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8-Chloromethyl-5-(2,5-dioxooxolan-3-yl)-3,3a,4,5-tetrahydro-1*H*-naphtho-[1,2-*c*]furan-1,3-dione

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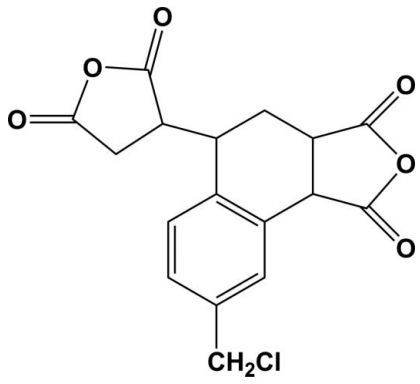
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.108; data-to-parameter ratio = 14.9.

The title compound, $C_{17}H_{13}ClO_6$, is an asymmetric alicyclic dianhydride containing a chloromethyl-substituted tetrahydronaphthalene moiety. The cyclohexene ring in the tetrahydronaphthalene moiety exhibits an envelope conformation with the tertiary C atom as the flap The dihedral angle between the two anhydride rings is 79.96 (6)°, while those between the benzene ring and the non-fused and fused anhydride rings are 71.03 (5) and 42.57 (7)°, respectively. In the crystal, molecules are connected by weak C—H···O interactions, forming a three-dimensional supramolecular structure.

Related literature

For background to polyimides, see: Li *et al.* (2005); Liaw *et al.* (2012); Zhang *et al.* (2003); Zhong *et al.* (2004). For background to and applications of tetrahydronaphthalene-containing alicyclic dianhydrides, see: Guo, Shen *et al.* (2013). For the structure of a related compound, see: Guo, Liu & Yang (2013) and for its synthesis, see: Hall *et al.* (1982); Guo *et al.* (2012). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{17}H_{13}ClO_6$
M_r = 348.72
Triclinic, $P\overline{1}$
a = 6.8988 (15) Å
b = 9.140 (2) Å
c = 11.950 (3) Å
α = 80.937 (9)°
β = 75.365 (8)°
γ = 79.614 (8)°
V = 712.1 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 173 K
0.41 × 0.21 × 0.15 mm

Data collection

Rigaku Saturn724+ CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.702, T_{max} = 1.000
9192 measured reflections
3238 independent reflections
3034 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.10
3238 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3*B*···O4^{i}	0.99	2.51	3.420 (2)	153
C5—H5···O1^{ii}	1.00	2.59	3.386 (2)	136
C7—H7···O4^{i}	1.00	2.51	3.468 (2)	160

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

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZP2004).

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supporting information

Acta Cryst. (2013). E**69**, o1031–o1032 [https://doi.org/10.1107/S1600536813014943]

8-Chloromethyl-5-(2,5-dioxooxolan-3-yl)-3,3a,4,5-tetrahydro-1*H*-naphtho[1,2-*c*]furan-1,3-dione

Y. Z. Guo, Y. Z. Song, J. G. Liu and S. Y. Yang

S1. Comment

Polyimide (PI) is an important class of high performance polymers in the current industry. Functional PI materials have been widely used in microelectronic, optoelectronic and advanced display areas (Liaw *et al.*, 2012). Chloromethyl is an important active species for functionalization of PI materials (Li *et al.*, 2005). For instance, PIs which are highly sensitive to ultraviolet lights of high-pressure mercury lamps have been successfully developed *via* the reaction of chloromethyl substituted in the PI molecules with photosensitive substances, such as cinnamic acid (Zhang *et al.*, 2003). In addition, chloromethyl-containing PIs exhibited good sensitivity to linearly polarized ultraviolet light, which making it possible using the PIs for the photoalignment fabrication of liquid crystal molecules in advanced liquid crystal display devices (Zhong *et al.*, 2004). In the current work, we reported a novel chloromethyl-containing alicyclic dianhydride monomer. The molecular structure of the title compound is shown in Fig. 1. The compound has an asymmetrical structure and the dihedral angle between the two anhydride rings is 79.96 (6)° while the dihedral angles between the benzene ring and the anhydride ring 1(C1—C2—C3—C4—O2) and anhydride ring 2 (C7—C8—C9—C10—O5) are 71.03 (5)° and 42.57 (7)°, respectively. The six-membered cyclohexene ring in the tetra-hydronaphthalene residue exhibits an envelope conformation with puckering parameters of Q = 0.4805 (17) Å, θ=57.46 (19)° and φ =58.9 (2)°. =122.8 (2)° and φ=300.7 (2)° (Cremer & Pople, 1975). There is an intramolecular C—H···Cl hydrogen bond in the molecule, while in the crystal, molecules are connected by week C—H···O intermolecular interactions, as shown in Table 1.

S2. Experimental

Into a 500 ml three-necked flask equipped with a mechanical stirrer, a nitric oxide inlet, and a condenser, 43.75 g(0.446 mol) of maleic anhydride, 104.09 g(0.682 mol) of 4-chloromethylstyrene, 0.1138 g(0.5 mmol) of 2,5-di-*tert*-butyl hydroquinone were added. The reaction mixture was heated to 120°C and maintained for 6 h under nitric oxide. The produced red-brown nitrogen oxide gas was trapped by passing through an aqueous solution of 20 wt% sodium hydroxide. White needle crystals were formed. After the reaction was completed, 60 ml of acetonitrile was added and the solution was refluxed for about 0.5 h. Then 60 ml of toluene was added and the reactino mixture was cooled to room temperature. The produced white needle crystals was collected by filtration and the solid was washed with toluene and petroleum ether in succession. After being dried in vacuum, the pure MCTDA was obtained as white crystals. Yield: 59.49 g(76.5%). Elemental analysis: calculated for $C_{17}H_{13}ClO_6$:*C*,58.55; H:3.76%. Found: C:58.71; H:3.85%. EI—MS, m/*z*:142(M^+-176, 100%). Colourless single crystals were grown by slow evaporation of an acetonitrile solution over a period of several days.

S3. Refinement

All H atoms were positioned geometrically (C-H=0.95-1.00 Å) and refined using a riding model with the U_{iso}(H)=1.2 U_{eq}C for both of the aromatic ring and aliphatic chain.

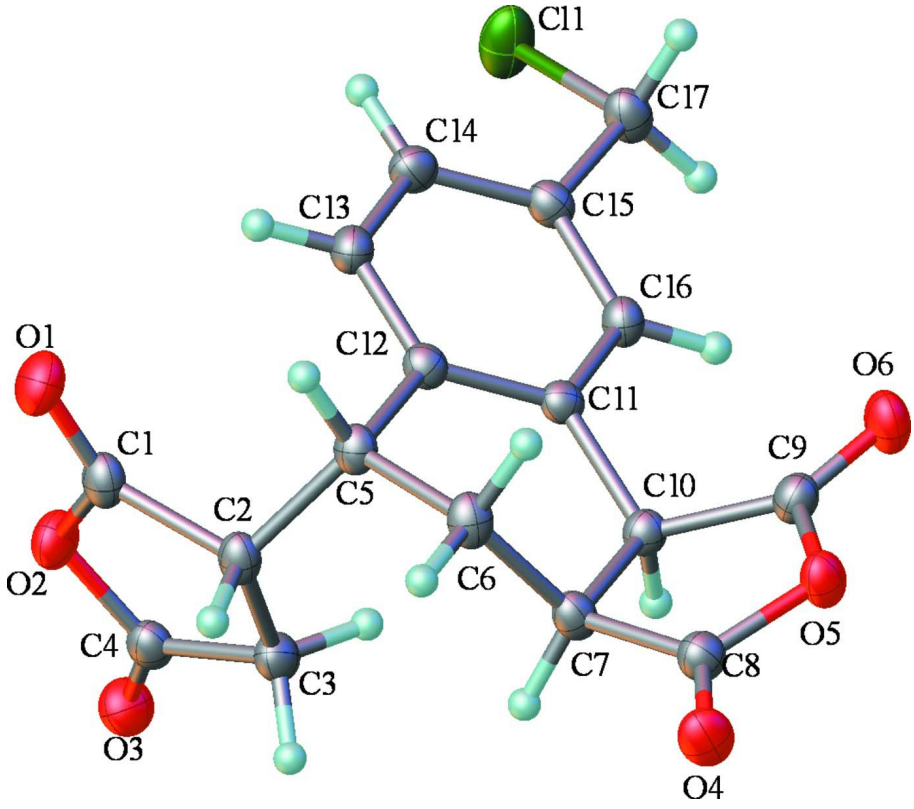

Figure 1

The molecular structure of the title compound, showing diaplacement ellipsoids at the 30% probability level.

8-Chloromethyl-5-(2,5-dioxooxolan-3-yl)-3,3a,4,5-tetrahydro-1*H*-naphtho[1,2-*c*]furan-1,3-dione

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c = 11.950 (3) Å
α = 80.937 (9)°
β = 75.365 (8)°
γ = 79.614 (8)°
V = 712.1 (3) Å^3

Z = 2
F(000) = 360
D_x = 1.626 Mg m^{-3}
Melting point: 502 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2542 reflections
θ = 2.3–27.5°
μ = 0.30 mm^{-1}
T = 173 K
Block, colourless
0.41 × 0.21 × 0.15 mm

Data collection

Rigaku Saturn724+ CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
ω scans at fixed χ = 45°

Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.702, T_{max} = 1.000
9192 measured reflections
3238 independent reflections

3034 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.108$
$S = 1.10$
3238 reflections
217 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.3488P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.05131 (7)	−0.07996 (5)	0.86631 (4)	0.03800 (15)
O1	0.26974 (19)	0.57365 (14)	0.98000 (10)	0.0314 (3)
O2	0.50528 (18)	0.64807 (13)	0.82479 (10)	0.0277 (3)
O3	0.70203 (18)	0.68985 (14)	0.64654 (11)	0.0303 (3)
O4	−0.16049 (18)	0.33284 (13)	0.54844 (11)	0.0301 (3)
O5	0.05290 (17)	0.11884 (12)	0.56476 (10)	0.0258 (3)
O6	0.31175 (19)	−0.05753 (13)	0.59407 (11)	0.0307 (3)
C1	0.3305 (2)	0.58452 (17)	0.87724 (14)	0.0236 (3)
C2	0.2441 (2)	0.53951 (17)	0.78490 (14)	0.0217 (3)
H2	0.1206	0.6131	0.7772	0.026*
C3	0.4071 (2)	0.56388 (18)	0.67298 (14)	0.0241 (3)
H3A	0.4742	0.4670	0.6448	0.029*
H3B	0.3475	0.6268	0.6112	0.029*
C4	0.5553 (2)	0.64167 (17)	0.70584 (14)	0.0229 (3)
C5	0.1782 (2)	0.38204 (17)	0.82204 (13)	0.0198 (3)
H5	0.1048	0.3789	0.9058	0.024*
C6	0.0298 (2)	0.35351 (18)	0.75498 (14)	0.0228 (3)
H6A	−0.0792	0.4403	0.7555	0.027*
H6B	−0.0331	0.2643	0.7946	0.027*
C7	0.1347 (2)	0.32835 (17)	0.62825 (14)	0.0209 (3)
H7	0.1755	0.4237	0.5823	0.025*
C8	−0.0087 (2)	0.26947 (18)	0.57545 (14)	0.0235 (3)

C9	0.2381 (2)	0.07047 (18)	0.59505 (13)	0.0226 (3)
C10	0.3176 (2)	0.20368 (16)	0.61997 (13)	0.0194 (3)
H10	0.4219	0.2337	0.5491	0.023*
C11	0.4192 (2)	0.17137 (16)	0.72211 (13)	0.0183 (3)
C12	0.3571 (2)	0.25765 (16)	0.81480 (13)	0.0190 (3)
C13	0.4641 (2)	0.22721 (17)	0.90297 (13)	0.0222 (3)
H13	0.4250	0.2865	0.9658	0.027*
C14	0.6257 (2)	0.11244 (17)	0.90047 (14)	0.0237 (3)
H14	0.6960	0.0934	0.9614	0.028*
C15	0.6854 (2)	0.02504 (17)	0.80893 (14)	0.0213 (3)
C16	0.5840 (2)	0.05678 (17)	0.71949 (13)	0.0206 (3)
H16	0.6274	−0.0003	0.6554	0.025*
C17	0.8514 (2)	−0.10779 (18)	0.80455 (15)	0.0259 (3)
H17A	0.9082	−0.1267	0.7225	0.031*
H17B	0.7930	−0.1975	0.8474	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0321 (2)	0.0391 (3)	0.0504 (3)	0.00849 (18)	−0.0251 (2)	−0.0182 (2)
O1	0.0324 (6)	0.0352 (7)	0.0283 (6)	−0.0042 (5)	−0.0050 (5)	−0.0130 (5)
O2	0.0287 (6)	0.0309 (6)	0.0285 (6)	−0.0087 (5)	−0.0100 (5)	−0.0079 (5)
O3	0.0303 (6)	0.0306 (6)	0.0324 (7)	−0.0097 (5)	−0.0082 (5)	−0.0032 (5)
O4	0.0269 (6)	0.0288 (6)	0.0394 (7)	−0.0020 (5)	−0.0181 (5)	−0.0038 (5)
O5	0.0256 (6)	0.0227 (6)	0.0339 (6)	−0.0028 (4)	−0.0137 (5)	−0.0070 (5)
O6	0.0334 (6)	0.0226 (6)	0.0396 (7)	0.0017 (5)	−0.0136 (5)	−0.0118 (5)
C1	0.0232 (7)	0.0202 (7)	0.0292 (8)	0.0000 (6)	−0.0082 (6)	−0.0084 (6)
C2	0.0205 (7)	0.0191 (7)	0.0277 (8)	0.0003 (6)	−0.0092 (6)	−0.0072 (6)
C3	0.0286 (8)	0.0213 (7)	0.0256 (8)	−0.0070 (6)	−0.0101 (6)	−0.0025 (6)
C4	0.0249 (8)	0.0184 (7)	0.0271 (8)	−0.0007 (6)	−0.0105 (6)	−0.0031 (6)
C5	0.0172 (7)	0.0202 (7)	0.0224 (7)	−0.0011 (5)	−0.0041 (6)	−0.0062 (6)
C6	0.0180 (7)	0.0226 (7)	0.0293 (8)	−0.0020 (6)	−0.0062 (6)	−0.0074 (6)
C7	0.0199 (7)	0.0183 (7)	0.0269 (8)	−0.0023 (5)	−0.0096 (6)	−0.0032 (6)
C8	0.0241 (8)	0.0225 (7)	0.0257 (8)	−0.0041 (6)	−0.0088 (6)	−0.0028 (6)
C9	0.0237 (7)	0.0238 (8)	0.0220 (7)	−0.0023 (6)	−0.0075 (6)	−0.0055 (6)
C10	0.0190 (7)	0.0198 (7)	0.0204 (7)	−0.0026 (5)	−0.0059 (5)	−0.0035 (6)
C11	0.0182 (7)	0.0174 (7)	0.0202 (7)	−0.0046 (5)	−0.0057 (5)	−0.0009 (5)
C12	0.0184 (7)	0.0177 (7)	0.0214 (7)	−0.0036 (5)	−0.0049 (5)	−0.0018 (5)
C13	0.0266 (8)	0.0203 (7)	0.0207 (7)	−0.0045 (6)	−0.0059 (6)	−0.0040 (6)
C14	0.0261 (8)	0.0223 (7)	0.0253 (8)	−0.0038 (6)	−0.0116 (6)	−0.0010 (6)
C15	0.0202 (7)	0.0183 (7)	0.0263 (8)	−0.0027 (5)	−0.0076 (6)	−0.0015 (6)
C16	0.0209 (7)	0.0191 (7)	0.0229 (7)	−0.0028 (6)	−0.0054 (6)	−0.0054 (6)
C17	0.0254 (8)	0.0209 (7)	0.0345 (9)	−0.0002 (6)	−0.0137 (7)	−0.0050 (6)

Geometric parameters (Å, º)

Cl1—C17	1.7920 (16)	C6—H6A	0.9900
O1—C1	1.187 (2)	C6—H6B	0.9900

O2—C4	1.384 (2)	C7—C8	1.510 (2)
O2—C1	1.393 (2)	C7—C10	1.535 (2)
O3—C4	1.192 (2)	C7—H7	1.0000
O4—C8	1.1957 (19)	C9—C10	1.520 (2)
O5—C8	1.3818 (19)	C10—C11	1.520 (2)
O5—C9	1.3923 (19)	C10—H10	1.0000
O6—C9	1.189 (2)	C11—C12	1.395 (2)
C1—C2	1.518 (2)	C11—C16	1.398 (2)
C2—C3	1.529 (2)	C12—C13	1.399 (2)
C2—C5	1.552 (2)	C13—C14	1.384 (2)
C2—H2	1.0000	C13—H13	0.9500
C3—C4	1.503 (2)	C14—C15	1.390 (2)
C3—H3A	0.9900	C14—H14	0.9500
C3—H3B	0.9900	C15—C16	1.386 (2)
C5—C12	1.515 (2)	C15—C17	1.509 (2)
C5—C6	1.528 (2)	C16—H16	0.9500
C5—H5	1.0000	C17—H17A	0.9900
C6—C7	1.538 (2)	C17—H17B	0.9900

C4—O2—C1	110.80 (12)	C6—C7—H7	110.6
C8—O5—C9	110.77 (12)	O4—C8—O5	120.53 (14)
O1—C1—O2	120.33 (14)	O4—C8—C7	129.30 (15)
O1—C1—C2	129.76 (15)	O5—C8—C7	110.11 (13)
O2—C1—C2	109.90 (13)	O6—C9—O5	120.05 (15)
C1—C2—C3	103.52 (12)	O6—C9—C10	130.51 (15)
C1—C2—C5	110.96 (13)	O5—C9—C10	109.38 (13)
C3—C2—C5	118.62 (12)	C9—C10—C11	114.41 (12)
C1—C2—H2	107.8	C9—C10—C7	103.68 (12)
C3—C2—H2	107.8	C11—C10—C7	116.64 (12)
C5—C2—H2	107.8	C9—C10—H10	107.2
C4—C3—C2	105.08 (13)	C11—C10—H10	107.2
C4—C3—H3A	110.7	C7—C10—H10	107.2
C2—C3—H3A	110.7	C12—C11—C16	119.82 (13)
C4—C3—H3B	110.7	C12—C11—C10	121.42 (13)
C2—C3—H3B	110.7	C16—C11—C10	118.70 (13)
H3A—C3—H3B	108.8	C11—C12—C13	118.55 (14)
O3—C4—O2	120.22 (14)	C11—C12—C5	121.75 (13)
O3—C4—C3	129.78 (15)	C13—C12—C5	119.70 (13)
O2—C4—C3	109.95 (13)	C14—C13—C12	121.30 (14)
C12—C5—C6	110.91 (12)	C14—C13—H13	119.3
C12—C5—C2	112.48 (12)	C12—C13—H13	119.3
C6—C5—C2	112.64 (13)	C13—C14—C15	120.07 (14)
C12—C5—H5	106.8	C13—C14—H14	120.0
C6—C5—H5	106.8	C15—C14—H14	120.0
C2—C5—H5	106.8	C16—C15—C14	119.13 (14)
C5—C6—C7	111.94 (12)	C16—C15—C17	117.99 (14)
C5—C6—H6A	109.2	C14—C15—C17	122.83 (14)
C7—C6—H6A	109.2	C15—C16—C11	121.09 (14)

C5—C6—H6B	109.2	C15—C16—H16	119.5
C7—C6—H6B	109.2	C11—C16—H16	119.5
H6A—C6—H6B	107.9	C15—C17—Cl1	112.50 (11)
C8—C7—C10	103.64 (12)	C15—C17—H17A	109.1
C8—C7—C6	108.82 (13)	Cl1—C17—H17A	109.1
C10—C7—C6	112.36 (12)	C15—C17—H17B	109.1
C8—C7—H7	110.6	Cl1—C17—H17B	109.1
C10—C7—H7	110.6	H17A—C17—H17B	107.8

C4—O2—C1—O1	176.48 (15)	O6—C9—C10—C7	−170.26 (17)
C4—O2—C1—C2	−4.14 (16)	O5—C9—C10—C7	12.71 (16)
O1—C1—C2—C3	−172.78 (17)	C8—C7—C10—C9	−15.08 (15)
O2—C1—C2—C3	7.90 (16)	C6—C7—C10—C9	102.23 (14)
O1—C1—C2—C5	−44.5 (2)	C8—C7—C10—C11	−141.81 (13)
O2—C1—C2—C5	136.19 (13)	C6—C7—C10—C11	−24.50 (18)
C1—C2—C3—C4	−8.38 (15)	C9—C10—C11—C12	−125.35 (15)
C5—C2—C3—C4	−131.77 (13)	C7—C10—C11—C12	−4.1 (2)
C1—O2—C4—O3	−179.38 (14)	C9—C10—C11—C16	57.57 (18)
C1—O2—C4—C3	−1.65 (17)	C7—C10—C11—C16	178.79 (13)
C2—C3—C4—O3	−175.99 (16)	C16—C11—C12—C13	0.5 (2)
C2—C3—C4—O2	6.56 (17)	C10—C11—C12—C13	−176.56 (13)
C1—C2—C5—C12	−72.89 (16)	C16—C11—C12—C5	−179.44 (13)
C3—C2—C5—C12	46.72 (18)	C10—C11—C12—C5	3.5 (2)
C1—C2—C5—C6	160.87 (12)	C6—C5—C12—C11	25.70 (19)
C3—C2—C5—C6	−79.51 (16)	C2—C5—C12—C11	−101.46 (16)
C12—C5—C6—C7	−54.14 (17)	C6—C5—C12—C13	−154.22 (14)
C2—C5—C6—C7	72.94 (16)	C2—C5—C12—C13	78.62 (17)
C5—C6—C7—C8	168.26 (12)	C11—C12—C13—C14	−1.2 (2)
C5—C6—C7—C10	54.08 (17)	C5—C12—C13—C14	178.68 (14)
C9—O5—C8—O4	176.79 (15)	C12—C13—C14—C15	0.3 (2)
C9—O5—C8—C7	−5.78 (17)	C13—C14—C15—C16	1.5 (2)
C10—C7—C8—O4	−169.45 (17)	C13—C14—C15—C17	−176.01 (14)
C6—C7—C8—O4	70.8 (2)	C14—C15—C16—C11	−2.3 (2)
C10—C7—C8—O5	13.41 (16)	C17—C15—C16—C11	175.37 (14)
C6—C7—C8—O5	−106.35 (14)	C12—C11—C16—C15	1.3 (2)
C8—O5—C9—O6	177.93 (15)	C10—C11—C16—C15	178.39 (14)
C8—O5—C9—C10	−4.67 (17)	C16—C15—C17—Cl1	147.27 (13)
O6—C9—C10—C11	−42.1 (2)	C14—C15—C17—Cl1	−35.2 (2)
O5—C9—C10—C11	140.82 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*B*···O4^{i}	0.99	2.51	3.420 (2)	153
C5—H5···O1^{ii}	1.00	2.59	3.386 (2)	136

C7—H7···O4^{i}	1.00	2.51	3.468 (2)	160
C14—H14···Cl1	0.95	2.75	3.1045 (17)	103

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