metal-organic compounds

catena-Poly[[bis(4-methoxybenzoato)-copper(II)]-*μ*-1,1′-(oxydiethylene)-diimidazole-*κ²N³:N³'*]

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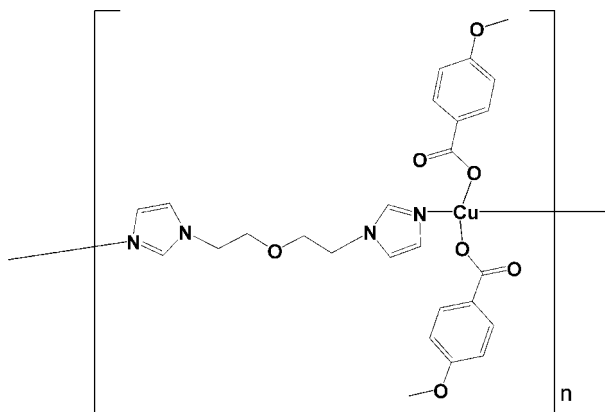Correspondence e-mail: yangjinnenu@yahoo.com.cn

In the title compound, $[Cu(C_7H_4O_3)_2(C_{10}H_{14}N_4O)]_n$, the Cu^{II} atom lies on a centre of symmetry and is four-coordinated by two N atoms from two 1,1′-(oxydiethylene)diimidazole (BIE) ligands and two O atoms from two 4-methoxybenzoate anions in a square-planar geometry. Each BIE ligand links two Cu^{II} atoms to form an infinite chain structure along the c axis. The 4-methoxybenzoate anion, as a terminal ligand, attaches to both sides of the BIE–Cu^{II} chains.

Related literature

For related literature, see: Cao *et al.* (2002); Ma *et al.* (2000); Yang *et al.* (2006); Zhang *et al.* (2004).

Experimental

Crystal data

$[Cu(C_7H_4O_3)_2(C_{10}H_{14}N_4O)]$
$M_r = 572.06$
Monoclinic, $C2/c$
$a = 21.866 (13)$ Å
$b = 7.699 (4)$ Å
$c = 15.519 (8)$ Å
$\beta = 101.44 (2)°$

$V = 2561 (2)$ Å³
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.91$ mm⁻¹
$T = 293 (2)$ K
$0.49 \times 0.48 \times 0.06$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.65$, $T_{max} = 0.950$

11978 measured reflections
2899 independent reflections
2106 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.155$
$S = 1.05$
2899 reflections

196 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.41$ e Å⁻³
$\Delta\rho_{min} = -0.49$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.980 (2)	Cu1—N1	2.003 (3)
O3—Cu1—N1	89.95 (10)		

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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supplementary materials

catena-Poly[[bis(4-methoxybenzoato)copper(II)]-*$^\mu$*-1,1'-(oxydiethylene)diimidazole-*$\kappa^2 N^3$:$N^{3'}$*]

G.-H. Wei, L.-P. Zhang, J.-C. Ma and J. Yang

Comment

Coordination polymers constructed by substituted benzimidazole or imidazole have received increasing interests (Yang *et al.*, 2006; Ma *et al.*, 2000). We have selected 2,2'-bis(imidazol)ether (BIE) as a bridging ligand, *p*-methoxybenzoate as an anion, and Cu^{II} as a central metal, generating a new chain coordination polymer, [Cu(*p*-MB)$_2$(BIE)]$_n$, (I), which is reported here. In this structure the Cu^{II} atom lies on a centre of symmetry and is four-coordinated by two nitrogen atoms from two BIE molecules and two oxygen atoms from two different *p*-MB anions (Cu–N 2.003 (3) Å and Cu–O 1.980 (2) Å) in a square-planar coordination geometry (Fig. 1). The Cu–O and Cu–N bond lengths are all within normal ranges (Zhang *et al.*, 2004; Cao *et al.*, 2002). The two nitrogen atoms of the BIE ligand bridge two Cu^{II} centers, leading to a one-dimensional chain structure (Fig. 2). The monocarboxylate *p*-MB anion, as a terminal ligand, attaches to both sides of the BIE-Cu^{II} chains.

Experimental

A mixture of CuCl$_2$·2H$_2$O (86.0 mg, 0.5 mmol) and NaOH (40 mg, 1 mmol) in 20 ml water was stirred for 10 min at room temperature, then the Cu(OH)$_2$ solid was filtered. *p*-HMB (152.0 mg, 1 mmol) was added to the Cu(OH)$_2$ suspension in water with constant stirring for 1 h and a blue precipitate was obtained. It was filtered off and washed with water. Then BIE (103.1 mg, 0.5 mmol) was added to the precipitatie with stirring for 1 h and a blue solution was obtained. Blue crystals of (I) were obtained by evaporation of the solution at room temperature.

Refinement

All H atoms attached to C were positioned geometrically and refined in the riding aproximation, with C–H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The methyl groups were allowed to rotate but not to tip. The disordered C atoms of the BIE ligand were refined using isotropic C atoms split over two sites, with half occupancy each, and their hydrogen atoms not included in the model.
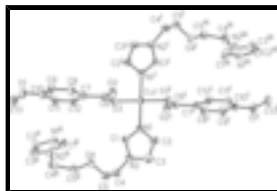
Figures

Fig. 1. Ellipsoid plot of (I), drawn at the 30% probability level, showing the local coordination environment of Cu^{II} (Hydrogen atoms are omitted for clarity). Symmetry codes: (i) −*x*, −*y*, −*z* + 1; (ii) −*x*, *y*, −*z* + 3/2; (iii) *x*, −*y*, *z* − 1/2.
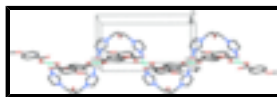

Fig. 2. View of the infinite zigzag polymeric chain of (I) along the *c* axis.

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Crystal data

$[Cu(C_7H_4O_3)_2(C_{10}H_{14}N_4O)]$	$F_{000} = 1188$
$M_r = 572.06$	$D_x = 1.484$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
Hall symbol: -C 2yc	Cell parameters from 8430 reflections
$a = 21.866$ (13) Å	$\theta = 3.0–24.4º$
$b = 7.699$ (4) Å	$\mu = 0.91$ mm^{-1}
$c = 15.519$ (8) Å	$T = 293$ (2) K
$\beta = 101.44$ (2)º	Plate, blue
$V = 2561$ (2) Å^3	$0.49 \times 0.48 \times 0.06$ mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	2899 independent reflections
Radiation source: rotor target	2106 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.051$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.4º$
$T = 293(2)$ K	$\theta_{min} = 3.0º$
ω scans	$h = -28 \rightarrow 28$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -9 \rightarrow 9$
$T_{min} = 0.65$, $T_{max} = 0.950$	$l = -20 \rightarrow 20$
11978 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
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.155$	$w = 1/[\sigma^2(F_o^2) + (0.0869P)^2 + 1.4878P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2899 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
196 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 ($Å^2$)

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
Cu1	0.0000	0.0000	0.5000	0.0411 (2)	
C1	0.03679 (17)	0.3163 (5)	0.6067 (3)	0.0674 (10)	
H1	0.0143	0.2802	0.6484	0.081*	
C2	0.07700 (18)	0.3296 (5)	0.4927 (2)	0.0638 (9)	
H2	0.0878	0.3015	0.4393	0.077*	
C3	0.0962 (2)	0.4710 (5)	0.5402 (3)	0.0743 (12)	
H3	0.1217	0.5587	0.5261	0.089*	
C4	0.0739 (5)	0.6360 (11)	0.6582 (7)	0.073 (2)	0.50
C4'	0.0884 (5)	0.5482 (14)	0.7085 (6)	0.066 (2)	0.50
C5	0.0754 (5)	0.5791 (16)	0.7487 (7)	0.076 (3)	0.50
C5'	0.0296 (5)	0.6503 (10)	0.7251 (5)	0.0632 (19)	0.50
C6	−0.09631 (15)	0.0740 (4)	0.5710 (2)	0.0451 (7)	
C7	−0.13921 (14)	0.0973 (4)	0.63396 (19)	0.0438 (7)	
C8	−0.19905 (16)	0.1591 (6)	0.6029 (2)	0.0641 (10)	
H8	−0.2118	0.1832	0.5433	0.077*	
C9	−0.23998 (16)	0.1856 (6)	0.6589 (2)	0.0689 (11)	
H9	−0.2798	0.2283	0.6370	0.083*	
C10	−0.22173 (15)	0.1485 (5)	0.7478 (2)	0.0539 (8)	
C11	−0.16211 (16)	0.0878 (5)	0.7807 (2)	0.0535 (8)	
H11	−0.1494	0.0636	0.8403	0.064*	
C12	−0.12126 (15)	0.0635 (5)	0.7230 (2)	0.0488 (7)	
H12	−0.0810	0.0236	0.7449	0.059*	
C13	−0.2490 (2)	0.1688 (7)	0.8892 (3)	0.0852 (14)	
H13A	−0.2851	0.1888	0.9144	0.128*	
H13B	−0.2184	0.2568	0.9091	0.128*	
H13C	−0.2318	0.0567	0.9071	0.128*	
N1	0.03890 (11)	0.2319 (3)	0.53434 (16)	0.0475 (6)	
N2	0.07111 (15)	0.4613 (5)	0.6132 (3)	0.0815 (12)	
O1	−0.26625 (11)	0.1746 (4)	0.79675 (16)	0.0749 (8)	
O2	−0.11383 (11)	0.1160 (3)	0.49215 (14)	0.0567 (6)	
O3	−0.04254 (10)	0.0090 (3)	0.60132 (15)	0.0479 (5)	
O4	0.0158 (2)	0.5193 (6)	0.7619 (6)	0.0626 (18)	0.50

supplementary materials

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0408 (3)	0.0455 (3)	0.0388 (3)	0.0011 (2)	0.0126 (2)	−0.0031 (2)
C1	0.051 (2)	0.078 (3)	0.079 (2)	−0.0133 (19)	0.0260 (17)	−0.036 (2)
C2	0.074 (2)	0.061 (2)	0.0566 (19)	−0.0173 (19)	0.0136 (17)	0.0050 (18)
C3	0.065 (3)	0.057 (2)	0.097 (3)	−0.0103 (18)	0.006 (2)	−0.003 (2)
C4	0.101 (7)	0.059 (5)	0.069 (5)	−0.019 (5)	0.037 (5)	−0.023 (4)
C4'	0.081 (6)	0.077 (6)	0.039 (4)	−0.022 (5)	0.007 (4)	−0.015 (5)
C5	0.077 (6)	0.098 (8)	0.055 (5)	−0.037 (6)	0.018 (5)	−0.018 (6)
C5'	0.087 (6)	0.055 (5)	0.051 (4)	0.008 (4)	0.019 (4)	−0.006 (3)
C6	0.0496 (18)	0.0423 (16)	0.0457 (16)	−0.0027 (14)	0.0146 (13)	−0.0032 (14)
C7	0.0413 (16)	0.0480 (18)	0.0442 (15)	0.0001 (13)	0.0132 (12)	−0.0008 (13)
C8	0.0505 (19)	0.095 (3)	0.0467 (17)	0.0130 (19)	0.0089 (14)	0.0061 (18)
C9	0.0415 (18)	0.104 (3)	0.061 (2)	0.0192 (19)	0.0102 (15)	0.004 (2)
C10	0.0453 (17)	0.066 (2)	0.0545 (17)	0.0018 (15)	0.0206 (14)	−0.0035 (16)
C11	0.0517 (18)	0.067 (2)	0.0437 (16)	0.0055 (16)	0.0139 (13)	0.0009 (16)
C12	0.0420 (16)	0.0594 (18)	0.0455 (16)	0.0054 (14)	0.0100 (13)	0.0014 (15)
C13	0.083 (3)	0.119 (4)	0.063 (2)	0.004 (3)	0.037 (2)	−0.010 (2)
N1	0.0432 (14)	0.0485 (14)	0.0510 (14)	0.0023 (11)	0.0098 (11)	−0.0034 (12)
N2	0.0501 (18)	0.079 (2)	0.120 (3)	−0.0167 (16)	0.027 (2)	−0.057 (2)
O1	0.0518 (14)	0.114 (2)	0.0656 (15)	0.0114 (15)	0.0276 (12)	−0.0026 (15)
O2	0.0643 (14)	0.0632 (15)	0.0444 (12)	0.0041 (12)	0.0154 (10)	0.0031 (11)
O3	0.0445 (12)	0.0568 (14)	0.0446 (11)	0.0027 (10)	0.0140 (9)	−0.0034 (9)
O4	0.066 (5)	0.070 (3)	0.057 (5)	−0.001 (2)	0.025 (4)	−0.007 (3)

Geometric parameters (Å, °)

Cu1—O3	1.980 (2)	C5'—O4ii	1.457 (10)
Cu1—O3i	1.980 (2)	C5'—C5'iii	1.637 (17)
Cu1—N1	2.003 (3)	C6—O2	1.249 (4)
Cu1—N1i	2.003 (3)	C6—O3	1.279 (4)
C1—N1	1.306 (4)	C6—C7	1.494 (4)
C1—N2	1.338 (5)	C7—C12	1.384 (4)
C1—H1	0.9300	C7—C8	1.386 (5)
C2—C3	1.335 (5)	C8—C9	1.380 (5)
C2—N1	1.376 (4)	C8—H8	0.9300
C2—H2	0.9300	C9—C10	1.388 (5)
C3—N2	1.354 (6)	C9—H9	0.9300
C3—H3	0.9300	C10—O1	1.363 (4)
C4—C4'	1.034 (12)	C10—C11	1.383 (5)
C4—C5	1.466 (13)	C11—C12	1.397 (4)
C4—N2	1.511 (8)	C11—H11	0.9300
C4—C5'	1.557 (11)	C12—H12	0.9300
C4'—C5	0.773 (10)	C13—O1	1.410 (4)
C4'—C5'	1.570 (14)	C13—H13A	0.9600
C4'—N2	1.599 (9)	C13—H13B	0.9600

C5—C5'	1.136 (13)	C13—H13C	0.9600
C5—O4	1.435 (11)	O4—O4^{ii}	0.715 (10)
C5'—O4	1.227 (10)	O4—C5$^{\prime ii}$	1.457 (10)
O3—Cu1—O3^{i}	180.0	O3—C6—C7	117.2 (3)
O3—Cu1—N1	89.95 (10)	C12—C7—C8	118.3 (3)
O3^{i}—Cu1—N1	90.05 (10)	C12—C7—C6	122.7 (3)
O3—Cu1—N1^{i}	90.05 (10)	C8—C7—C6	119.0 (3)
O3^{i}—Cu1—N1^{i}	89.95 (10)	C9—C8—C7	121.1 (3)
N1—Cu1—N1^{i}	180.00 (13)	C9—C8—H8	119.4
N1—C1—N2	111.4 (3)	C7—C8—H8	119.4
N1—C1—H1	124.3	C8—C9—C10	120.1 (3)
N2—C1—H1	124.3	C8—C9—H9	120.0
C3—C2—N1	109.9 (4)	C10—C9—H9	120.0
C3—C2—H2	125.1	O1—C10—C11	124.7 (3)
N1—C2—H2	125.1	O1—C10—C9	115.3 (3)
C2—C3—N2	106.4 (4)	C11—C10—C9	120.0 (3)
C2—C3—H3	126.8	C10—C11—C12	119.0 (3)
N2—C3—H3	126.8	C10—C11—H11	120.5
C4'—C4—N2	75.3 (8)	C12—C11—H11	120.5
C5—C4—N2	99.7 (8)	C7—C12—C11	121.6 (3)
N2—C4—C5'	113.5 (6)	C7—C12—H12	119.2
C5—C4'—C4	107.5 (18)	C11—C12—H12	119.2
C4—C4'—C5'	70.0 (9)	O1—C13—H13A	109.5
C5—C4'—N2	144.9 (14)	O1—C13—H13B	109.5
C4—C4'—N2	66.0 (6)	H13A—C13—H13B	109.5
C5'—C4'—N2	108.0 (6)	O1—C13—H13C	109.5
C4'—C5—C5'	109.2 (16)	H13A—C13—H13C	109.5
C4'—C5—O4	120.5 (13)	H13B—C13—H13C	109.5
C5'—C5—O4	55.6 (6)	C1—N1—C2	105.0 (3)
C5'—C5—C4	72.3 (8)	C1—N1—Cu1	125.9 (2)
O4—C5—C4	112.6 (9)	C2—N1—Cu1	128.9 (2)
C5—C5'—O4	74.7 (8)	C1—N2—C3	107.3 (3)
C5—C5'—O4^{ii}	101.6 (8)	C1—N2—C4	138.4 (4)
C5—C5'—C4	63.7 (7)	C3—N2—C4	110.6 (5)
O4—C5'—C4	119.8 (8)	C1—N2—C4'	116.4 (5)
O4^{ii}—C5'—C4	125.0 (6)	C3—N2—C4'	133.6 (5)
O4—C5'—C4'	87.2 (7)	C10—O1—C13	119.1 (3)
O4^{ii}—C5'—C4'	106.1 (6)	C6—O3—Cu1	105.27 (19)
C5—C5'—C5$^{\prime ii}$	125.2 (9)	O4^{ii}—O4—C5'	93.5 (10)
O4—C5'—C5$^{\prime ii}$	59.1 (5)	O4^{ii}—O4—C5	137.4 (16)
O4^{ii}—C5'—C5$^{\prime ii}$	46.3 (5)	C5'—O4—C5	49.8 (6)
C4—C5'—C5$^{\prime ii}$	166.1 (10)	O4^{ii}—O4—C5$^{\prime ii}$	57.2 (8)
C4'—C5'—C5$^{\prime ii}$	145.9 (6)	C5'—O4—C5$^{\prime ii}$	74.6 (7)
O2—C6—O3	122.9 (3)	C5—O4—C5$^{\prime ii}$	117.5 (8)
O2—C6—C7	119.9 (3)		

N1—C2—C3—N2	1.1 (5)	C7—C8—C9—C10	−0.7 (7)
N2—C4—C4'—C5	−143.0 (14)	C8—C9—C10—O1	−178.3 (4)
C5'—C4—C4'—C5	−21.5 (12)	C8—C9—C10—C11	1.1 (6)
C5—C4—C4'—C5'	21.5 (12)	O1—C10—C11—C12	178.8 (3)
N2—C4—C4'—C5'	−121.5 (6)	C9—C10—C11—C12	−0.6 (6)
C5—C4—C4'—N2	143.0 (14)	C8—C7—C12—C11	0.9 (5)
C5'—C4—C4'—N2	121.5 (6)	C6—C7—C12—C11	179.4 (3)
C4—C4'—C5—C5'	30.3 (17)	C10—C11—C12—C7	−0.5 (5)
N2—C4'—C5—C5'	−43 (3)	N2—C1—N1—C2	0.1 (4)
C4—C4'—C5—O4	90.9 (17)	N2—C1—N1—Cu1	175.4 (3)
C5'—C4'—C5—O4	60.7 (12)	C3—C2—N1—C1	−0.7 (4)
N2—C4'—C5—O4	18 (4)	C3—C2—N1—Cu1	−175.9 (3)
C5'—C4'—C5—C4	−30.3 (17)	O3—Cu1—N1—C1	8.2 (3)
N2—C4'—C5—C4	−73 (3)	O3^i—Cu1—N1—C1	−171.8 (3)
N2—C4—C5—C4'	36.2 (13)	O3—Cu1—N1—C2	−177.6 (3)
C5'—C4—C5—C4'	150.0 (17)	O3^i—Cu1—N1—C2	2.4 (3)
C4'—C4—C5—C5'	−150.0 (17)	N1—C1—N2—C3	0.6 (5)
N2—C4—C5—C5'	−113.8 (8)	N1—C1—N2—C4	155.5 (8)
C4'—C4—C5—O4	−111.0 (17)	N1—C1—N2—C4'	−163.3 (5)
N2—C4—C5—O4	−74.8 (10)	C2—C3—N2—C1	−1.0 (5)
C5'—C4—C5—O4	39.1 (7)	C2—C3—N2—C4	−163.5 (5)
C4'—C5—C5'—O4	114.3 (15)	C2—C3—N2—C4'	159.0 (7)
C4—C5—C5'—O4	135.2 (7)	C4'—C4—N2—C1	70.4 (12)
C4'—C5—C5'—O4^{ii}	102.7 (15)	C5—C4—N2—C1	52.5 (12)
O4—C5—C5'—O4^{ii}	−11.7 (8)	C5'—C4—N2—C1	8.7 (14)
C4—C5—C5'—O4^{ii}	123.5 (7)	C4'—C4—N2—C3	−135.2 (8)
C4'—C5—C5'—C4	−20.8 (13)	C5—C4—N2—C3	−153.1 (6)
O4—C5—C5'—C4	−135.2 (7)	C5'—C4—N2—C3	163.1 (7)
O4—C5—C5'—C4'	−114.3 (15)	C5—C4—N2—C4'	−17.9 (8)
C4—C5—C5'—C4'	20.8 (13)	C5'—C4—N2—C4'	−61.7 (8)
C4'—C5—C5'—C5'^{ii}	146.7 (13)	C5—C4'—N2—C1	−49 (3)
O4—C5—C5'—C5'^{ii}	32.4 (8)	C4—C4'—N2—C1	−135.7 (7)
C4—C5—C5'—C5'^{ii}	167.6 (9)	C5'—C4'—N2—C1	−78.3 (8)
C4'—C4—C5'—C5	15.4 (9)	C5—C4'—N2—C3	152 (3)
N2—C4—C5'—C5	79.4 (11)	C4—C4'—N2—C3	65.7 (11)
C4'—C4—C5'—O4	−36.2 (10)	C5'—C4'—N2—C3	123.1 (7)
C5—C4—C5'—O4	−51.6 (9)	C5—C4'—N2—C4	87 (3)
N2—C4—C5'—O4	27.8 (14)	C5'—C4'—N2—C4	57.4 (8)
C4'—C4—C5'—O4^{ii}	−70.5 (10)	C11—C10—O1—C13	11.3 (6)
C5—C4—C5'—O4^{ii}	−85.9 (10)	C9—C10—O1—C13	−169.4 (4)
N2—C4—C5'—O4^{ii}	−6.5 (14)	O2—C6—O3—Cu1	1.0 (4)
C5—C4—C5'—C4'	−15.4 (9)	C7—C6—O3—Cu1	−179.7 (2)
N2—C4—C5'—C4'	64.0 (8)	N1—Cu1—O3—C6	93.6 (2)
C4'—C4—C5'—C5'^{ii}	−118 (2)	N1^i—Cu1—O3—C6	−86.4 (2)
C5—C4—C5'—C5'^{ii}	−133 (2)	C5—C5'—O4—O4^{ii}	−156.1 (15)
N2—C4—C5'—C5'^{ii}	−54 (3)	C4—C5'—O4—O4^{ii}	−109.4 (14)

C4—C4'—C5'—C5	−149.3 (19)	C4'—C5'—O4—O4^{ii}	−131.0 (13)
N2—C4'—C5'—C5	155.7 (19)	C5^{iii}—C5'—O4—O4^{ii}	54.6 (12)
C5—C4'—C5'—O4	−61.6 (15)	O4^{ii}—C5'—O4—C5	156.1 (15)
C4—C4'—C5'—O4	149.1 (9)	C4—C5'—O4—C5	46.7 (8)
N2—C4'—C5'—O4	94.1 (8)	C4'—C5'—O4—C5	25.1 (6)
C5—C4'—C5'—O4^{ii}	−84.2 (16)	C5^{iii}—C5'—O4—C5	−149.3 (10)
C4—C4'—C5'—O4^{ii}	126.5 (9)	C5—C5'—O4—C5^{iii}	149.3 (10)
N2—C4'—C5'—O4^{ii}	71.5 (8)	O4^{ii}—C5'—O4—C5^{iii}	−54.6 (12)
C5—C4'—C5'—C4	149.3 (19)	C4—C5'—O4—C5^{iii}	−163.9 (12)
N2—C4'—C5'—C4	−55.0 (6)	C4'—C5'—O4—C5^{iii}	174.4 (8)
C5—C4'—C5'—C5^{iii}	−53 (2)	C4'—C5—O4—O4^{ii}	−57 (3)
C4—C4'—C5'—C5^{iii}	157.7 (16)	C5'—C5—O4—O4^{ii}	36.7 (14)
N2—C4'—C5'—C5^{iii}	102.7 (16)	C4—C5—O4—O4^{ii}	−10.0 (18)
O2—C6—C7—C12	−175.9 (3)	C4'—C5—O4—C5'	−93.4 (19)
O3—C6—C7—C12	4.8 (5)	C4—C5—O4—C5'	−46.7 (8)
O2—C6—C7—C8	2.6 (5)	C4'—C5—O4—C5^{iii}	−127.1 (19)
O3—C6—C7—C8	−176.8 (3)	C5'—C5—O4—C5^{iii}	−33.7 (10)
C12—C7—C8—C9	−0.4 (6)	C4—C5—O4—C5^{iii}	−80.3 (12)
C6—C7—C8—C9	−178.9 (4)		

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

Fig. 1

Fig. 2