catena-Poly[[(2,2′-bipyridine)copper(II)]-μ-5-*tert*-butylisophthalato]

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In the crystal structure of the title polymeric compound, $[Cu(C_{12}H_{12}O_4)(C_{10}H_8N_2)]_n$, the asymmetric unit consists of one Cu^{II} ion, one 5-*tert*-butylisophthalate (tbip) and one 2,2′-bipyridine (bpy) ligand. The copper(II) ion is four-coordinated by two N atoms from bipy and two O atoms from two tbip ligands, leading to a distorted tetrahedral coordination. Each tbip ligand adopts a bis-monodentate coordination mode to connect two symmetry-related copper(II) ions, so forming a zigzag polymer chain parallel to [001]. The *tert*-butyl methyl groups are disordered over two positions with occupancies of 0.506 (6)/0.494 (6)

Related literature

For related literature on the synthesis of flexible organic ligands, see: Chang *et al.* (2005); Ma, Chen *et al.* (2008); Xu *et al.* (2006). For related literature on coordination polymers, see: Ma, Wang, Huo *et al.* (2008); Ma, Wang, Wang *et al.* (2008); Pan *et al.* (2006); Yang *et al.* (2002). For bond-length data, see: Allen *et al.* (1987).
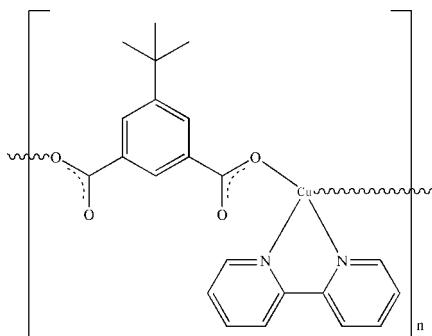
Experimental

Crystal data

[Cu(C₁₂H₁₂O₄)(C₁₀H₈N₂)]
$[Cu(C_{12}H_{12}O_4)(C_{10}H_8N_2)]$
$M_r = 439.94$
Monoclinic, $P2_1/c$
$a = 8.905$ (2) Å
$b = 20.875$ (5) Å
$c = 11.564$ (3) Å
$\beta = 98.188$ (3)°

$V = 2127.8$ (9) Å³
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.06$ mm⁻¹
$T = 296$ (2) K
$0.29 \times 0.22 \times 0.16$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.716$, $T_{max} = 0.845$

15716 measured reflections
3949 independent reflections
3021 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.130$
$S = 1.05$
3949 reflections
260 parameters

91 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.64$ e Å⁻³
$\Delta\rho_{min} = -0.55$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.933 (2)	Cu1—N1	1.985 (3)
Cu1—O3ⁱ	1.956 (2)	Cu1—N2	1.983 (3)
O1—Cu1—O3ⁱ	88.17 (11)	O1—Cu1—N2	173.34 (11)
O1—Cu1—N1	94.83 (11)	O3ⁱ—Cu1—N2	96.69 (11)
O3ⁱ—Cu1—N1	172.79 (11)	N1—Cu1—N2	80.88 (11)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

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metal-organic compounds

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supplementary materials

catena-Poly[[(2,2'-bipyridine)copper(II)]-*μ*-5-*tert*-butylisophthalato]

X.-L. Li and M.-L. Huang

Comment

It is well known that organic ligands play a crucial role in the design and construction of desirable frameworks. The changes in flexibility, length and symmetry of organic ligands can result in a remarkable class of materials bearing diverse architectures and functions. Thus, the construction of target molecules is a challenge for synthetic chemists (Ma *et al.*, 2008; Chang *et al.*, 2005; Xu *et al.*, 2006). Benzene-1,3-dicarboxylic acid (isophthalic acid, H2isop) and its derivatives, with special conformations such as, an angle of 120° between two carboxylic groups, present versatile coordination modes that can yield predetermined networks. Such ligands have been widely used to construct coordination polymers (Pan *et al.*, 2006; Yang *et al.*, 2002; Ma *et al.*, 2008).

   The title compound, (I), was prepared by hydrothermal synthesis using 5-tert-butyl isophthalic acid, 2,2'-bipyridine and copper(II) actate. The asymmetric unit of (I) consists of one copper(II) ion, one tbip and one bipy ligand molecules (Fig. 1). Each copper(II) ion is four-coordinated by two nitrogen atoms from one bipy molecule and two oxygen atoms from two tbip ligands (Table 1). The coordination geometry of the copper(II) ion is distorted tetrahedral. The Cu—O bond lengths [1.933 (2)–1.965 (2) Å] are within the range reported for tetrahedral environments, and the Cu—N bond lengths [1.983 (3)–1.985 (3) Å] are also similar to those found in other tetrahedral copper complexes of bipy (Allen *et al.*, 1987). Each tbip ligand adopts the bis-monodentated coordination mode to connect two symmetry related copper(II) ions so forming a zigzag polymer chain (Fig. 2).

Experimental

A mixture of 5-*tert*-butyl isophthalic acid (0.1 mmol, 23.1 mg), 2,2'-bipyridine (0.1 mmol, 15.8 mg), Cu(OAc).2.4H$_2$O (0.05 mmol, 11.5 mg), NaOH (0.1 mmol, 4.0 mg) and H$_2$O (15 ml) was placed in a Teflon-lined stainless steel vessel, and heated to 160 °C for 4 days. It was then cooled to room temperature over a period of 24 h. Blue block-like crystals of compound (I) were obtained.

Refinement

The tertiary butyl methyl groups are disordered over two almost equally occupied positions: 0.506 (6)/0.494 (6). The H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.93–0.96 Å with U$_{iso}$(H) = 1.2 or 1.5U$_{eq}$(parent C-atom).

supplementary materials

Figures
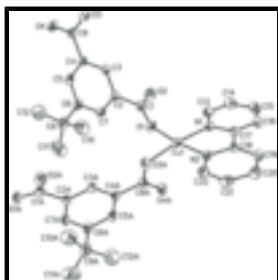
Fig. 1. A view of the asymmetric unit of compound (I), with thermal ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. Atoms with label A are related to those without by symmetry operation (x, $-y+1.5$, $z+0.5$).
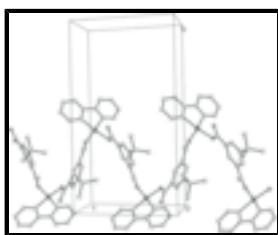
Fig. 2. A partial view, along the a axis, of the crystal packing of compound (I) showing the zigzag polymer chain. H atoms have been omitted for clarity.

catena-Poly[[(2,2'-bipyridine)copper(II)]-μ-5-*tert*-butylisophthalato]

Crystal data

$[Cu(C_{12}H_{12}O_4)(C_{10}H_8N_2)]$	$F_{000} = 908$
$M_r = 439.94$	$D_x = 1.373$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
	$\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3455 reflections
$a = 8.905$ (2) Å	$\theta = 2.5–22.5°$
$b = 20.875$ (5) Å	$\mu = 1.06$ mm^{-1}
$c = 11.564$ (3) Å	$T = 296$ (2) K
$\beta = 98.188$ (3)°	Block, blue
$V = 2127.8$ (9) Å^3	$0.29 \times 0.22 \times 0.16$ mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3949 independent reflections
Radiation source: fine-focus sealed tube	3021 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
$T = 296(2)$ K	$\theta_{max} = 25.5°$
φ and ω scans	$\theta_{min} = 2.5°$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -10 \rightarrow 10$
$T_{min} = 0.716$, $T_{max} = 0.845$	$k = -25 \rightarrow 25$
15716 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 1.7017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
3949 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
260 parameters	$\Delta\rho_{min} = -0.54$ e Å^{-3}
91 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
C10	−0.2988 (8)	0.7849 (4)	0.0801 (8)	0.0991 (17)	0.50
H10A	−0.3808	0.7876	0.1255	0.149*	0.50
H10B	−0.2580	0.7422	0.0851	0.149*	0.50
H10C	−0.3355	0.7948	0.0000	0.149*	0.50
C11	−0.1382 (9)	0.8222 (4)	0.2581 (6)	0.1033 (17)	0.50
H11A	−0.0577	0.8506	0.2893	0.155*	0.50
H11B	−0.1070	0.7786	0.2736	0.155*	0.50
H11C	−0.2266	0.8310	0.2943	0.155*	0.50
C12	−0.2268 (8)	0.9003 (3)	0.1063 (7)	0.1019 (19)	0.50
H12A	−0.3113	0.9085	0.1473	0.153*	0.50
H12B	−0.2570	0.9071	0.0242	0.153*	0.50
H12C	−0.1450	0.9288	0.1341	0.153*	0.50
C10'	−0.2432 (9)	0.7777 (3)	0.1868 (8)	0.0991 (17)	0.50
H10D	−0.2073	0.7791	0.2691	0.149*	0.50
H10E	−0.2138	0.7378	0.1553	0.149*	0.50
H10F	−0.3518	0.7813	0.1743	0.149*	0.50
C11'	−0.1082 (9)	0.8784 (4)	0.2317 (7)	0.1033 (17)	0.50

H11D	−0.0967	0.9208	0.2021	0.155*	0.50
H11E	−0.0112	0.8626	0.2671	0.155*	0.50
H11F	−0.1764	0.8796	0.2890	0.155*	0.50
C12'	−0.2878 (8)	0.8749 (4)	0.0548 (7)	0.1019 (19)	0.50
H12D	−0.3658	0.8871	0.0998	0.153*	0.50
H12E	−0.3324	0.8523	−0.0138	0.153*	0.50
H12F	−0.2371	0.9125	0.0323	0.153*	0.50
Cu1	0.30126 (5)	0.570966 (18)	0.17572 (3)	0.03784 (16)	
O1	0.1606 (3)	0.63474 (11)	0.1038 (2)	0.0497 (6)	
O2	0.3724 (3)	0.67027 (13)	0.0490 (3)	0.0598 (7)	
O3	0.3259 (3)	0.87708 (12)	−0.1821 (2)	0.0507 (6)	
O4	0.1347 (3)	0.94173 (12)	−0.1635 (2)	0.0542 (7)	
N1	0.2646 (3)	0.50997 (13)	0.0430 (2)	0.0368 (6)	
N2	0.4556 (3)	0.50539 (13)	0.2322 (2)	0.0371 (6)	
C1	0.2394 (5)	0.67826 (18)	0.0641 (3)	0.0510 (8)	
C2	0.1631 (4)	0.74186 (15)	0.0367 (3)	0.0397 (8)	
C3	0.2214 (4)	0.78533 (16)	−0.0351 (3)	0.0394 (8)	
H3	0.3084	0.7756	−0.0676	0.047*	
C4	0.1487 (4)	0.84380 (15)	−0.0584 (3)	0.0378 (8)	
C5	0.0213 (4)	0.85804 (16)	−0.0065 (3)	0.0430 (8)	
H5	−0.0261	0.8974	−0.0220	0.052*	
C6	−0.0377 (4)	0.81567 (17)	0.0678 (3)	0.0460 (9)	
C7	0.0343 (4)	0.75671 (16)	0.0860 (3)	0.0448 (9)	
H7	−0.0050	0.7264	0.1325	0.054*	
C8	0.2057 (4)	0.89150 (16)	−0.1391 (3)	0.0422 (8)	
C9	−0.1753 (6)	0.8323 (2)	0.1271 (5)	0.0809 (12)	
C13	0.1605 (4)	0.51736 (18)	−0.0526 (3)	0.0469 (9)	
H13	0.1031	0.5547	−0.0608	0.056*	
C14	0.1365 (4)	0.4717 (2)	−0.1382 (3)	0.0541 (10)	
H14	0.0625	0.4775	−0.2026	0.065*	
C15	0.2233 (5)	0.4176 (2)	−0.1271 (4)	0.0575 (11)	
H15	0.2087	0.3860	−0.1842	0.069*	
C16	0.3328 (4)	0.40997 (18)	−0.0308 (3)	0.0485 (9)	
H16	0.3938	0.3736	−0.0230	0.058*	
C17	0.3503 (4)	0.45690 (16)	0.0533 (3)	0.0352 (7)	
C18	0.4614 (4)	0.45458 (16)	0.1610 (3)	0.0353 (7)	
C19	0.5640 (4)	0.40508 (18)	0.1901 (3)	0.0478 (9)	
H19	0.5675	0.3703	0.1402	0.057*	
C20	0.6603 (5)	0.4085 (2)	0.2941 (4)	0.0556 (10)	
H20	0.7289	0.3755	0.3156	0.067*	
C21	0.6549 (5)	0.4606 (2)	0.3664 (3)	0.0548 (10)	
H21	0.7203	0.4638	0.4364	0.066*	
C22	0.5505 (4)	0.50766 (18)	0.3323 (3)	0.0475 (9)	
H22	0.5457	0.5428	0.3811	0.057*	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C10	0.081 (4)	0.096 (3)	0.134 (4)	0.009 (3)	0.061 (3)	0.009 (3)
C11	0.101 (4)	0.102 (4)	0.118 (4)	0.020 (3)	0.058 (3)	−0.004 (3)
C12	0.087 (4)	0.084 (3)	0.144 (5)	0.035 (3)	0.048 (3)	0.007 (3)
C10'	0.081 (4)	0.096 (3)	0.134 (4)	0.009 (3)	0.061 (3)	0.009 (3)
C11'	0.101 (4)	0.102 (4)	0.118 (4)	0.020 (3)	0.058 (3)	−0.004 (3)
C12'	0.087 (4)	0.084 (3)	0.144 (5)	0.035 (3)	0.048 (3)	0.007 (3)
Cu1	0.0495 (3)	0.0268 (2)	0.0376 (3)	0.00568 (18)	0.00751 (18)	0.00124 (16)
O1	0.0618 (16)	0.0312 (13)	0.0578 (16)	0.0093 (12)	0.0143 (13)	0.0113 (11)
O2	0.0639 (14)	0.0477 (13)	0.0722 (16)	0.0222 (12)	0.0247 (13)	0.0112 (12)
O3	0.0599 (17)	0.0424 (14)	0.0514 (16)	−0.0017 (12)	0.0132 (13)	0.0113 (12)
O4	0.0725 (18)	0.0373 (14)	0.0517 (16)	0.0066 (13)	0.0042 (13)	0.0124 (12)
N1	0.0414 (16)	0.0347 (15)	0.0340 (15)	0.0035 (12)	0.0042 (12)	0.0052 (12)
N2	0.0448 (16)	0.0336 (15)	0.0322 (14)	−0.0010 (12)	0.0029 (12)	0.0018 (12)
C1	0.0611 (16)	0.0381 (16)	0.0573 (18)	0.0190 (15)	0.0207 (15)	0.0079 (14)
C2	0.051 (2)	0.0288 (17)	0.0407 (19)	0.0085 (15)	0.0102 (16)	0.0041 (14)
C3	0.046 (2)	0.0351 (18)	0.0373 (18)	0.0047 (15)	0.0085 (15)	0.0008 (15)
C4	0.046 (2)	0.0293 (16)	0.0363 (18)	0.0006 (14)	0.0008 (15)	0.0015 (14)
C5	0.046 (2)	0.0299 (18)	0.051 (2)	0.0079 (15)	−0.0001 (16)	0.0030 (15)
C6	0.047 (2)	0.0335 (18)	0.059 (2)	0.0083 (16)	0.0106 (17)	0.0025 (17)
C7	0.051 (2)	0.0324 (18)	0.055 (2)	0.0062 (16)	0.0187 (17)	0.0105 (16)
C8	0.058 (2)	0.0337 (18)	0.0317 (17)	−0.0047 (17)	−0.0048 (16)	0.0022 (14)
C9	0.075 (3)	0.062 (2)	0.118 (3)	0.021 (2)	0.054 (3)	0.011 (2)
C13	0.047 (2)	0.049 (2)	0.043 (2)	0.0062 (17)	0.0025 (16)	0.0034 (17)
C14	0.047 (2)	0.070 (3)	0.043 (2)	−0.009 (2)	−0.0010 (17)	−0.0015 (19)
C15	0.062 (3)	0.060 (3)	0.049 (2)	−0.009 (2)	0.0051 (19)	−0.020 (2)
C16	0.052 (2)	0.042 (2)	0.052 (2)	0.0024 (17)	0.0075 (18)	−0.0099 (17)
C17	0.0374 (18)	0.0351 (17)	0.0343 (17)	−0.0003 (14)	0.0090 (14)	0.0010 (14)
C18	0.0388 (18)	0.0322 (17)	0.0367 (18)	0.0022 (14)	0.0112 (14)	0.0039 (14)
C19	0.053 (2)	0.043 (2)	0.048 (2)	0.0117 (18)	0.0132 (17)	0.0019 (17)
C20	0.055 (2)	0.058 (2)	0.053 (2)	0.020 (2)	0.0061 (19)	0.012 (2)
C21	0.057 (2)	0.061 (3)	0.044 (2)	0.004 (2)	−0.0044 (18)	0.0116 (19)
C22	0.057 (2)	0.043 (2)	0.041 (2)	−0.0016 (18)	0.0012 (17)	0.0005 (16)

Geometric parameters (Å, °)

C10—C9	1.521 (9)	N1—C17	1.341 (4)
C10—H10A	0.9600	N1—C13	1.347 (4)
C10—H10B	0.9600	N2—C22	1.333 (4)
C10—H10C	0.9600	N2—C18	1.348 (4)
C11—C9	1.519 (9)	C1—C2	1.505 (5)
C11—H11A	0.9600	C2—C3	1.381 (5)
C11—H11B	0.9600	C2—C7	1.386 (5)
C11—H11C	0.9600	C3—C4	1.390 (5)
C12—C9	1.501 (7)	C3—H3	0.9300
C12—H12A	0.9600	C4—C5	1.389 (5)
C12—H12B	0.9600	C4—C8	1.502 (5)
C12—H12C	0.9600	C5—C6	1.387 (5)
C10'—C9	1.504 (8)	C5—H5	0.9300
C10'—H10D	0.9600	C6—C7	1.390 (5)

C10'—H10E	0.9600	C6—C9	1.527 (6)
C10'—H10F	0.9600	C7—H7	0.9300
C11'—C9	1.595 (9)	C8—Cu1^{ii}	2.538 (4)
C11'—H11D	0.9600	C13—C14	1.368 (5)
C11'—H11E	0.9600	C13—H13	0.9300
C11'—H11F	0.9600	C14—C15	1.365 (6)
C12'—C9	1.502 (8)	C14—H14	0.9300
C12'—H12D	0.9600	C15—C16	1.382 (6)
C12'—H12E	0.9600	C15—H15	0.9300
C12'—H12F	0.9600	C16—C17	1.373 (5)
Cu1—O1	1.933 (2)	C16—H16	0.9300
Cu1—O3^{i}	1.956 (2)	C17—C18	1.477 (5)
Cu1—N1	1.985 (3)	C18—C19	1.388 (5)
Cu1—N2	1.983 (3)	C19—C20	1.376 (5)
Cu1—C8^{i}	2.538 (4)	C19—H19	0.9300
O1—C1	1.273 (4)	C20—C21	1.377 (6)
O2—C1	1.233 (5)	C20—H20	0.9300
O3—C8	1.279 (5)	C21—C22	1.372 (5)
O3—Cu1^{ii}	1.956 (2)	C21—H21	0.9300
O4—C8	1.236 (4)	C22—H22	0.9300
C9—C10—H10A	109.5	C6—C5—C4	122.4 (3)
C9—C10—H10B	109.5	C6—C5—H5	118.8
H10A—C10—H10B	109.5	C4—C5—H5	118.8
C9—C10—H10C	109.5	C5—C6—C7	116.8 (3)
H10A—C10—H10C	109.5	C5—C6—C9	122.1 (3)
H10B—C10—H10C	109.5	C7—C6—C9	121.0 (4)
C9—C11—H11A	109.5	C2—C7—C6	121.8 (3)
C9—C11—H11B	109.5	C2—C7—H7	119.1
H11A—C11—H11B	109.5	C6—C7—H7	119.1
C9—C11—H11C	109.5	O4—C8—O3	122.7 (3)
H11A—C11—H11C	109.5	O4—C8—C4	119.8 (4)
H11B—C11—H11C	109.5	O3—C8—C4	117.5 (3)
C9—C12—H12A	109.5	O4—C8—Cu1^{ii}	76.6 (2)
C9—C12—H12B	109.5	O3—C8—Cu1^{ii}	49.07 (17)
H12A—C12—H12B	109.5	C4—C8—Cu1^{ii}	155.9 (2)
C9—C12—H12C	109.5	C12—C9—C10'	131.1 (4)
H12A—C12—H12C	109.5	C12'—C9—C10'	115.1 (5)
H12B—C12—H12C	109.5	C12—C9—C11	108.0 (5)
C9—C10'—H10D	109.5	C12'—C9—C11	132.1 (5)
C9—C10'—H10E	109.5	C10'—C9—C11	58.7 (3)
H10D—C10'—H10E	109.5	C12—C9—C10	111.7 (5)
C9—C10'—H10F	109.5	C12'—C9—C10	78.2 (4)
H10D—C10'—H10F	109.5	C10'—C9—C10	49.7 (2)
H10E—C10'—H10F	109.5	C11—C9—C10	108.0 (4)
C9—C11'—H11D	109.5	C12—C9—C6	112.9 (4)
C9—C11'—H11E	109.5	C12'—C9—C6	113.5 (5)
H11D—C11'—H11E	109.5	C10'—C9—C6	115.8 (4)

C9—C11'—H11F	109.5	C11—C9—C6	110.0 (5)
H11D—C11'—H11F	109.5	C10—C9—C6	106.1 (5)
H11E—C11'—H11F	109.5	C12—C9—C11'	67.9 (3)
C9—C12'—H12D	109.5	C12'—C9—C11'	102.3 (4)
C9—C12'—H12E	109.5	C10'—C9—C11'	103.9 (5)
H12D—C12'—H12E	109.5	C11—C9—C11'	47.3 (2)
C9—C12'—H12F	109.5	C10—C9—C11'	146.9 (5)
H12D—C12'—H12F	109.5	C6—C9—C11'	103.9 (5)
H12E—C12'—H12F	109.5	N1—C13—C14	122.2 (4)
O1—Cu1—O3^i	88.17 (11)	N1—C13—H13	118.9
O1—Cu1—N1	94.83 (11)	C14—C13—H13	118.9
O3^i—Cu1—N1	172.79 (11)	C15—C14—C13	118.7 (4)
O1—Cu1—N2	173.34 (11)	C15—C14—H14	120.6
O3^i—Cu1—N2	96.69 (11)	C13—C14—H14	120.6
N1—Cu1—N2	80.88 (11)	C14—C15—C16	119.8 (4)
O1—Cu1—C8^i	82.87 (11)	C14—C15—H15	120.1
O3^i—Cu1—C8^i	29.60 (11)	C16—C15—H15	120.1
N2—Cu1—C8^i	103.60 (11)	C17—C16—C15	119.0 (4)
N1—Cu1—C8^i	144.33 (12)	C17—C16—H16	120.5
C1—O1—Cu1	106.8 (2)	C15—C16—H16	120.5
C8—O3—Cu1^{ii}	101.3 (2)	N1—C17—C16	121.4 (3)
C17—N1—C13	118.9 (3)	N1—C17—C18	114.0 (3)
C17—N1—Cu1	115.6 (2)	C16—C17—C18	124.6 (3)
C13—N1—Cu1	125.4 (2)	N2—C18—C19	121.3 (3)
C22—N2—C18	118.9 (3)	N2—C18—C17	114.2 (3)
C22—N2—Cu1	125.8 (2)	C19—C18—C17	124.5 (3)
C18—N2—Cu1	115.3 (2)	C20—C19—C18	118.7 (4)
O2—C1—O1	123.0 (3)	C20—C19—H19	120.7
O2—C1—C2	120.3 (3)	C18—C19—H19	120.7
O1—C1—C2	116.7 (3)	C19—C20—C21	120.0 (4)
C3—C2—C7	120.3 (3)	C19—C20—H20	120.0
C3—C2—C1	120.6 (3)	C21—C20—H20	120.0
C7—C2—C1	119.1 (3)	C22—C21—C20	118.2 (4)
C2—C3—C4	119.3 (3)	C22—C21—H21	120.9
C2—C3—H3	120.4	C20—C21—H21	120.9
C4—C3—H3	120.4	N2—C22—C21	123.0 (4)
C5—C4—C3	119.4 (3)	N2—C22—H22	118.5
C5—C4—C8	119.7 (3)	C21—C22—H22	118.5
C3—C4—C8	120.9 (3)		
O3^i—Cu1—O1—C1	84.9 (3)	C3—C4—C8—Cu1^{ii}	47.6 (8)
N1—Cu1—O1—C1	−101.7 (3)	C5—C6—C9—C12	−6.0 (7)
C8^i—Cu1—O1—C1	114.1 (3)	C7—C6—C9—C12	174.1 (5)
O1—Cu1—N1—C17	176.4 (2)	C5—C6—C9—C12'	32.7 (7)
N2—Cu1—N1—C17	1.5 (2)	C7—C6—C9—C12'	−147.2 (5)
C8^i—Cu1—N1—C17	−99.1 (3)	C5—C6—C9—C10'	169.2 (6)
N2—Cu1—N1—C13	−180.0 (3)	C7—C6—C9—C10'	−10.7 (8)

C8^i—Cu1—N1—C13	79.4 (3)	C5—C6—C9—C11	−126.8 (5)
O3^i—Cu1—N2—C22	−7.2 (3)	C7—C6—C9—C11	53.3 (7)
N1—Cu1—N2—C22	179.6 (3)	C5—C6—C9—C10	116.6 (5)
C8^i—Cu1—N2—C22	−36.5 (3)	C7—C6—C9—C10	−63.3 (6)
O3^i—Cu1—N2—C18	172.5 (2)	C5—C6—C9—C11'	−77.6 (6)
N1—Cu1—N2—C18	−0.6 (2)	C7—C6—C9—C11'	102.6 (5)
C8^i—Cu1—N2—C18	143.3 (2)	C17—N1—C13—C14	1.8 (5)
Cu1—O1—C1—O2	17.2 (5)	Cu1—N1—C13—C14	−176.7 (3)
Cu1—O1—C1—C2	−162.2 (3)	N1—C13—C14—C15	−1.4 (6)
O2—C1—C2—C3	18.7 (6)	C13—C14—C15—C16	−0.1 (6)
O1—C1—C2—C3	−162.0 (3)	C14—C15—C16—C17	1.1 (6)
O2—C1—C2—C7	−160.4 (4)	C13—N1—C17—C16	−0.7 (5)
O1—C1—C2—C7	19.0 (5)	Cu1—N1—C17—C16	178.0 (3)
C7—C2—C3—C4	−0.7 (5)	C13—N1—C17—C18	179.3 (3)
C1—C2—C3—C4	−179.7 (3)	Cu1—N1—C17—C18	−2.1 (4)
C2—C3—C4—C5	1.7 (5)	C15—C16—C17—N1	−0.7 (6)
C2—C3—C4—C8	−178.1 (3)	C15—C16—C17—C18	179.3 (3)
C3—C4—C5—C6	−0.5 (5)	C22—N2—C18—C19	−0.1 (5)
C8—C4—C5—C6	179.3 (3)	Cu1—N2—C18—C19	−179.8 (3)
C4—C5—C6—C7	−1.7 (6)	C22—N2—C18—C17	179.5 (3)
C4—C5—C6—C9	178.4 (4)	Cu1—N2—C18—C17	−0.3 (4)
C3—C2—C7—C6	−1.7 (6)	N1—C17—C18—N2	1.5 (4)
C1—C2—C7—C6	177.4 (4)	C16—C17—C18—N2	−178.5 (3)
C5—C6—C7—C2	2.8 (6)	N1—C17—C18—C19	−178.9 (3)
C9—C6—C7—C2	−177.3 (4)	C16—C17—C18—C19	1.1 (5)
Cu1^{ii}—O3—C8—O4	−22.7 (4)	N2—C18—C19—C20	0.4 (5)
Cu1^{ii}—O3—C8—C4	155.6 (2)	C17—C18—C19—C20	−179.2 (3)
C5—C4—C8—O4	−3.7 (5)	C18—C19—C20—C21	−0.8 (6)
C3—C4—C8—O4	176.1 (3)	C19—C20—C21—C22	0.9 (6)
C5—C4—C8—O3	178.0 (3)	C18—N2—C22—C21	0.2 (5)
C3—C4—C8—O3	−2.2 (5)	Cu1—N2—C22—C21	180.0 (3)
C5—C4—C8—Cu1^{ii}	−132.2 (6)	C20—C21—C22—N2	−0.6 (6)

Symmetry codes: (i) x, −y+3/2, z+1/2; (ii) x, −y+3/2, z−1/2.

Fig. 1

Fig. 2