)	C41—H41	0.9300
C4—H4	0.9300	C42—C43	1.402 (6)
C5—C6	1.404 (8)	C42—C44	1.451 (6)

C5—H5	0.9300	C43—C49	1.429 (6)
C6—C7	1.367 (8)	C44—C47	1.403 (8)
C6—H6	0.9300	C45—C46	1.334 (10)
C7—C8	1.422 (7)	C45—H45	0.9300
C7—H7	0.9300	C46—H46	0.9300
C8—C9	1.423 (6)	C47—C48	1.450 (7)
C9—C10	1.358 (7)	C48—C50	1.373 (7)
C9—C12	1.511 (6)	C48—C49	1.391 (5)
C10—C11	1.396 (6)	C50—C51	1.373 (8)
C10—H10	0.9300	C50—H50	0.9300
C11—H11	0.9300	C51—C52	1.396 (6)
C13—C14	1.515 (5)	C51—H51	0.9300
C14—C23	1.363 (7)	C52—H52	0.9300
C14—C15	1.412 (7)		
O1—Cu1—O5	91.2 (1)	C20—C19—H19	119.1
O1—Cu1—N1	171.5 (1)	C21—C20—C19	123.7 (4)
O5—Cu1—N1	96.2 (1)	C21—C20—C15	118.5 (4)
O1—Cu1—N4	92.4 (1)	C19—C20—C15	117.7 (4)
O5—Cu1—N4	171.8 (1)	C22—C21—C20	120.1 (4)
N1—Cu1—N4	80.8 (1)	C22—C21—C24	119.6 (4)
O1—Cu1—O5^{i}	86.7 (1)	C20—C21—C24	120.3 (3)
O5—Cu1—O5^{i}	72.8 (1)	C21—C22—C23	121.6 (5)
N1—Cu1—O5^{i}	91.5 (1)	C21—C22—H22	119.2
N4—Cu1—O5^{i}	114.8 (1)	C23—C22—H22	119.2
O7^{ii}—Cu2—O3	89.5 (1)	C14—C23—C22	120.1 (4)
O7^{ii}—Cu2—N5	98.1 (1)	C14—C23—H23	120.0
O3—Cu2—N5	172.4 (1)	C22—C23—H23	120.0
O7^{ii}—Cu2—N8	173.9 (1)	O8—C24—O7	124.7 (3)
O3—Cu2—N8	91.7 (1)	O8—C24—C21	119.6 (4)
N5—Cu2—N8	80.8 (1)	O7—C24—C21	115.7 (3)
O7^{ii}—Cu2—O7^{iii}	74.6 (1)	N1—C25—C26	121.4 (4)
O3—Cu2—O7^{iii}	87.0 (1)	N1—C25—H25	119.3
N5—Cu2—O7^{iii}	94.3 (1)	C26—C25—H25	119.3
N8—Cu2—O7^{iii}	111.4 (1)	C27—C26—C25	121.1 (4)
C1—O1—Cu1	120.8 (3)	C27—C26—H26	119.5
C12—O3—Cu2	120.9 (3)	C25—C26—H26	119.5
C13—O5—Cu1	120.1 (3)	C26—C27—C28	118.4 (4)
C13—O5—Cu1^{i}	132.6 (2)	C26—C27—H27	120.8
Cu1—O5—Cu1^{i}	107.22 (12)	C28—C27—H27	120.8
C24—O7—Cu2^{iv}	121.6 (2)	C29—C28—C27	117.8 (4)
C24—O7—Cu2^{iii}	129.8 (2)	C29—C28—C30	118.6 (4)
Cu2^{iv}—O7—Cu2^{iii}	105.40 (11)	C27—C28—C30	123.5 (4)
C25—N1—C29	118.1 (3)	N1—C29—C28	123.1 (4)
C25—N1—Cu1	128.0 (3)	N1—C29—C35	115.7 (3)
C29—N1—Cu1	113.8 (2)	C28—C29—C35	121.1 (3)

C31—N2—C30	114.0 (5)	N2—C30—C33	122.1 (4)
C32—N3—C33	116.1 (5)	N2—C30—C28	118.0 (4)
C38—N4—C35	117.6 (3)	C33—C30—C28	119.9 (4)
C38—N4—Cu1	129.1 (3)	N2—C31—C32	123.8 (5)
C35—N4—Cu1	113.3 (2)	N2—C31—H31	118.1
C39—N5—C43	117.6 (4)	C32—C31—H31	118.1
C39—N5—Cu2	128.9 (3)	N3—C32—C31	122.7 (5)
C43—N5—Cu2	113.5 (3)	N3—C32—H32	118.7
C45—N6—C44	115.2 (6)	C31—C32—H32	118.7
C46—N7—C47	113.0 (6)	N3—C33—C30	121.2 (4)
C52—N8—C49	117.4 (4)	N3—C33—C34	118.0 (4)
C52—N8—Cu2	128.8 (3)	C30—C33—C34	120.8 (3)
C49—N8—Cu2	113.8 (3)	C36—C34—C35	117.7 (4)
O2—C1—O1	124.3 (4)	C36—C34—C33	123.5 (4)
O2—C1—C2	120.3 (4)	C35—C34—C33	118.8 (4)
O1—C1—C2	115.4 (4)	N4—C35—C34	123.4 (4)
C11—C2—C3	119.7 (4)	N4—C35—C29	116.0 (3)
C11—C2—C1	116.2 (4)	C34—C35—C29	120.6 (4)
C3—C2—C1	124.1 (4)	C37—C36—C34	119.2 (4)
C2—C3—C4	123.1 (4)	C37—C36—H36	120.4
C2—C3—C8	118.9 (4)	C34—C36—H36	120.4
C4—C3—C8	118.0 (4)	C36—C37—C38	119.5 (4)
C5—C4—C3	122.4 (5)	C36—C37—H37	120.3
C5—C4—H4	118.8	C38—C37—H37	120.3
C3—C4—H4	118.8	N4—C38—C37	122.6 (4)
C4—C5—C6	120.3 (5)	N4—C38—H38	118.7
C4—C5—H5	119.9	C37—C38—H38	118.7
C6—C5—H5	119.9	N5—C39—C40	122.8 (4)
C7—C6—C5	120.0 (6)	N5—C39—H39	118.6
C7—C6—H6	120.0	C40—C39—H39	118.6
C5—C6—H6	120.0	C41—C40—C39	120.3 (5)
C6—C7—C8	121.8 (5)	C41—C40—H40	119.9
C6—C7—H7	119.1	C39—C40—H40	119.9
C8—C7—H7	119.1	C40—C41—C42	118.7 (4)
C7—C8—C9	123.2 (4)	C40—C41—H41	120.6
C7—C8—C3	117.5 (4)	C42—C41—H41	120.6
C9—C8—C3	119.3 (4)	C41—C42—C43	118.1 (4)
C10—C9—C8	119.4 (4)	C41—C42—C44	123.3 (4)
C10—C9—C12	117.3 (4)	C43—C42—C44	118.6 (5)
C8—C9—C12	123.3 (4)	N5—C43—C42	122.4 (4)
C9—C10—C11	121.7 (4)	N5—C43—C49	116.0 (4)
C9—C10—H10	119.2	C42—C43—C49	121.6 (4)
C11—C10—H10	119.2	N6—C44—C47	121.9 (4)
C2—C11—C10	121.1 (4)	N6—C44—C42	118.7 (5)
C2—C11—H11	119.5	C47—C44—C42	119.4 (4)
C10—C11—H11	119.5	N6—C45—C46	123.2 (6)
O4—C12—O3	124.6 (4)	N6—C45—H45	118.4
O4—C12—C9	121.6 (4)	C46—C45—H45	118.4
O3—C12—C9	113.8 (4)	C45—C46—N7	124.9 (5)

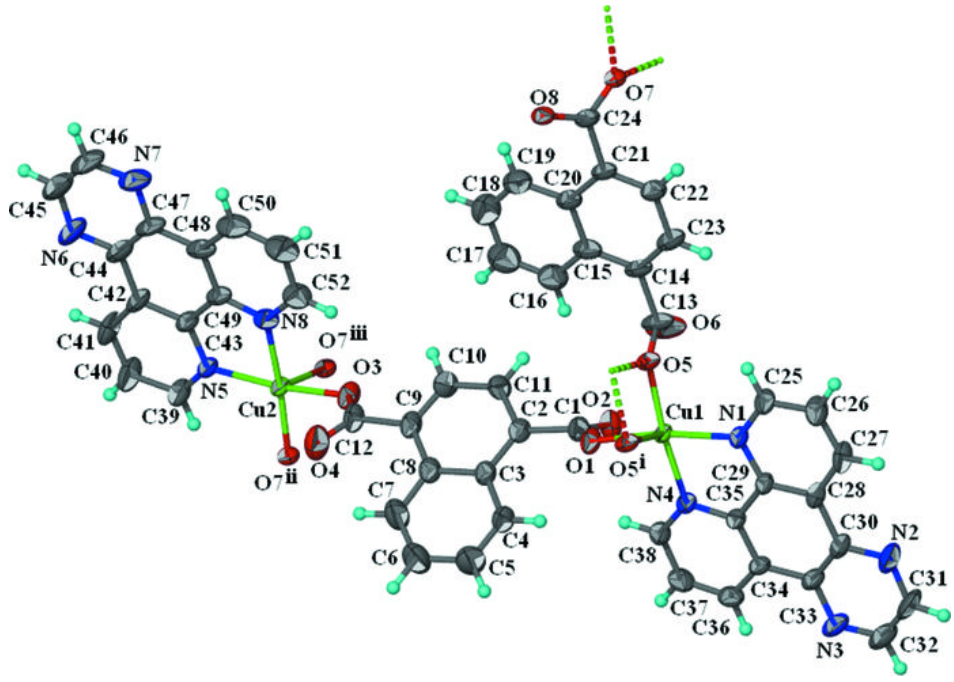
O6—C13—O5	122.5 (4)	C45—C46—H46	117.6
O6—C13—C14	121.4 (4)	N7—C46—H46	117.6
O5—C13—C14	116.1 (4)	N7—C47—C44	121.8 (5)
C23—C14—C15	120.5 (4)	N7—C47—C48	116.9 (5)
C23—C14—C13	119.3 (4)	C44—C47—C48	121.3 (4)
C15—C14—C13	120.2 (4)	C50—C48—C49	117.6 (5)
C14—C15—C16	122.5 (4)	C50—C48—C47	123.9 (4)
C14—C15—C20	119.1 (4)	C49—C48—C47	118.6 (4)
C16—C15—C20	118.4 (5)	N8—C49—C48	123.7 (4)
C17—C16—C15	121.6 (5)	N8—C49—C43	115.8 (3)
C17—C16—H16	119.2	C48—C49—C43	120.5 (4)
C15—C16—H16	119.2	C51—C50—C48	119.8 (4)
C16—C17—C18	120.1 (6)	C51—C50—H50	120.1
C16—C17—H17	119.9	C48—C50—H50	120.1
C18—C17—H17	119.9	C50—C51—C52	119.3 (5)
C19—C18—C17	120.3 (6)	C50—C51—H51	120.3
C19—C18—H18	119.8	C52—C51—H51	120.3
C17—C18—H18	119.8	N8—C52—C51	122.3 (5)
C18—C19—C20	121.8 (5)	N8—C52—H52	118.8
C18—C19—H19	119.1	C51—C52—H52	118.8
O5—Cu1—O1—C1	93.3 (2)	Cu2^{iii}—O7—C24—C21	33.8 (3)
N4—Cu1—O1—C1	−79.3 (2)	C22—C21—C24—O8	−120.2 (4)
O5^{i}—Cu1—O1—C1	166.0 (2)	C20—C21—C24—O8	61.2 (4)
O7^{ii}—Cu2—O3—C12	−90.6 (2)	C22—C21—C24—O7	60.2 (4)
N8—Cu2—O3—C12	83.4 (2)	C20—C21—C24—O7	−118.5 (4)
O7^{iii}—Cu2—O3—C12	−165.2 (2)	C29—N1—C25—C26	−0.2 (7)
O1—Cu1—O5—C13	−94.3 (3)	Cu1—N1—C25—C26	177.2 (4)
N1—Cu1—O5—C13	89.8 (3)	N1—C25—C26—C27	−0.8 (8)
O5^{i}—Cu1—O5—C13	179.4 (3)	C25—C26—C27—C28	0.9 (8)
O1—Cu1—O5—Cu1^{i}	86.21 (14)	C26—C27—C28—C29	−0.1 (7)
N1—Cu1—O5—Cu1^{i}	−89.68 (14)	C26—C27—C28—C30	178.1 (4)
O5^{i}—Cu1—O5—Cu1^{i}	0.0	C25—N1—C29—C28	0.9 (6)
O5—Cu1—N1—C25	4.6 (4)	Cu1—N1—C29—C28	−176.8 (3)
N4—Cu1—N1—C25	176.9 (4)	C25—N1—C29—C35	−176.4 (4)
O5^{i}—Cu1—N1—C25	−68.3 (4)	Cu1—N1—C29—C35	5.9 (4)
O5—Cu1—N1—C29	−178.0 (3)	C27—C28—C29—N1	−0.8 (6)
N4—Cu1—N1—C29	−5.7 (3)	C30—C28—C29—N1	−179.1 (4)
O5^{i}—Cu1—N1—C29	109.2 (3)	C27—C28—C29—C35	176.4 (4)
O1—Cu1—N4—C38	11.1 (4)	C30—C28—C29—C35	−2.0 (6)
N1—Cu1—N4—C38	−174.0 (4)	C31—N2—C30—C33	−0.1 (7)
O5^{i}—Cu1—N4—C38	98.6 (4)	C31—N2—C30—C28	−178.6 (4)
O1—Cu1—N4—C35	−170.4 (3)	C29—C28—C30—N2	−177.6 (4)
N1—Cu1—N4—C35	4.5 (3)	C27—C28—C30—N2	4.1 (7)
O5^{i}—Cu1—N4—C35	−82.9 (3)	C29—C28—C30—C33	3.8 (6)
O7^{ii}—Cu2—N5—C39	−7.6 (4)	C27—C28—C30—C33	−174.4 (4)
N8—Cu2—N5—C39	178.5 (4)	C30—N2—C31—C32	1.8 (8)

O7^{iii}—Cu2—N5—C39	67.5 (4)	C33—N3—C32—C31	0.0 (8)
O7^{ii}—Cu2—N5—C43	175.6 (3)	N2—C31—C32—N3	−1.9 (9)
N8—Cu2—N5—C43	1.6 (3)	C32—N3—C33—C30	1.7 (6)
O7^{iii}—Cu2—N5—C43	−109.4 (3)	C32—N3—C33—C34	−179.3 (4)
O3—Cu2—N8—C52	−1.7 (4)	N2—C30—C33—N3	−1.7 (7)
N5—Cu2—N8—C52	179.9 (4)	C28—C30—C33—N3	176.8 (4)
O7^{iii}—Cu2—N8—C52	−89.1 (4)	N2—C30—C33—C34	179.3 (4)
O3—Cu2—N8—C49	178.0 (3)	C28—C30—C33—C34	−2.2 (6)
N5—Cu2—N8—C49	−0.4 (3)	N3—C33—C34—C36	−0.4 (6)
O7^{iii}—Cu2—N8—C49	90.5 (3)	C30—C33—C34—C36	178.6 (4)
Cu1—O1—C1—O2	6.7 (3)	N3—C33—C34—C35	179.8 (4)
Cu1—O1—C1—C2	−173.3 (2)	C30—C33—C34—C35	−1.2 (6)
O2—C1—C2—C11	−47.7 (4)	C38—N4—C35—C34	−2.0 (6)
O1—C1—C2—C11	132.3 (4)	Cu1—N4—C35—C34	179.3 (3)
O2—C1—C2—C3	132.6 (4)	C38—N4—C35—C29	176.0 (4)
O1—C1—C2—C3	−47.4 (4)	Cu1—N4—C35—C29	−2.7 (4)
C11—C2—C3—C4	179.7 (4)	C36—C34—C35—N4	1.1 (6)
C1—C2—C3—C4	−0.6 (6)	C33—C34—C35—N4	−179.1 (4)
C11—C2—C3—C8	0.5 (6)	C36—C34—C35—C29	−176.8 (4)
C1—C2—C3—C8	−179.8 (3)	C33—C34—C35—C29	3.1 (6)
C2—C3—C4—C5	−177.5 (5)	N1—C29—C35—N4	−2.1 (5)
C8—C3—C4—C5	1.7 (7)	C28—C29—C35—N4	−179.5 (4)
C3—C4—C5—C6	−1.2 (10)	N1—C29—C35—C34	175.9 (3)
C4—C5—C6—C7	0.6 (11)	C28—C29—C35—C34	−1.5 (6)
C5—C6—C7—C8	−0.6 (10)	C35—C34—C36—C37	0.6 (6)
C6—C7—C8—C9	178.7 (5)	C33—C34—C36—C37	−179.2 (4)
C6—C7—C8—C3	1.2 (8)	C34—C36—C37—C38	−1.4 (7)
C2—C3—C8—C7	177.6 (4)	C35—N4—C38—C37	1.1 (7)
C4—C3—C8—C7	−1.6 (6)	Cu1—N4—C38—C37	179.6 (3)
C2—C3—C8—C9	−0.1 (6)	C36—C37—C38—N4	0.5 (7)
C4—C3—C8—C9	−179.3 (4)	C43—N5—C39—C40	−2.5 (7)
C7—C8—C9—C10	−178.1 (5)	Cu2—N5—C39—C40	−179.3 (4)
C3—C8—C9—C10	−0.6 (6)	N5—C39—C40—C41	2.9 (9)
C7—C8—C9—C12	2.1 (7)	C39—C40—C41—C42	−1.4 (9)
C3—C8—C9—C12	179.6 (3)	C40—C41—C42—C43	−0.2 (8)
C8—C9—C10—C11	0.8 (7)	C40—C41—C42—C44	−179.1 (5)
C12—C9—C10—C11	−179.3 (4)	C39—N5—C43—C42	0.8 (6)
C3—C2—C11—C10	−0.3 (6)	Cu2—N5—C43—C42	178.1 (3)
C1—C2—C11—C10	180.0 (4)	C39—N5—C43—C49	−179.8 (4)
C9—C10—C11—C2	−0.4 (7)	Cu2—N5—C43—C49	−2.6 (4)
Cu2—O3—C12—O4	−3.8 (3)	C41—C42—C43—N5	0.5 (7)
Cu2—O3—C12—C9	176.4 (2)	C44—C42—C43—N5	179.5 (4)
C10—C9—C12—O4	−142.3 (4)	C41—C42—C43—C49	−178.8 (4)
C8—C9—C12—O4	37.5 (4)	C44—C42—C43—C49	0.2 (6)
C10—C9—C12—O3	37.5 (4)	C45—N6—C44—C47	1.4 (7)
C8—C9—C12—O3	−142.7 (4)	C45—N6—C44—C42	−179.9 (5)
Cu1—O5—C13—O6	−7.4 (4)	C41—C42—C44—N6	−0.2 (7)
Cu1^{i}—O5—C13—O6	171.9 (4)	C43—C42—C44—N6	−179.1 (4)

Cu1—O5—C13—C14	172.7 (3)	C41—C42—C44—C47	178.6 (5)
Cu1^{i}—O5—C13—C14	−8.0 (4)	C43—C42—C44—C47	−0.4 (6)
O6—C13—C14—C23	−91.8 (5)	C44—N6—C45—C46	−0.4 (9)
O5—C13—C14—C23	88.0 (5)	N6—C45—C46—N7	−1.4 (11)
O6—C13—C14—C15	88.7 (5)	C47—N7—C46—C45	1.9 (9)
O5—C13—C14—C15	−91.4 (5)	C46—N7—C47—C44	−0.8 (7)
C23—C14—C15—C16	178.7 (5)	C46—N7—C47—C48	179.9 (5)
C13—C14—C15—C16	−1.8 (7)	N6—C44—C47—N7	−0.8 (7)
C23—C14—C15—C20	−2.2 (7)	C42—C44—C47—N7	−179.5 (4)
C13—C14—C15—C20	177.2 (4)	N6—C44—C47—C48	178.5 (4)
C14—C15—C16—C17	179.5 (5)	C42—C44—C47—C48	−0.3 (7)
C20—C15—C16—C17	0.5 (8)	N7—C47—C48—C50	−1.1 (7)
C15—C16—C17—C18	0.0 (9)	C44—C47—C48—C50	179.6 (5)
C16—C17—C18—C19	−0.7 (9)	N7—C47—C48—C49	−179.7 (4)
C17—C18—C19—C20	1.0 (9)	C44—C47—C48—C49	1.1 (7)
C18—C19—C20—C21	177.7 (5)	C52—N8—C49—C48	−0.1 (6)
C18—C19—C20—C15	−0.5 (7)	Cu2—N8—C49—C48	−179.8 (3)
C14—C15—C20—C21	2.4 (6)	C52—N8—C49—C43	178.9 (4)
C16—C15—C20—C21	−178.5 (4)	Cu2—N8—C49—C43	−0.8 (5)
C14—C15—C20—C19	−179.3 (4)	C50—C48—C49—N8	−0.9 (7)
C16—C15—C20—C19	−0.2 (7)	C47—C48—C49—N8	177.7 (4)
C19—C20—C21—C22	−178.3 (4)	C50—C48—C49—C43	−179.9 (4)
C15—C20—C21—C22	−0.1 (6)	C47—C48—C49—C43	−1.2 (6)
C19—C20—C21—C24	0.3 (6)	N5—C43—C49—N8	2.2 (5)
C15—C20—C21—C24	178.5 (4)	C42—C43—C49—N8	−178.4 (4)
C20—C21—C22—C23	−2.4 (7)	N5—C43—C49—C48	−178.7 (4)
C24—C21—C22—C23	178.9 (4)	C42—C43—C49—C48	0.6 (6)
C15—C14—C23—C22	−0.3 (7)	C49—C48—C50—C51	1.5 (7)
C13—C14—C23—C22	−179.7 (4)	C47—C48—C50—C51	−177.1 (5)
C21—C22—C23—C14	2.7 (7)	C48—C50—C51—C52	−1.0 (8)
Cu2^{iv}—O7—C24—O8	10.8 (3)	C49—N8—C52—C51	0.6 (7)
Cu2^{iii}—O7—C24—O8	−145.8 (3)	Cu2—N8—C52—C51	−179.8 (4)
Cu2^{iv}—O7—C24—C21	−169.6 (2)	C50—C51—C52—N8	0.0 (8)

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

Fig. 1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C26
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Fig. 2