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catena-Poly[[bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene-$\kappa^2N^4:N^{4'}$]copper(I)] perchlorate]

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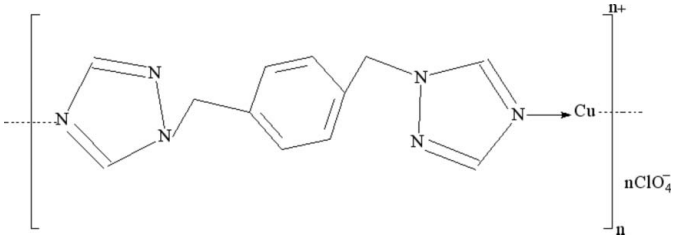
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.046; wR factor = 0.107; data-to-parameter ratio = 9.7.

The crystal structure of the title compound, $\{[Cu(C_{12}H_{12}N_6)]ClO_4\}_n$, consists of a one-dimensional cationic copper(I) chain and uncoordinated ClO_4^- anions. In the cationic chain, the Cu^I center, which lies on a crystallographic twofold rotation axis, is coordinated by two N atoms from two 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene ligands, giving a linear coordination geometry, and the 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene ligand adopts a bis-monodentate bridging mode, linking Cu^I atoms. The anion O atoms are disordered equally over two sites.

Related literature

The corresponding copper(II) coordination polymer has a double-stranded chain structure (Li *et al.*, 2005).



Experimental

Crystal data

$[Cu(C_{12}H_{12}N_6)]ClO_4$
M_r = 403.28
Monoclinic, $C2/c$
a = 16.098 (6) Å
b = 11.550 (4) Å
c = 10.687 (4) Å
β = 128.349 (5)°
V = 1558.4 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.684, T_{max} = 0.788
4433 measured reflections
1595 independent reflections
1106 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.107
S = 1.10
1595 reflections
165 parameters
188 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2171).

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supplementary materials

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catena-Poly[[bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene-$\kappa^2N^4:N^{4'}$]copper(I)] perchlorate]

J. Lin and G.-Y. Dong

Comment

The crystal structure of (I) comprises a one-dimensional cationic $[CuL]_n$ chain [*L* is 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene] and uncoordinated [ClO_4] anion. Within the chain, the coordination geometry of each Cu^I atom is linear (Fig.1 and Table 1). The Cu^I atom, which is two-coordinated by two N atoms from two symmetry-related *L* liagands, with a unique Cu—N distance of 1.867 (3) Å. The N1—Cu1—N1A bond angles is 174.79 (18) °. Each *L* ligand coordinates to two Cu^I atoms, acting as a bridging ligand, forming an extended cationic chain structure (Fig.2). the distance between the closest Cu^I atoms in the chain is 13.1559 (2) Å and the dihedral angle between the benzene with 1,2,4-triazole plane in one *L* ligand is 91 (3) °.

The corresponding copper(II) coordination polymer has double-stranded chain structures. (Li *et al.*, 2005).

Experimental

The ligand *L* was prepared according to the reported procedure (Li *et al.*, 2005). Copper(II) perchlorate hexahydrate (37.1 mg, 0.10 mmol) and copper plates (12.8 mg, 0.2 mmol) were stirred in acetone (5 cm^3) under an ethylene atmosphere for 1 h, and to the resulting colourless solution was added an acetone solution (5 cm^3) containing *L* (48 mg, 0.20 mmol) under argon. The yellow mixture was stirred, and the filtrate transferred to a 10 mm diameter glass tube and layered with n-pentane (2 cm^3) as a diffusion solvent. After standing for 2 weeks at 278 K, pale yellow crystal was obtained in 62% Yield. Analysis calculated for $C_{12}H_{12}$ CuN_6O_4Cl: C 35.74, H 3.00, N 20.84%; found: C 35.63, H 2.94, N 20.78%).

Refinement

The perchlorate O atoms show positional disorder, and they were refined as two groups sharing the same Cl atom. As the occupancy could not be satisfactorily refined, the eight O atoms were each given site occupancy of 0.5. The C—O(1.45 (1) Å) and O —O distances were restrained with approximate equality. The displacement parameters of the disordered O atoms were also restrained weakly to be approximately isotropic. The aromatic [C —H = 0.93 Å and U_{iso}(H) =1.2U_{eq}(C)] and methylene H atoms [C—H= 0.96 Å and U_{iso}(H) =1.5U_{eq}(C)] were included in the refinement in the riding-model approximation.

Figures

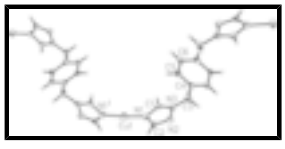

Fig. 1. Part of the structure of (I) showing the coordination environment of atom Cu^I. Displacement ellipsoids are shown at the 30% probability level.[symmetry codes: (i) $x + 2$, y, $-z + 3/2$}

Fig. 2. A view of the one-dimensional structure of (I).

catena-Poly[[bis[μ-1,4-bis(1,2,4-triazol-1-ylmethyl)benzene- $\kappa^2N^4:N^{4'}$]copper(I)] perchlorate]

Crystal data

$[Cu(C_{12}H_{12}N_6)]ClO_4$	F_{000} = 816
M_r = 403.28	D_x = 1.719 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 670 reflections
a = 16.098 (6) Å	θ = 3.2–25.2º
b = 11.550 (4) Å	μ = 1.61 mm^{-1}
c = 10.687 (4) Å	*T* = 293 (2) K
β = 128.349 (5)º	Block, colorless
V = 1558.4 (10) Å^3	0.25 × 0.20 × 0.15 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1595 independent reflections
Radiation source: fine-focus sealed tube	1106 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 293(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	*h* = −20→15
T_{min} = 0.684, T_{max} = 0.788	*k* = −11→14
4433 measured reflections	*l* = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.107	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 2.5014P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.077
1595 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
165 parameters	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
188 restraints	Extinction correction: none

Primary atom site location: structure-invariant direct methods

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	1.0000	0.55003 (7)	0.7500	0.0571 (3)	
C1	0.8162 (3)	0.4702 (3)	0.7079 (4)	0.0428 (9)	
H1	0.7953	0.4219	0.6234	0.051*	
C2	0.8950 (3)	0.5942 (3)	0.8917 (4)	0.0424 (9)	
H2	0.9431	0.6509	0.9610	0.051*	
C3	0.6806 (3)	0.4100 (4)	0.7408 (5)	0.0500 (11)	
H3A	0.6478	0.3664	0.6430	0.060*	
H3B	0.6279	0.4623	0.7258	0.060*	
C4	0.7177 (3)	0.3277 (3)	0.8767 (4)	0.0386 (9)	
C5	0.8028 (3)	0.2532 (3)	0.9363 (5)	0.0435 (10)	
H5	0.8388	0.2551	0.8940	0.052*	
C6	0.8344 (3)	0.1764 (3)	1.0581 (4)	0.0419 (9)	
H6	0.8912	0.1269	1.0965	0.050*	
N1	0.8975 (3)	0.5426 (3)	0.7800 (4)	0.0428 (8)	
N2	0.8187 (3)	0.5572 (3)	0.8931 (4)	0.0444 (8)	
N3	0.7692 (3)	0.4769 (3)	0.7740 (3)	0.0397 (8)	
Cl1	0.5000	0.67676 (13)	0.7500	0.0635 (5)	
O1	0.4610 (15)	0.7125 (15)	0.840 (2)	0.079 (7)	0.188 (7)
O2	0.5716 (14)	0.5829 (14)	0.838 (2)	0.107 (9)	0.188 (7)
O3	0.4091 (12)	0.6380 (15)	0.5978 (12)	0.088 (7)	0.188 (7)
O4	0.5486 (13)	0.7722 (13)	0.7406 (19)	0.081 (7)	0.188 (7)
O1'	0.5238 (10)	0.5799 (9)	0.8375 (14)	0.090 (5)	0.312 (7)
O2'	0.3811 (6)	0.6946 (11)	0.6356 (13)	0.095 (5)	0.312 (7)
O3'	0.5456 (10)	0.7812 (9)	0.8234 (14)	0.138 (7)	0.312 (7)
O4'	0.5214 (9)	0.6559 (11)	0.6319 (11)	0.076 (4)	0.312 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0644 (6)	0.0653 (6)	0.0645 (5)	0.000	0.0513 (5)	0.000
C1	0.055 (3)	0.042 (2)	0.037 (2)	0.005 (2)	0.032 (2)	0.0051 (17)

C2	0.049 (2)	0.040 (2)	0.040 (2)	0.0024 (18)	0.029 (2)	0.0043 (17)
C3	0.046 (3)	0.060 (3)	0.041 (2)	−0.006 (2)	0.025 (2)	0.0061 (19)
C4	0.039 (2)	0.038 (2)	0.0359 (19)	−0.0073 (17)	0.0221 (18)	−0.0034 (16)
C5	0.048 (2)	0.050 (2)	0.046 (2)	−0.0082 (19)	0.036 (2)	−0.0047 (18)
C6	0.038 (2)	0.041 (2)	0.044 (2)	−0.0012 (17)	0.0241 (19)	−0.0026 (17)
N1	0.050 (2)	0.0454 (18)	0.0406 (17)	0.0073 (17)	0.0319 (16)	0.0091 (15)
N2	0.057 (2)	0.0431 (19)	0.0416 (17)	−0.0015 (17)	0.0351 (17)	−0.0014 (15)
N3	0.051 (2)	0.0395 (18)	0.0338 (16)	0.0006 (15)	0.0288 (16)	0.0054 (13)
Cl1	0.0879 (13)	0.0418 (8)	0.0572 (10)	0.000	0.0432 (10)	0.000
O1	0.086 (10)	0.068 (11)	0.093 (11)	0.016 (8)	0.060 (8)	−0.013 (8)
O2	0.119 (13)	0.097 (12)	0.114 (12)	0.041 (9)	0.076 (9)	0.015 (9)
O3	0.097 (11)	0.095 (10)	0.047 (8)	−0.018 (9)	0.032 (7)	−0.019 (8)
O4	0.091 (10)	0.070 (9)	0.058 (9)	−0.044 (7)	0.034 (7)	−0.001 (7)
O1'	0.080 (8)	0.079 (7)	0.108 (8)	0.011 (6)	0.057 (7)	0.045 (6)
O2'	0.070 (7)	0.108 (9)	0.110 (8)	0.011 (6)	0.057 (6)	0.000 (7)
O3'	0.154 (11)	0.116 (9)	0.141 (10)	−0.042 (8)	0.090 (8)	−0.034 (8)
O4'	0.087 (8)	0.085 (8)	0.057 (6)	0.010 (6)	0.046 (5)	−0.002 (5)

Geometric parameters (Å, °)

Cu1—N1^{i}	1.868 (3)	Cl1—O3'^{iii}	1.377 (7)
Cu1—N1	1.868 (3)	Cl1—O4	1.391 (9)
C1—N3	1.318 (5)	Cl1—O4^{iii}	1.391 (9)
C1—N1	1.325 (5)	Cl1—O2^{iii}	1.429 (9)
C1—H1	0.9300	Cl1—O2	1.429 (9)
C2—N2	1.309 (5)	Cl1—O3	1.426 (8)
C2—N1	1.358 (5)	Cl1—O3^{iii}	1.426 (8)
C2—H2	0.9300	Cl1—O1	1.496 (9)
C3—N3	1.459 (5)	Cl1—O1^{iii}	1.496 (9)
C3—C4	1.515 (5)	O1—O4^{iii}	1.04 (3)
C3—H3A	0.9700	O2—O3^{iii}	0.84 (3)
C3—H3B	0.9700	O2—O2^{iii}	1.86 (3)
C4—C6^{ii}	1.385 (5)	O3—O2^{iii}	0.84 (3)
C4—C5	1.392 (5)	O4—O1^{iii}	1.04 (3)
C5—C6	1.385 (5)	O4—O4^{iii}	1.70 (3)
C5—H5	0.9300	O1'—O4'^{iii}	1.30 (2)
C6—C4^{ii}	1.385 (5)	O1'—O1'^{iii}	1.52 (2)
C6—H6	0.9300	O2'—O3'^{iii}	1.39 (2)
N2—N3	1.362 (4)	O3'—O3'^{iii}	1.33 (2)
Cl1—O1'^{iii}	1.352 (7)	O3'—O2'^{iii}	1.39 (2)
Cl1—O1'	1.352 (7)	O4'—O1'^{iii}	1.30 (2)
Cl1—O3'	1.377 (8)		
N1^{i}—Cu1—N1	174.7 (2)	O2^{iii}—Cl1—O2	81.3 (17)
N3—C1—N1	109.9 (3)	O1'^{iii}—Cl1—O3	45.7 (8)
N3—C1—H1	125.1	O1'—Cl1—O3	100.3 (10)

N1—C1—H1	125.1	O3'—Cl1—O3	137.0 (10)
N2—C2—N1	114.0 (4)	O3'^{iii}—Cl1—O3	79.5 (9)
N2—C2—H2	123.0	O4—Cl1—O3	113.0 (6)
N1—C2—H2	123.0	O4^{iii}—Cl1—O3	96.1 (12)
N3—C3—C4	110.8 (3)	O2^{iii}—Cl1—O3	34.4 (12)
N3—C3—H3A	109.5	O2—Cl1—O3	110.5 (7)
C4—C3—H3A	109.5	O1'^{iii}—Cl1—O3^{iii}	100.3 (10)
N3—C3—H3B	109.5	O1'—Cl1—O3^{iii}	45.7 (8)
C4—C3—H3B	109.5	O3'—Cl1—O3^{iii}	79.5 (9)
H3A—C3—H3B	108.1	O3'^{iii}—Cl1—O3^{iii}	137.0 (10)
C6^{ii}—C4—C5	118.7 (3)	O4—Cl1—O3^{iii}	96.1 (12)
C6^{ii}—C4—C3	120.1 (4)	O4^{iii}—Cl1—O3^{iii}	113.0 (6)
C5—C4—C3	121.2 (4)	O2^{iii}—Cl1—O3^{iii}	110.5 (7)
C6—C5—C4	120.6 (4)	O2—Cl1—O3^{iii}	34.4 (12)
C6—C5—H5	119.7	O3—Cl1—O3^{iii}	143.5 (14)
C4—C5—H5	119.7	O1'^{iii}—Cl1—O1	128.4 (9)
C4^{ii}—C6—C5	120.7 (4)	O1'—Cl1—O1	80.5 (9)
C4^{ii}—C6—H6	119.7	O3'—Cl1—O1	71.3 (9)
C5—C6—H6	119.7	O3'^{iii}—Cl1—O1	80.6 (8)
C1—N1—C2	103.3 (3)	O4—Cl1—O1	107.9 (6)
C1—N1—Cu1	126.1 (3)	O4^{iii}—Cl1—O1	41.9 (11)
C2—N1—Cu1	130.0 (3)	O2^{iii}—Cl1—O1	98.1 (11)
C2—N2—N3	102.8 (3)	O2—Cl1—O1	106.1 (6)
C1—N3—N2	110.1 (3)	O3—Cl1—O1	106.0 (7)
C1—N3—C3	129.6 (3)	O3^{iii}—Cl1—O1	84.1 (7)
N2—N3—C3	120.3 (3)	O1'^{iii}—Cl1—O1^{iii}	80.5 (9)
O1'^{iii}—Cl1—O1'	68.4 (12)	O1'—Cl1—O1^{iii}	128.4 (9)
O1'^{iii}—Cl1—O3'	160.2 (8)	O3'—Cl1—O1^{iii}	80.6 (9)
O1'—Cl1—O3'	120.6 (6)	O3'^{iii}—Cl1—O1^{iii}	71.3 (9)
O1'^{iii}—Cl1—O3'^{iii}	120.6 (6)	O4—Cl1—O1^{iii}	41.9 (11)
O1'—Cl1—O3'^{iii}	160.2 (8)	O4^{iii}—Cl1—O1^{iii}	107.9 (6)
O3'—Cl1—O3'^{iii}	57.6 (12)	O2^{iii}—Cl1—O1^{iii}	106.1 (6)
O1'^{iii}—Cl1—O4	122.4 (9)	O2—Cl1—O1^{iii}	98.1 (11)
O1'—Cl1—O4	140.8 (10)	O3—Cl1—O1^{iii}	84.1 (7)
O3'—Cl1—O4	38.9 (7)	O3^{iii}—Cl1—O1^{iii}	106.0 (7)
O3'^{iii}—Cl1—O4	52.4 (8)	O1—Cl1—O1^{iii}	147.9 (14)
O1'^{iii}—Cl1—O4^{iii}	140.8 (10)	O4^{iii}—O1—Cl1	63.6 (9)
O1'—Cl1—O4^{iii}	122.4 (9)	O3^{iii}—O2—Cl1	72.6 (9)
O3'—Cl1—O4^{iii}	52.4 (8)	O3^{iii}—O2—O2^{iii}	114.9 (16)
O3'^{iii}—Cl1—O4^{iii}	38.9 (7)	Cl1—O2—O2^{iii}	49.3 (9)
O4—Cl1—O4^{iii}	75.2 (17)	O2^{iii}—O3—Cl1	73.0 (12)
O1'^{iii}—Cl1—O2^{iii}	32.0 (9)	O1^{iii}—O4—Cl1	74.5 (9)

O1'—Cl1—O2^{iii}	66.0 (8)	O1^{iii}—O4—O4^{iii}	115.1 (15)
O3'—Cl1—O2^{iii}	165.2 (9)	Cl1—O4—O4^{iii}	52.4 (8)
O3'^{iii}—Cl1—O2^{iii}	111.3 (12)	O4'^{iii}—O1'—Cl1	69.8 (6)
O4—Cl1—O2^{iii}	144.6 (9)	O4'^{iii}—O1'—O1'^{iii}	112.0 (10)
O4^{iii}—Cl1—O2^{iii}	112.8 (7)	Cl1—O1'—O1'^{iii}	55.8 (6)
O1'^{iii}—Cl1—O2	66.0 (8)	O3'^{iii}—O2'—Cl1	56.3 (6)
O1'—Cl1—O2	32.0 (9)	O3'^{iii}—O3'—O2'^{iii}	118.1 (10)
O3'—Cl1—O2	111.3 (12)	O3'^{iii}—O3'—Cl1	61.2 (6)
O3'^{iii}—Cl1—O2	165.2 (9)	O2'^{iii}—O3'—Cl1	66.3 (6)
O4—Cl1—O2	112.8 (7)	O1'^{iii}—O4'—Cl1	56.6 (6)
O4^{iii}—Cl1—O2	144.6 (9)		
N3—C3—C4—C6^{ii}	130.3 (4)	O3'^{iii}—Cl1—O4—O4^{iii}	35.7 (10)
N3—C3—C4—C5	−51.0 (5)	O2^{iii}—Cl1—O4—O4^{iii}	109 (2)
C6^{ii}—C4—C5—C6	0.2 (6)	O2—Cl1—O4—O4^{iii}	−143.4 (10)
C3—C4—C5—C6	−178.5 (4)	O3—Cl1—O4—O4^{iii}	90.4 (12)
C4—C5—C6—C4^{ii}	−0.2 (6)	O3^{iii}—Cl1—O4—O4^{iii}	−112.3 (8)
N3—C1—N1—C2	−0.9 (4)	O1—Cl1—O4—O4^{iii}	−26.6 (12)
N3—C1—N1—Cu1	170.7 (2)	O1^{iii}—Cl1—O4—O4^{iii}	140 (2)
N2—C2—N1—C1	0.7 (4)	O1'^{iii}—Cl1—O1'—O4'^{iii}	−137.2 (12)
N2—C2—N1—Cu1	−170.5 (3)	O3'—Cl1—O1'—O4'^{iii}	62.5 (11)
N1^{i}—Cu1—N1—C1	−41.6 (3)	O3'^{iii}—Cl1—O1'—O4'^{iii}	−16 (3)
N1^{i}—Cu1—N1—C2	127.8 (3)	O4—Cl1—O1'—O4'^{iii}	107.6 (15)
N1—C2—N2—N3	−0.2 (4)	O4^{iii}—Cl1—O1'—O4'^{iii}	0.2 (12)
N1—C1—N3—N2	0.9 (4)	O2^{iii}—Cl1—O1'—O4'^{iii}	−102.5 (11)
N1—C1—N3—C3	−176.4 (3)	O2—Cl1—O1'—O4'^{iii}	144 (3)
C2—N2—N3—C1	−0.4 (4)	O3—Cl1—O1'—O4'^{iii}	−103.8 (13)
C2—N2—N3—C3	177.2 (3)	O3^{iii}—Cl1—O1'—O4'^{iii}	91.9 (15)
C4—C3—N3—C1	108.9 (4)	O1—Cl1—O1'—O4'^{iii}	0.9 (11)
C4—C3—N3—N2	−68.1 (5)	O1^{iii}—Cl1—O1'—O4'^{iii}	165.5 (11)
O1'^{iii}—Cl1—O1—O4^{iii}	−126.6 (18)	O3'—Cl1—O1'—O1'^{iii}	−160.3 (8)
O1'—Cl1—O1—O4^{iii}	−179.1 (16)	O3'^{iii}—Cl1—O1'—O1'^{iii}	121 (3)
O3'—Cl1—O1—O4^{iii}	54.0 (14)	O4—Cl1—O1'—O1'^{iii}	−115.2 (12)
O3'^{iii}—Cl1—O1—O4^{iii}	−4.9 (18)	O4^{iii}—Cl1—O1'—O1'^{iii}	137.4 (10)
O4—Cl1—O1—O4^{iii}	40 (2)	O2^{iii}—Cl1—O1'—O1'^{iii}	34.7 (11)
O2^{iii}—Cl1—O1—O4^{iii}	−115.3 (14)	O2—Cl1—O1'—O1'^{iii}	−79 (2)
O2—Cl1—O1—O4^{iii}	162 (2)	O3—Cl1—O1'—O1'^{iii}	33.3 (12)
O3—Cl1—O1—O4^{iii}	−81 (2)	O3^{iii}—Cl1—O1'—O1'^{iii}	−131.0 (16)
O3^{iii}—Cl1—O1—O4^{iii}	134.8 (15)	O1—Cl1—O1'—O1'^{iii}	138.1 (11)
O1^{iii}—Cl1—O1—O4^{iii}	23.9 (14)	O1^{iii}—Cl1—O1'—O1'^{iii}	−57.3 (14)
O1'^{iii}—Cl1—O2—O3^{iii}	−178 (3)	O1'^{iii}—Cl1—O2'—O3'^{iii}	−133.2 (9)

O1'—Cl1—O2—O3^{iii}	−90 (2)	O1'—Cl1—O2'—O3''^{iii}	162.8 (11)
O3'—Cl1—O2—O3^{iii}	24 (2)	O3'—Cl1—O2'—O3''^{iii}	29.7 (14)
O3''^{iii}—Cl1—O2—O3^{iii}	63 (4)	O4—Cl1—O2'—O3''^{iii}	−11.3 (13)
O4—Cl1—O2—O3^{iii}	66 (2)	O4^{iii}—Cl1—O2'—O3''^{iii}	46.5 (9)
O4^{iii}—Cl1—O2—O3^{iii}	−31 (4)	O2^{iii}—Cl1—O2'—O3''^{iii}	−154.7 (13)
O2^{iii}—Cl1—O2—O3^{iii}	−148 (3)	O2—Cl1—O2'—O3''^{iii}	−176.2 (12)
O3—Cl1—O2—O3^{iii}	−166.7 (15)	O3—Cl1—O2'—O3''^{iii}	−115.2 (16)
O1—Cl1—O2—O3^{iii}	−52 (2)	O3^{iii}—Cl1—O2'—O3''^{iii}	128.2 (15)
O1^{iii}—Cl1—O2—O3^{iii}	107 (2)	O1—Cl1—O2'—O3''^{iii}	91.5 (11)
O1''^{iii}—Cl1—O2—O2^{iii}	−29.4 (9)	O1^{iii}—Cl1—O2'—O3''^{iii}	−55.1 (10)
O1'—Cl1—O2—O2^{iii}	57.9 (19)	O1''^{iii}—Cl1—O3'—O3''^{iii}	91 (3)
O3'—Cl1—O2—O2^{iii}	171.8 (8)	O1'—Cl1—O3'—O3''^{iii}	−156.9 (10)
O3''^{iii}—Cl1—O2—O2^{iii}	−149 (3)	O4—Cl1—O3'—O3''^{iii}	68.6 (17)
O4—Cl1—O2—O2^{iii}	−146.1 (10)	O4^{iii}—Cl1—O3'—O3''^{iii}	−47.6 (11)
O4^{iii}—Cl1—O2—O2^{iii}	117 (2)	O2^{iii}—Cl1—O3'—O3''^{iii}	−44 (4)
O3—Cl1—O2—O2^{iii}	−18.5 (14)	O2—Cl1—O3'—O3''^{iii}	168.9 (10)
O3^{iii}—Cl1—O2—O2^{iii}	148 (3)	O3—Cl1—O3'—O3''^{iii}	3.2 (18)
O1—Cl1—O2—O2^{iii}	96.0 (11)	O3^{iii}—Cl1—O3'—O3''^{iii}	−177.8 (13)
O1^{iii}—Cl1—O2—O2^{iii}	−105.2 (7)	O1—Cl1—O3'—O3''^{iii}	−90.5 (12)
O1''^{iii}—Cl1—O3—O2^{iii}	47.7 (18)	O1^{iii}—Cl1—O3'—O3''^{iii}	73.8 (12)
O1'—Cl1—O3—O2^{iii}	2(2)	O1''^{iii}—Cl1—O3'—O2''^{iii}	−55 (3)
O3'—Cl1—O3—O2^{iii}	−160.5 (17)	O1'—Cl1—O3'—O2''^{iii}	57.1 (10)
O3''^{iii}—Cl1—O3—O2^{iii}	−158 (2)	O3''^{iii}—Cl1—O3'—O2''^{iii}	−146.0 (15)
O4—Cl1—O3—O2^{iii}	161 (2)	O4—Cl1—O3'—O2''^{iii}	−77.4 (16)
O4^{iii}—Cl1—O3—O2^{iii}	−122.3 (19)	O4^{iii}—Cl1—O3'—O2''^{iii}	166.4 (16)
O2—Cl1—O3—O2^{iii}	34 (3)	O2^{iii}—Cl1—O3'—O2''^{iii}	170 (3)
O3^{iii}—Cl1—O3—O2^{iii}	21.2 (19)	O2—Cl1—O3'—O2''^{iii}	22.9 (12)
O1—Cl1—O3—O2^{iii}	−81 (2)	O3—Cl1—O3'—O2''^{iii}	−142.8 (13)
O1^{iii}—Cl1—O3—O2^{iii}	130.2 (19)	O3^{iii}—Cl1—O3'—O2''^{iii}	36.2 (10)
O1''^{iii}—Cl1—O4—O1^{iii}	1.0 (19)	O1—Cl1—O3'—O2''^{iii}	123.5 (11)
O1'—Cl1—O4—O1^{iii}	96.0 (17)	O1^{iii}—Cl1—O3'—O2''^{iii}	−72.2 (10)
O3'—Cl1—O4—O1^{iii}	172 (3)	O1'—Cl1—O4'—O1''^{iii}	42.1 (14)
O3''^{iii}—Cl1—O4—O1^{iii}	−104.7 (15)	O3'—Cl1—O4'—O1''^{iii}	174.3 (11)
O4^{iii}—Cl1—O4—O1^{iii}	−140 (2)	O3''^{iii}—Cl1—O4'—O1''^{iii}	−130.2 (9)
O2^{iii}—Cl1—O4—O1^{iii}	−32 (4)	O4—Cl1—O4'—O1''^{iii}	−179.8 (11)
O2—Cl1—O4—O1^{iii}	76.2 (15)	O4^{iii}—Cl1—O4'—O1''^{iii}	−130.3 (13)
O3—Cl1—O4—O1^{iii}	−50.0 (16)	O2^{iii}—Cl1—O4'—O1''^{iii}	−18.4 (14)
O3^{iii}—Cl1—O4—O1^{iii}	107.3 (15)	O2—Cl1—O4'—O1''^{iii}	63.5 (10)
O1—Cl1—O4—O1^{iii}	−166.9 (11)	O3—Cl1—O4'—O1''^{iii}	−51.2 (10)
O1''^{iii}—Cl1—O4—O4^{iii}	141.4 (8)	O3^{iii}—Cl1—O4'—O1''^{iii}	90.3 (13)
O1'—Cl1—O4—O4^{iii}	−123.6 (12)	O1—Cl1—O4'—O1''^{iii}	−105 (4)

O3'—Cl1—O4—O4^{iii}	−47.3 (14)	O1^{iii}—Cl1—O4'—O1'^{iii}	−178 (2)

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

Fig. 1

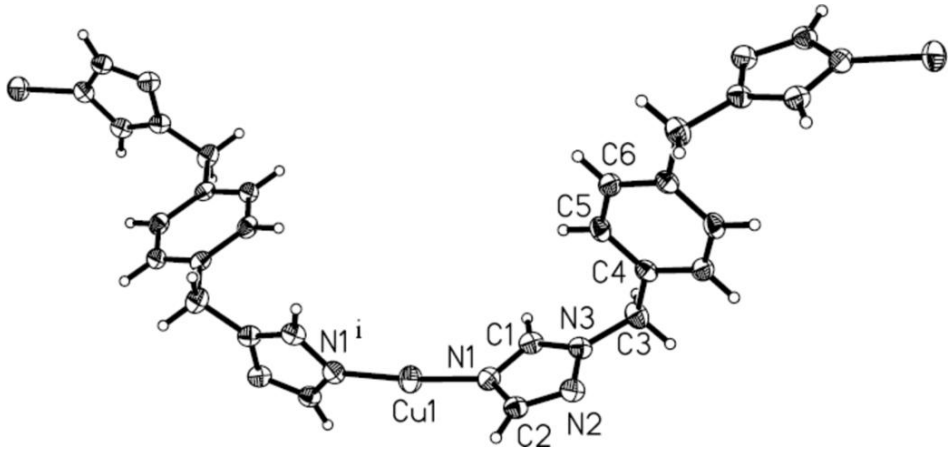

Fig. 2