catena-Poly[[[bis(1H-benzimidazole-κN³)copper(II)]-μ-3-(4-carboxylatophenoxy)propionato-κ²O:O'] N,N-dimethylformamide solvate pentahydrate]

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In the crystal structure of the polymeric title compound, $\{[Cu(C_7H_5N_2)_2(C_{10}H_8O_5)]\cdot C_3H_7NO\cdot 5H_2O\}_n$, the 3-(4-carboxylatophenoxy)propionate dianion links the bis(benzimidazole)copper groups into a linear chain running along the a axis of the monoclinic unit cell, with the dianion binding through one O atom of each carboxylate end to confer a distorted square-planar environment on the copper center.

Related literature

For the 2,2′-bipyridine chelated transition metal derivatives of 3-(4-carboxylatophenoxy)propionic acid, see: Kong *et al.* (2007a,b).
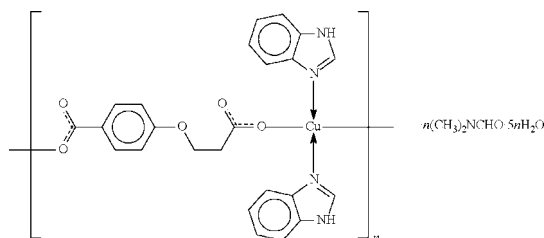
Experimental

Crystal data

$[Cu(C_7H_5N_2)_2(C_{10}H_8O_5)]\cdot C_3H_7NO\cdot 5H_2O$	β = 102.834 (4)°
M_r = 671.16	V = 3099.9 (8) Å^3
Monoclinic, $P2_1/n$	Z = 4
a = 12.179 (2) Å	Mo $K\alpha$ radiation
b = 15.898 (2) Å	μ = 0.77 mm^{-1}
c = 16.420 (2) Å	T = 295 (2) K
	0.38 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	23434 measured reflections
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	5460 independent reflections
	3293 reflections with $I > 2\sigma(I)$
T_{min} = 0.590, T_{max} = 0.880	R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071	66 restraints
$wR(F^2)$ = 0.247	H-atom parameters constrained
S = 1.11	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
5460 reflections	$\Delta\rho_{min}$ = −0.51 e Å^{-3}
399 parameters	

Data collection: *RAPID-AUTO* (Rigaku, 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); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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supplementary materials

catena-Poly[[[bis(1*H*-benzimidazole-κN^3)copper(II)]-μ-3-(4-carboxylatophenoxy)propionato-κ^2O:*O'*] *N,N*-dimethylformamide solvate pentahydrate]

L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Comment

The present report follows our studies on the transition metal derivatives of 3-(4-carboxylatophenoxy)propionic acid. Previous reports (Kong *et al.*, 2007*a*,b) describe the crystal structures of isostrutural manganese(II) and cobalt(II) adducts with 2,2'-bipyridine. In the present work, DMF, which was used as a co-solvent, is incorporated into the crystal structure.

The 3-(4-carboxylatophenoxy)propionate dianion links the di(benzimidazole)copper groups into a linear chain running along the *a* axis of the monoclinic unit cell, with the dianion binding through one O atom each from both carboxylate ends to confer a distorted square-planar environment to the copper center.

Experimental

Copper nitrate hexahydrate (5 mmol), benzimidazole (10 mmol) and 3-(4-carboxylatophenoxy)propionic acid were dissolved in DMF-water (1:1, *v*/*v*) solution, and the pH was adjusted to 7 with 0.1 *M* sodium hydroxide. The solution was fltered and then set aside for the growth of crystals over a week.

Refinement

The displacement parameters of the water and *N,N*-dimethylformamide (DMF) molecules were restrained to be nearly isotropic. The non-H atoms of the DMF molecule were restrained to lie in an approximately flat plane, and the C25—O6, C25—N5 and N5—C26 (= N5—C27) bond distances were restrained to 1.25 (1), 1.35 (1) and 1.45 (1) Å, respectively. C-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 were placed in chemically sensible positions, however, not all of them form hydrogen bonds. Since the positions of the water H atoms cannot be unambiguously determined, a table of hydrogen bond is not included.
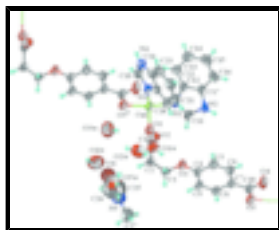
Figures

Fig. 1. Part of the polymeric structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. Symmetry code: (i) $x - 1$, y, z.

supplementary materials

catena-Poly[[[bis(1*H*-benzimidazole-κN^3)copper(II)]-μ- 3-(4-carboxylatophenoxy)propionato-κ^2O:O'] *N,N*-di-methylformamide solvate pentahydrate]

Crystal data

[Cu(C$_7$H$_5$N$_2$)$_2$(C$_{10}$H$_8$O$_5$)]·C$_3$H$_7$NO·5H$_2$O	F_{000} = 1404
M_r = 671.16	D_x = 1.438 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 12961 reflections
a = 12.179 (2) Å	θ = 3.0–27.5º
b = 15.898 (2) Å	μ = 0.77 mm^{-1}
c = 16.420 (2) Å	T = 295 (2) K
β = 102.834 (4)º	Block, blue
V = 3099.9 (8) Å^3	0.38 × 0.25 × 0.17 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	5460 independent reflections
Radiation source: fine-focus sealed tube	3293 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 25.0º
T = 295(2) K	θ_{min} = 3.0º
ω scans	$h = -14\rightarrow13$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -18\rightarrow18$
T_{min} = 0.590, T_{max} = 0.880	$l = -19\rightarrow19$
23434 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
$R[F^2 > 2\sigma(F^2)]$ = 0.071	H-atom parameters constrained
$wR(F^2)$ = 0.247	$w = 1/[\sigma^2(F_o^2) + (0.1404P)^2 + 1.2497P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.11	$(\Delta/\sigma)_{max}$ = 0.001
5460 reflections	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
399 parameters	$\Delta\rho_{min}$ = −0.51 e Å^{-3}
66 restraints	Extinction correction: SHELXL, Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0080 (18)

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.

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

	x	y	z	$U_{iso}*/U_{eq}$
Cu1	0.42338 (5)	0.38523 (4)	0.21419 (4)	0.0554 (3)
O1	0.4755 (3)	0.2807 (3)	0.1671 (2)	0.0630 (10)
O2	0.5993 (4)	0.2998 (3)	0.2855 (3)	0.0785 (13)
O3	0.7685 (3)	0.2409 (3)	0.1683 (3)	0.0663 (11)
O4	1.2319 (4)	0.3954 (3)	0.1235 (3)	0.0865 (15)
O5	1.2925 (3)	0.3207 (3)	0.2359 (3)	0.0663 (11)
O6	0.4539 (7)	0.0029 (5)	0.2326 (6)	0.169 (3)
O1W	0.8142 (4)	0.3305 (3)	0.5698 (3)	0.0871 (14)
H1W1	0.8856	0.3333	0.5841	0.131*
H1W2	0.7928	0.2797	0.5711	0.131*
O2W	0.6657 (6)	0.2406 (4)	0.4455 (4)	0.124 (2)
H2W1	0.6472	0.2499	0.3933	0.186*
H2W2	0.6073	0.2235	0.4609	0.186*
O3W	0.3860 (6)	0.2179 (5)	0.3771 (5)	0.156 (3)
H3W1	0.4473	0.2443	0.3950	0.233*
H3W2	0.3542	0.2355	0.3288	0.233*
O4W	0.4405 (7)	0.0577 (5)	0.3838 (6)	0.180 (3)
H4W1	0.3869	0.0384	0.3462	0.270*
H4W2	0.4198	0.0559	0.4299	0.270*
O5W	0.6616 (4)	0.0497 (4)	0.4591 (3)	0.1076 (18)
H5W1	0.6344	0.0923	0.4303	0.161*
H5W2	0.7053	0.0653	0.5044	0.161*
N1	0.5139 (4)	0.4592 (3)	0.1570 (3)	0.0579 (12)
N2	0.6480 (4)	0.5091 (3)	0.0992 (3)	0.0628 (13)
H2N	0.7116	0.5125	0.0849	0.075*
N3	0.4082 (4)	0.4714 (3)	0.2970 (3)	0.0619 (12)
N4	0.3327 (4)	0.5670 (3)	0.3673 (3)	0.0685 (14)
H4N	0.2825	0.5977	0.3824	0.082*
N5	0.5337 (6)	−0.0769 (4)	0.1470 (5)	0.119 (2)
C1	0.5601 (5)	0.2565 (4)	0.2215 (4)	0.0602 (14)
C2	0.6158 (5)	0.1738 (4)	0.2072 (4)	0.0638 (15)
H2A	0.5943	0.1307	0.2425	0.077*
H2B	0.5892	0.1566	0.1495	0.077*
C3	0.7430 (5)	0.1814 (4)	0.2266 (4)	0.0646 (16)
H3A	0.7709	0.2010	0.2834	0.078*
H3B	0.7772	0.1274	0.2202	0.078*
C4	0.8798 (4)	0.2598 (4)	0.1730 (4)	0.0562 (14)
C5	0.8999 (5)	0.3188 (4)	0.1135 (4)	0.0636 (15)

H5	0.8399	0.3412	0.0744	0.076*
C6	1.0065 (5)	0.3428 (4)	0.1136 (4)	0.0622 (15)
H6	1.0191	0.3801	0.0731	0.075*
C7	1.0973 (4)	0.3128 (4)	0.1728 (3)	0.0538 (13)
C8	1.0759 (4)	0.2543 (4)	0.2300 (3)	0.0581 (14)
H8	1.1361	0.2331	0.2697	0.070*
C9	0.9696 (4)	0.2267 (4)	0.2302 (4)	0.0595 (14)
H9	0.9581	0.1862	0.2683	0.071*
C10	1.2128 (5)	0.3447 (4)	0.1763 (4)	0.0606 (14)
C11	0.6153 (5)	0.4466 (4)	0.1434 (4)	0.0604 (14)
H11	0.6592	0.3997	0.1623	0.072*
C12	0.4764 (5)	0.5357 (4)	0.1179 (3)	0.0552 (13)
C13	0.3774 (5)	0.5787 (4)	0.1105 (3)	0.0619 (14)
H13	0.3205	0.5588	0.1349	0.074*
C14	0.3653 (6)	0.6521 (4)	0.0657 (4)	0.0758 (18)
H14	0.2991	0.6828	0.0599	0.091*
C15	0.4500 (7)	0.6816 (4)	0.0286 (4)	0.0807 (19)
H15	0.4388	0.7315	−0.0016	0.097*
C16	0.5487 (6)	0.6396 (4)	0.0355 (4)	0.0727 (17)
H16	0.6050	0.6595	0.0104	0.087*
C17	0.5617 (5)	0.5667 (4)	0.0808 (3)	0.0582 (14)
C18	0.3140 (5)	0.5081 (4)	0.3077 (4)	0.0694 (16)
H18	0.2427	0.4941	0.2770	0.083*
C19	0.4946 (5)	0.5092 (4)	0.3561 (3)	0.0579 (14)
C20	0.6081 (5)	0.4948 (4)	0.3737 (4)	0.0706 (17)
H20	0.6400	0.4548	0.3447	0.085*
C21	0.6737 (6)	0.5429 (5)	0.4372 (5)	0.084 (2)
H21	0.7512	0.5343	0.4511	0.101*
C22	0.6276 (7)	0.6027 (4)	0.4801 (5)	0.083 (2)
H22	0.6747	0.6343	0.5212	0.100*
C23	0.5131 (7)	0.6168 (4)	0.4634 (4)	0.0771 (19)
H23	0.4815	0.6563	0.4933	0.093*
C24	0.4475 (6)	0.5696 (4)	0.4002 (4)	0.0640 (15)
C25	0.5381 (9)	−0.0393 (5)	0.2196 (7)	0.140 (4)
H25	0.6030	−0.0435	0.2617	0.168*
C26	0.4364 (13)	−0.0725 (14)	0.0809 (11)	0.336 (12)
H26A	0.4120	−0.0151	0.0727	0.504*
H26B	0.3773	−0.1058	0.0948	0.504*
H26C	0.4539	−0.0937	0.0306	0.504*
C27	0.6256 (8)	−0.1250 (6)	0.1309 (7)	0.134 (4)
H27A	0.6911	−0.1156	0.1747	0.201*
H27B	0.6409	−0.1081	0.0784	0.201*
H27C	0.6064	−0.1837	0.1287	0.201*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0417 (5)	0.0649 (5)	0.0626 (5)	−0.0028 (3)	0.0181 (3)	0.0022 (3)

O1	0.046 (2)	0.073 (3)	0.069 (2)	−0.0064 (19)	0.0104 (19)	0.001 (2)
O2	0.076 (3)	0.078 (3)	0.076 (3)	0.009 (2)	0.005 (2)	−0.008 (2)
O3	0.039 (2)	0.079 (3)	0.082 (3)	−0.0037 (19)	0.0169 (18)	0.017 (2)
O4	0.051 (3)	0.128 (4)	0.075 (3)	−0.027 (2)	0.004 (2)	0.030 (3)
O5	0.047 (2)	0.079 (3)	0.074 (3)	−0.002 (2)	0.015 (2)	0.008 (2)
O6	0.151 (6)	0.150 (6)	0.209 (7)	−0.001 (5)	0.044 (5)	0.004 (5)
O1W	0.084 (3)	0.089 (3)	0.086 (3)	0.026 (3)	0.015 (2)	0.000 (3)
O2W	0.154 (5)	0.127 (5)	0.087 (3)	0.010 (4)	0.018 (3)	0.001 (3)
O3W	0.136 (5)	0.181 (6)	0.149 (5)	−0.012 (5)	0.031 (4)	0.041 (5)
O4W	0.136 (5)	0.165 (6)	0.225 (7)	0.023 (5)	0.011 (5)	−0.010 (6)
O5W	0.078 (3)	0.148 (5)	0.102 (3)	0.019 (3)	0.032 (3)	−0.020 (3)
N1	0.051 (3)	0.065 (3)	0.062 (3)	−0.001 (2)	0.021 (2)	0.001 (2)
N2	0.052 (3)	0.074 (3)	0.069 (3)	−0.015 (2)	0.027 (2)	0.000 (3)
N3	0.043 (3)	0.073 (3)	0.073 (3)	0.001 (2)	0.020 (2)	0.007 (3)
N4	0.061 (3)	0.073 (3)	0.077 (3)	0.014 (3)	0.027 (3)	0.002 (3)
N5	0.104 (5)	0.116 (5)	0.126 (5)	0.014 (4)	0.000 (4)	−0.004 (5)
C1	0.047 (3)	0.065 (4)	0.072 (4)	−0.005 (3)	0.021 (3)	0.002 (3)
C2	0.047 (3)	0.058 (3)	0.091 (4)	−0.002 (3)	0.024 (3)	−0.001 (3)
C3	0.050 (3)	0.059 (3)	0.089 (4)	0.003 (3)	0.024 (3)	0.012 (3)
C4	0.041 (3)	0.063 (3)	0.068 (3)	−0.007 (2)	0.018 (3)	−0.001 (3)
C5	0.048 (3)	0.074 (4)	0.067 (3)	−0.001 (3)	0.010 (3)	0.014 (3)
C6	0.055 (4)	0.068 (4)	0.065 (3)	−0.004 (3)	0.017 (3)	0.013 (3)
C7	0.043 (3)	0.063 (3)	0.058 (3)	−0.003 (2)	0.015 (3)	0.004 (3)
C8	0.042 (3)	0.068 (4)	0.064 (3)	0.005 (3)	0.013 (3)	0.010 (3)
C9	0.040 (3)	0.072 (4)	0.069 (3)	0.005 (3)	0.017 (3)	0.019 (3)
C10	0.046 (3)	0.072 (4)	0.066 (4)	−0.004 (3)	0.016 (3)	0.006 (3)
C11	0.048 (3)	0.072 (4)	0.065 (3)	−0.003 (3)	0.018 (3)	−0.004 (3)
C12	0.055 (3)	0.061 (3)	0.051 (3)	−0.008 (3)	0.015 (2)	−0.009 (3)
C13	0.062 (4)	0.066 (4)	0.058 (3)	0.000 (3)	0.016 (3)	−0.003 (3)
C14	0.084 (5)	0.074 (4)	0.066 (4)	0.013 (4)	0.009 (3)	−0.011 (3)
C15	0.101 (6)	0.068 (4)	0.071 (4)	−0.008 (4)	0.015 (4)	0.009 (3)
C16	0.083 (5)	0.072 (4)	0.065 (4)	−0.016 (4)	0.021 (3)	−0.001 (3)
C17	0.062 (4)	0.060 (4)	0.054 (3)	−0.016 (3)	0.017 (3)	−0.004 (3)
C18	0.054 (4)	0.087 (4)	0.069 (4)	−0.001 (3)	0.018 (3)	0.005 (4)
C19	0.051 (3)	0.062 (3)	0.064 (3)	0.000 (3)	0.019 (3)	0.007 (3)
C20	0.059 (4)	0.075 (4)	0.080 (4)	−0.001 (3)	0.020 (3)	−0.010 (3)
C21	0.060 (4)	0.096 (5)	0.094 (5)	0.003 (4)	0.010 (4)	−0.008 (4)
C22	0.085 (5)	0.081 (5)	0.079 (5)	−0.006 (4)	0.012 (4)	−0.008 (4)
C23	0.095 (6)	0.066 (4)	0.071 (4)	0.003 (4)	0.021 (4)	−0.002 (3)
C24	0.077 (4)	0.051 (3)	0.070 (4)	0.006 (3)	0.031 (3)	0.003 (3)
C25	0.142 (7)	0.128 (7)	0.150 (7)	0.002 (6)	0.034 (6)	0.000 (6)
C26	0.327 (15)	0.329 (15)	0.330 (15)	0.029 (10)	0.028 (10)	−0.003 (10)
C27	0.119 (7)	0.136 (7)	0.156 (7)	0.005 (5)	0.048 (6)	0.009 (6)

Geometric parameters (Å, °)

Cu1—N3	1.967 (5)	C4—C9	1.378 (8)
Cu1—N1	1.984 (4)	C4—C5	1.415 (8)
Cu1—O5^i	1.993 (4)	C5—C6	1.353 (8)

Cu1—O1	1.995 (4)	C5—H5	0.93
O1—C1	1.264 (7)	C6—C7	1.385 (8)
O2—C1	1.259 (7)	C6—H6	0.93
O3—C4	1.374 (6)	C7—C8	1.386 (7)
O3—C3	1.428 (7)	C7—C10	1.485 (7)
O4—C10	1.242 (7)	C8—C9	1.369 (7)
O5—C10	1.275 (7)	C8—H8	0.93
O5—Cu1ⁱⁱ	1.993 (4)	C9—H9	0.93
O6—C25	1.283 (8)	C11—H11	0.93
O1W—H1W1	0.85	C12—C13	1.366 (8)
O1W—H1W2	0.85	C12—C17	1.405 (7)
O2W—H2W1	0.85	C13—C14	1.370 (9)
O2W—H2W2	0.85	C13—H13	0.93
O3W—H3W1	0.85	C14—C15	1.390 (9)
O3W—H3W2	0.85	C14—H14	0.93
O4W—H4W1	0.85	C15—C16	1.358 (9)
O4W—H4W2	0.85	C15—H15	0.93
O5W—H5W1	0.85	C16—C17	1.368 (9)
O5W—H5W2	0.85	C16—H16	0.93
N1—C11	1.318 (7)	C18—H18	0.93
N1—C12	1.405 (7)	C19—C20	1.367 (8)
N2—C11	1.342 (7)	C19—C24	1.401 (8)
N2—C17	1.376 (7)	C20—C21	1.394 (9)
N2—H2N	0.86	C20—H20	0.93
N3—C18	1.333 (7)	C21—C22	1.375 (10)
N3—C19	1.399 (7)	C21—H21	0.93
N4—C18	1.337 (8)	C22—C23	1.379 (10)
N4—C24	1.383 (8)	C22—H22	0.93
N4—H4N	0.86	C23—C24	1.383 (9)
N5—C25	1.324 (8)	C23—H23	0.93
N5—C26	1.420 (10)	C25—H25	0.93
N5—C27	1.428 (8)	C26—H26A	0.96
C1—C2	1.521 (8)	C26—H26B	0.96
C2—C3	1.516 (8)	C26—H26C	0.96
C2—H2A	0.97	C27—H27A	0.96
C2—H2B	0.97	C27—H27B	0.96
C3—H3A	0.97	C27—H27C	0.96
C3—H3B	0.97		
N3—Cu1—N1	93.53 (19)	C4—C9—H9	120.5
N3—Cu1—O5ⁱ	91.88 (18)	O4—C10—O5	120.1 (5)
N1—Cu1—O5ⁱ	160.05 (19)	O4—C10—C7	121.2 (5)
N3—Cu1—O1	159.18 (19)	O5—C10—C7	118.7 (5)
N1—Cu1—O1	92.98 (17)	N1—C11—N2	112.4 (5)
O5ⁱ—Cu1—O1	88.67 (16)	N1—C11—H11	123.8
C1—O1—Cu1	105.0 (4)	N2—C11—H11	123.8
C4—O3—C3	117.7 (4)	C13—C12—N1	131.6 (5)
C10—O5—Cu1ⁱⁱ	102.2 (3)	C13—C12—C17	120.6 (6)
H1W1—O1W—H1W2	110.2	N1—C12—C17	107.7 (5)

H2W1—O2W—H2W2	107.7	C12—C13—C14	117.5 (6)
H3W1—O3W—H3W2	110.2	C12—C13—H13	121.3
H4W1—O4W—H4W2	107.7	C14—C13—H13	121.3
H5W1—O5W—H5W2	110.2	C13—C14—C15	121.4 (7)
C11—N1—C12	106.0 (5)	C13—C14—H14	119.3
C11—N1—Cu1	129.1 (4)	C15—C14—H14	119.3
C12—N1—Cu1	124.8 (4)	C16—C15—C14	121.8 (6)
C11—N2—C17	107.9 (4)	C16—C15—H15	119.1
C11—N2—H2N	126.0	C14—C15—H15	119.1
C17—N2—H2N	126.0	C15—C16—C17	117.1 (6)
C18—N3—C19	104.9 (5)	C15—C16—H16	121.4
C18—N3—Cu1	127.8 (4)	C17—C16—H16	121.4
C19—N3—Cu1	127.3 (4)	C16—C17—N2	132.4 (6)
C18—N4—C24	107.4 (5)	C16—C17—C12	121.7 (6)
C18—N4—H4N	126.3	N2—C17—C12	105.9 (5)
C24—N4—H4N	126.3	N3—C18—N4	113.1 (6)
C25—N5—C26	121.7 (13)	N3—C18—H18	123.4
C25—N5—C27	122.2 (9)	N4—C18—H18	123.4
C26—N5—C27	116.1 (12)	C20—C19—N3	130.1 (6)
O2—C1—O1	121.5 (6)	C20—C19—C24	121.1 (6)
O2—C1—C2	120.1 (6)	N3—C19—C24	108.7 (5)
O1—C1—C2	118.4 (6)	C19—C20—C21	116.8 (6)
C3—C2—C1	111.6 (5)	C19—C20—H20	121.6
C3—C2—H2A	109.3	C21—C20—H20	121.6
C1—C2—H2A	109.3	C22—C21—C20	122.1 (7)
C3—C2—H2B	109.3	C22—C21—H21	119.0
C1—C2—H2B	109.3	C20—C21—H21	119.0
H2A—C2—H2B	108.0	C21—C22—C23	121.4 (7)
O3—C3—C2	106.1 (5)	C21—C22—H22	119.3
O3—C3—H3A	110.5	C23—C22—H22	119.3
C2—C3—H3A	110.5	C24—C23—C22	116.8 (6)
O3—C3—H3B	110.5	C24—C23—H23	121.6
C2—C3—H3B	110.5	C22—C23—H23	121.6
H3A—C3—H3B	108.7	C23—C24—N4	132.5 (6)
O3—C4—C9	125.4 (5)	C23—C24—C19	121.7 (6)
O3—C4—C5	115.2 (5)	N4—C24—C19	105.8 (5)
C9—C4—C5	119.4 (5)	O6—C25—N5	120.8 (11)
C6—C5—C4	120.0 (5)	O6—C25—H25	119.6
C6—C5—H5	120.0	N5—C25—H25	119.6
C4—C5—H5	120.0	N5—C26—H26A	109.5
C5—C6—C7	121.3 (5)	N5—C26—H26B	109.5
C5—C6—H6	119.3	H26A—C26—H26B	109.5
C7—C6—H6	119.3	N5—C26—H26C	109.5
C6—C7—C8	117.8 (5)	H26A—C26—H26C	109.5
C6—C7—C10	120.7 (5)	H26B—C26—H26C	109.5
C8—C7—C10	121.5 (5)	N5—C27—H27A	109.5
C9—C8—C7	122.5 (5)	N5—C27—H27B	109.5
C9—C8—H8	118.8	H27A—C27—H27B	109.5
C7—C8—H8	118.8	N5—C27—H27C	109.5

C8—C9—C4	119.0 (5)	H27A—C27—H27C	109.5
C8—C9—H9	120.5	H27B—C27—H27C	109.5
N3—Cu1—O1—C1	−15.1 (7)	C17—N2—C11—N1	−1.1 (7)
N1—Cu1—O1—C1	93.0 (4)	C11—N1—C12—C13	178.6 (6)
O5^{i}—Cu1—O1—C1	−106.9 (4)	Cu1—N1—C12—C13	1.9 (8)
N3—Cu1—N1—C11	122.8 (5)	C11—N1—C12—C17	0.0 (6)
O5^{i}—Cu1—N1—C11	−131.8 (6)	Cu1—N1—C12—C17	−176.7 (4)
O1—Cu1—N1—C11	−37.4 (5)	N1—C12—C13—C14	−178.3 (6)
N3—Cu1—N1—C12	−61.3 (4)	C17—C12—C13—C14	0.1 (8)
O5^{i}—Cu1—N1—C12	44.2 (8)	C12—C13—C14—C15	0.5 (9)
O1—Cu1—N1—C12	138.5 (4)	C13—C14—C15—C16	−0.4 (10)
N1—Cu1—N3—C18	116.4 (5)	C14—C15—C16—C17	−0.2 (10)
O5^{i}—Cu1—N3—C18	−44.4 (5)	C15—C16—C17—N2	179.0 (6)
O1—Cu1—N3—C18	−135.6 (5)	C15—C16—C17—C12	0.8 (9)
N1—Cu1—N3—C19	−61.8 (5)	C11—N2—C17—C16	−177.4 (6)
O5^{i}—Cu1—N3—C19	137.4 (5)	C11—N2—C17—C12	1.0 (6)
O1—Cu1—N3—C19	46.2 (7)	C13—C12—C17—C16	−0.8 (9)
Cu1—O1—C1—O2	−5.3 (6)	N1—C12—C17—C16	177.9 (5)
Cu1—O1—C1—C2	175.8 (4)	C13—C12—C17—N2	−179.4 (5)
O2—C1—C2—C3	−43.4 (8)	N1—C12—C17—N2	−0.7 (6)
O1—C1—C2—C3	135.4 (6)	C19—N3—C18—N4	1.2 (7)
C4—O3—C3—C2	179.5 (5)	Cu1—N3—C18—N4	−177.3 (4)
C1—C2—C3—O3	−63.4 (7)	C24—N4—C18—N3	−1.0 (7)
C3—O3—C4—C9	−0.7 (8)	C18—N3—C19—C20	178.8 (6)
C3—O3—C4—C5	179.8 (5)	Cu1—N3—C19—C20	−2.7 (9)
O3—C4—C5—C6	179.0 (5)	C18—N3—C19—C24	−0.9 (6)
C9—C4—C5—C6	−0.5 (9)	Cu1—N3—C19—C24	177.6 (4)
C4—C5—C6—C7	−2.2 (9)	N3—C19—C20—C21	−179.7 (6)
C5—C6—C7—C8	2.8 (9)	C24—C19—C20—C21	0.0 (9)
C5—C6—C7—C10	−175.1 (6)	C19—C20—C21—C22	−0.5 (11)
C6—C7—C8—C9	−0.8 (9)	C20—C21—C22—C23	1.4 (11)
C10—C7—C8—C9	177.1 (5)	C21—C22—C23—C24	−1.6 (10)
C7—C8—C9—C4	−1.9 (9)	C22—C23—C24—N4	179.9 (6)
O3—C4—C9—C8	−177.0 (5)	C22—C23—C24—C19	1.1 (9)
C5—C4—C9—C8	2.5 (9)	C18—N4—C24—C23	−178.6 (7)
Cu1^{ii}—O5—C10—O4	1.2 (7)	C18—N4—C24—C19	0.3 (6)
Cu1^{ii}—O5—C10—C7	−177.2 (4)	C20—C19—C24—C23	−0.3 (9)
C6—C7—C10—O4	−4.1 (9)	N3—C19—C24—C23	179.5 (5)
C8—C7—C10—O4	178.0 (6)	C20—C19—C24—N4	−179.4 (5)
C6—C7—C10—O5	174.3 (5)	N3—C19—C24—N4	0.4 (6)
C8—C7—C10—O5	−3.6 (9)	C26—N5—C25—O6	−0.2 (3)
C12—N1—C11—N2	0.6 (6)	C27—N5—C25—O6	−179.4 (3)
Cu1—N1—C11—N2	177.2 (4)		

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

Fig. 1