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10,13-Dimethyl-16-oxo-4,5,6,7,8,9,10,-11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl acetate

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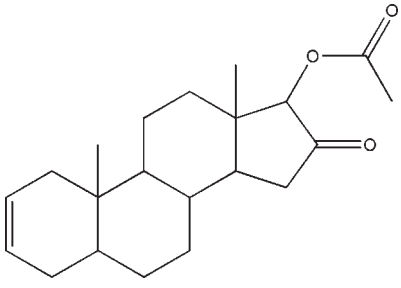
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.053; wR factor = 0.136; data-to-parameter ratio = 8.1.

In the title compound, $C_{21}H_{30}O_3$, the five-membered ring adopts an envelope conformation, the cyclohexene ring displays a half-chair conformation and the two cyclohexane rings have normal chair conformations. In the crystal structure, weak intermolecular C—H···O hydrogen bonding links the molecules into supramolecular chains running along [100].

Related literature

Rocuronium is a non-depolarizing neuromuscular blocking agent. The title compound was obtained as an intermediate during our ongoing investigation of the synthesis of rocuronium bromide; for further information on rocuronium bromide, see: Tuba *et al.* (2002); Auer (2007). For the synthesis, see: Tuba (1980); Newaz & Tcholakian (1984).



Experimental

Crystal data

$C_{21}H_{30}O_3$
M_r = 330.45
Monoclinic, $P2_1$
a = 7.383 (5) Å
b = 13.200 (9) Å
c = 9.843 (7) Å
β = 95.687 (10)°
V = 954.5 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.45 × 0.40 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
5527 measured reflections
1794 independent reflections
864 reflections with $I > 2\sigma(I)$
R_{int} = 0.102

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.136
S = 0.86
1794 reflections
221 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19C···O1^{i}	0.96	2.55	3.496 (11)	170

Symmetry code: (i) $x-1, y, z$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

The authors gratefully acknowledge computing time provided by the X-ray Diffraction Analysis Centre of the Key Laboratory of Medicinal Chemistry for Natural Resources (Ministry of Education), Yunnan University, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2791).

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supporting information

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S1. Comment

Rocuronium is a nondepolarizing neuromuscular blocking agent, which produces neuromuscular blockade by competing with acetylcholine for cholinergic receptors at the motor end plate (Tuba *et al.*, 2002; Auer, 2007). The title compound was obtained as an intermediate during our ongoing investigation of the synthese of rocuronium bromide. In this paper, we report the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. In the molecular structure, the cyclohexene ring displays a half-chair conformtion, the five ring adopts an envelope conformation, and two cyclohexane rings have the normal chair conformation. In the crystal structure weak intermolecular C—H···O hydrogen bonding links the molecules to form the supra-molecular chain running along the [1 0 0] direction (Table 1).

S2. Experimental

The title compound was synthesized according to the procedure reported by Tuba *et al.* (1980) and by Newaz & Tcholakian (1984). Single crystals were obtained from a mixture of ethyl acetate and petroleum ether by slow evaporation at room temperature.

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C). Friedel paris were merged as no significant anomalous scattering.

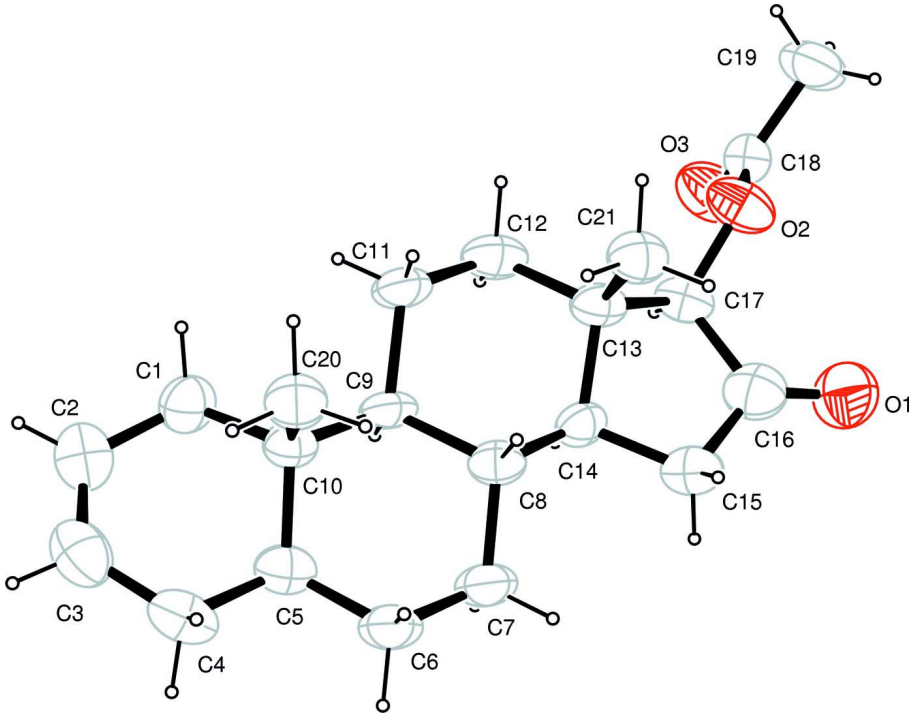

Figure 1

The molecular structure of the title compound, showing the atom labelling scheme and 30% probability displacement ellipsoids.

10,13-Dimethyl-16-oxo-4,5,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro- 1*H*-cyclopenta[*a*]phenanthren-17-yl acetate

Crystal data

$C_{21}H_{30}O_3$
$M_r = 330.45$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 7.383\ (5)$ Å
$b = 13.200\ (9)$ Å
$c = 9.843\ (7)$ Å
$\beta = 95.687\ (10)°$
$V = 954.5\ (11)$ Å^3
$Z = 2$
$F(000) = 360$
$D_x = 1.150$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 864 reflections
$\theta = 5.7–25.7°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, colorless
0.45 × 0.40 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
5527 measured reflections
1794 independent reflections
864 reflections with $I > 2\sigma(I)$
$R_{int} = 0.102$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.1°$
$h = -8\rightarrow8$
$k = -9\rightarrow15$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.136$
$S = 0.86$
1794 reflections
221 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (3)

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 $F^2 > \sigma(F^2)$ 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}
C1	0.2353 (9)	0.8413 (7)	0.3971 (7)	0.089 (2)
H1A	0.1047	0.8316	0.3809	0.107*
H1B	0.2756	0.8100	0.4841	0.107*
C2	0.2742 (13)	0.9525 (7)	0.4068 (8)	0.104 (3)
H2	0.1975	0.9938	0.4519	0.125*
C3	0.4149 (14)	0.9942 (7)	0.3531 (9)	0.109 (3)
H3	0.4306	1.0640	0.3597	0.130*
C4	0.5469 (11)	0.9345 (7)	0.2835 (8)	0.100 (2)
H4A	0.6690	0.9545	0.3187	0.120*
H4B	0.5318	0.9506	0.1868	0.120*
C5	0.5277 (9)	0.8189 (6)	0.3009 (7)	0.084 (2)
H5	0.5753	0.8028	0.3949	0.100*
C6	0.6463 (9)	0.7619 (6)	0.2068 (8)	0.090 (2)
H6A	0.6053	0.7772	0.1123	0.108*
H6B	0.7716	0.7842	0.2245	0.108*
C7	0.6356 (8)	0.6477 (6)	0.2303 (7)	0.087 (2)
H7A	0.7052	0.6129	0.1660	0.104*
H7B	0.6896	0.6319	0.3217	0.104*
C8	0.4396 (8)	0.6097 (5)	0.2132 (6)	0.0669 (18)
H8	0.3895	0.6192	0.1181	0.080*
C9	0.3222 (8)	0.6712 (6)	0.3088 (6)	0.0703 (19)
H9	0.3770	0.6599	0.4023	0.084*
C10	0.3266 (8)	0.7864 (5)	0.2843 (6)	0.0674 (18)

C11	0.1274 (8)	0.6266 (6)	0.3010 (7)	0.083 (2)
H11A	0.0603	0.6610	0.3673	0.100*
H11B	0.0660	0.6400	0.2111	0.100*
C12	0.1231 (9)	0.5120 (7)	0.3282 (7)	0.089 (2)
H12A	0.1719	0.4987	0.4217	0.107*
H12B	−0.0019	0.4884	0.3170	0.107*
C13	0.2347 (8)	0.4539 (5)	0.2304 (6)	0.0716 (19)
C14	0.4277 (8)	0.4979 (5)	0.2504 (6)	0.067 (2)
H14	0.4674	0.4928	0.3481	0.081*
C15	0.5425 (9)	0.4225 (6)	0.1788 (7)	0.091 (2)
H15A	0.5404	0.4378	0.0823	0.110*
H15B	0.6677	0.4223	0.2195	0.110*
C16	0.4499 (12)	0.3221 (8)	0.2014 (8)	0.100 (3)
C17	0.2753 (9)	0.3439 (6)	0.2690 (7)	0.0768 (19)
H17	0.3009	0.3385	0.3683	0.092*
C18	0.0718 (10)	0.2130 (6)	0.3117 (10)	0.084 (2)
C19	−0.0681 (10)	0.1408 (6)	0.2474 (8)	0.116 (3)
H19A	−0.0850	0.0864	0.3097	0.174*
H19B	−0.0276	0.1138	0.1650	0.174*
H19C	−0.1813	0.1758	0.2262	0.174*
C20	0.2325 (8)	0.8158 (5)	0.1428 (6)	0.083 (2)
H20A	0.1055	0.7990	0.1384	0.125*
H20B	0.2876	0.7794	0.0732	0.125*
H20C	0.2457	0.8873	0.1288	0.125*
C21	0.1481 (8)	0.4600 (5)	0.0849 (6)	0.083 (2)
H21A	0.2156	0.4187	0.0273	0.125*
H21B	0.1489	0.5290	0.0542	0.125*
H21C	0.0249	0.4361	0.0806	0.125*
O1	0.4948 (9)	0.2388 (5)	0.1678 (7)	0.129 (2)
O2	0.1340 (7)	0.2744 (4)	0.2230 (5)	0.0994 (16)
O3	0.1307 (8)	0.2124 (5)	0.4295 (6)	0.127 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.089 (5)	0.107 (7)	0.075 (5)	0.001 (5)	0.020 (4)	−0.015 (5)
C2	0.122 (7)	0.091 (7)	0.098 (6)	0.004 (5)	0.007 (5)	−0.003 (5)
C3	0.123 (7)	0.094 (7)	0.104 (7)	−0.012 (7)	−0.012 (6)	−0.010 (6)
C4	0.092 (6)	0.108 (7)	0.099 (6)	−0.036 (5)	0.000 (5)	0.003 (5)
C5	0.067 (5)	0.100 (7)	0.083 (5)	−0.012 (4)	0.000 (4)	0.001 (4)
C6	0.057 (4)	0.096 (6)	0.119 (6)	−0.014 (4)	0.016 (4)	0.008 (5)
C7	0.051 (4)	0.103 (6)	0.109 (6)	−0.010 (4)	0.016 (4)	0.003 (5)
C8	0.052 (4)	0.082 (6)	0.064 (4)	−0.001 (4)	−0.005 (3)	0.015 (4)
C9	0.041 (4)	0.102 (6)	0.069 (5)	−0.014 (4)	0.015 (3)	−0.002 (4)
C10	0.057 (4)	0.083 (6)	0.062 (4)	−0.005 (4)	0.001 (4)	−0.001 (4)
C11	0.047 (4)	0.114 (7)	0.091 (6)	−0.010 (4)	0.020 (4)	−0.005 (5)
C12	0.064 (5)	0.125 (7)	0.079 (5)	−0.025 (4)	0.016 (4)	0.011 (5)
C13	0.057 (4)	0.104 (6)	0.054 (4)	−0.014 (4)	0.005 (3)	−0.002 (4)

C14	0.056 (4)	0.090 (6)	0.058 (4)	−0.001 (4)	0.015 (3)	−0.005 (4)
C15	0.067 (5)	0.102 (6)	0.104 (6)	−0.006 (5)	0.005 (4)	0.009 (5)
C16	0.088 (6)	0.109 (8)	0.099 (6)	0.004 (6)	−0.010 (5)	0.012 (7)
C17	0.068 (5)	0.083 (6)	0.077 (5)	−0.018 (5)	−0.003 (4)	0.014 (4)
C18	0.076 (5)	0.083 (6)	0.094 (6)	−0.002 (5)	0.014 (5)	−0.020 (6)
C19	0.088 (6)	0.096 (6)	0.160 (8)	−0.033 (5)	−0.011 (5)	0.000 (5)
C20	0.076 (4)	0.095 (6)	0.077 (5)	0.000 (4)	−0.003 (4)	0.006 (4)
C21	0.075 (4)	0.104 (6)	0.069 (5)	−0.007 (4)	0.001 (4)	0.002 (4)
O1	0.124 (5)	0.096 (5)	0.168 (6)	0.011 (4)	0.022 (4)	0.013 (4)
O2	0.107 (4)	0.100 (4)	0.087 (4)	−0.037 (3)	−0.008 (3)	0.020 (3)
O3	0.141 (5)	0.142 (5)	0.100 (4)	−0.057 (4)	0.027 (4)	0.001 (4)

Geometric parameters (Å, º)

C1—C2	1.497 (11)	C11—H11B	0.9700
C1—C10	1.536 (8)	C12—C13	1.534 (8)
C1—H1A	0.9700	C12—H12A	0.9700
C1—H1B	0.9700	C12—H12B	0.9700
C2—C3	1.331 (10)	C13—C21	1.512 (8)
C2—H2	0.9300	C13—C17	1.522 (9)
C3—C4	1.473 (10)	C13—C14	1.534 (8)
C3—H3	0.9300	C14—C15	1.524 (9)
C4—C5	1.544 (10)	C14—H14	0.9800
C4—H4A	0.9700	C15—C16	1.517 (11)
C4—H4B	0.9700	C15—H15A	0.9700
C5—C6	1.533 (8)	C15—H15B	0.9700
C5—C10	1.538 (8)	C16—O1	1.204 (9)
C5—H5	0.9800	C16—C17	1.536 (10)
C6—C7	1.528 (9)	C17—O2	1.429 (7)
C6—H6A	0.9700	C17—H17	0.9800
C6—H6B	0.9700	C18—O3	1.197 (8)
C7—C8	1.525 (8)	C18—O2	1.306 (9)
C7—H7A	0.9700	C18—C19	1.500 (9)
C7—H7B	0.9700	C19—H19A	0.9600
C8—C14	1.525 (8)	C19—H19B	0.9600
C8—C9	1.568 (8)	C19—H19C	0.9600
C8—H8	0.9800	C20—H20A	0.9600
C9—C10	1.541 (8)	C20—H20B	0.9600
C9—C11	1.549 (7)	C20—H20C	0.9600
C9—H9	0.9800	C21—H21A	0.9600
C10—C20	1.543 (8)	C21—H21B	0.9600
C11—C12	1.536 (9)	C21—H21C	0.9600
C11—H11A	0.9700		
C2—C1—C10	114.4 (7)	C9—C11—H11B	108.8
C2—C1—H1A	108.7	H11A—C11—H11B	107.7
C10—C1—H1A	108.7	C13—C12—C11	111.2 (5)
C2—C1—H1B	108.7	C13—C12—H12A	109.4

C10—C1—H1B	108.7	C11—C12—H12A	109.4
H1A—C1—H1B	107.6	C13—C12—H12B	109.4
C3—C2—C1	122.2 (8)	C11—C12—H12B	109.4
C3—C2—H2	118.9	H12A—C12—H12B	108.0
C1—C2—H2	118.9	C21—C13—C17	110.0 (5)
C2—C3—C4	122.8 (8)	C21—C13—C12	111.4 (5)
C2—C3—H3	118.6	C17—C13—C12	115.2 (6)
C4—C3—H3	118.6	C21—C13—C14	113.6 (5)
C3—C4—C5	113.9 (7)	C17—C13—C14	99.9 (5)
C3—C4—H4A	108.8	C12—C13—C14	106.3 (5)
C5—C4—H4A	108.8	C15—C14—C8	118.2 (5)
C3—C4—H4B	108.8	C15—C14—C13	104.2 (5)
C5—C4—H4B	108.8	C8—C14—C13	114.3 (6)
H4A—C4—H4B	107.7	C15—C14—H14	106.4
C6—C5—C10	113.7 (6)	C8—C14—H14	106.4
C6—C5—C4	110.7 (6)	C13—C14—H14	106.4
C10—C5—C4	111.2 (6)	C16—C15—C14	102.9 (6)
C6—C5—H5	106.9	C16—C15—H15A	111.2
C10—C5—H5	106.9	C14—C15—H15A	111.2
C4—C5—H5	106.9	C16—C15—H15B	111.2
C7—C6—C5	110.6 (6)	C14—C15—H15B	111.2
C7—C6—H6A	109.5	H15A—C15—H15B	109.1
C5—C6—H6A	109.5	O1—C16—C15	128.1 (8)
C7—C6—H6B	109.5	O1—C16—C17	123.8 (9)
C5—C6—H6B	109.5	C15—C16—C17	108.1 (8)
H6A—C6—H6B	108.1	O2—C17—C13	114.5 (5)
C8—C7—C6	111.8 (6)	O2—C17—C16	111.1 (6)
C8—C7—H7A	109.3	C13—C17—C16	102.9 (6)
C6—C7—H7A	109.3	O2—C17—H17	109.4
C8—C7—H7B	109.3	C13—C17—H17	109.4
C6—C7—H7B	109.3	C16—C17—H17	109.4
H7A—C7—H7B	107.9	O3—C18—O2	122.2 (8)
C14—C8—C7	111.6 (5)	O3—C18—C19	125.0 (9)
C14—C8—C9	108.0 (5)	O2—C18—C19	112.7 (8)
C7—C8—C9	109.8 (5)	C18—C19—H19A	109.5
C14—C8—H8	109.1	C18—C19—H19B	109.5
C7—C8—H8	109.1	H19A—C19—H19B	109.5
C9—C8—H8	109.1	C18—C19—H19C	109.5
C10—C9—C11	113.7 (6)	H19A—C19—H19C	109.5
C10—C9—C8	113.3 (5)	H19B—C19—H19C	109.5
C11—C9—C8	109.9 (5)	C10—C20—H20A	109.5
C10—C9—H9	106.5	C10—C20—H20B	109.5
C11—C9—H9	106.5	H20A—C20—H20B	109.5
C8—C9—H9	106.5	C10—C20—H20C	109.5
C1—C10—C5	106.3 (6)	H20A—C20—H20C	109.5
C1—C10—C9	109.5 (6)	H20B—C20—H20C	109.5
C5—C10—C9	107.1 (5)	C13—C21—H21A	109.5
C1—C10—C20	110.1 (5)	C13—C21—H21B	109.5

C5—C10—C20	111.7 (5)	H21A—C21—H21B	109.5
C9—C10—C20	112.0 (5)	C13—C21—H21C	109.5
C12—C11—C9	113.6 (6)	H21A—C21—H21C	109.5
C12—C11—H11A	108.8	H21B—C21—H21C	109.5
C9—C11—H11A	108.8	C18—O2—C17	118.7 (6)
C12—C11—H11B	108.8		

C10—C1—C2—C3	−19.1 (10)	C11—C12—C13—C21	−67.3 (7)
C1—C2—C3—C4	−1.9 (13)	C11—C12—C13—C17	166.6 (5)
C2—C3—C4—C5	−10.3 (11)	C11—C12—C13—C14	57.0 (7)
C3—C4—C5—C6	170.4 (6)	C7—C8—C14—C15	−54.7 (8)
C3—C4—C5—C10	43.0 (8)	C9—C8—C14—C15	−175.5 (5)
C10—C5—C6—C7	−57.3 (8)	C7—C8—C14—C13	−177.9 (5)
C4—C5—C6—C7	176.7 (6)	C9—C8—C14—C13	61.3 (6)
C5—C6—C7—C8	55.4 (8)	C21—C13—C14—C15	−70.3 (7)
C6—C7—C8—C14	−174.4 (6)	C17—C13—C14—C15	46.7 (6)
C6—C7—C8—C9	−54.7 (7)	C12—C13—C14—C15	166.8 (5)
C14—C8—C9—C10	178.5 (5)	C21—C13—C14—C8	60.2 (7)
C7—C8—C9—C10	56.5 (7)	C17—C13—C14—C8	177.3 (5)
C14—C8—C9—C11	−53.2 (7)	C12—C13—C14—C8	−62.7 (7)
C7—C8—C9—C11	−175.1 (6)	C8—C14—C15—C16	−161.0 (5)
C2—C1—C10—C5	49.1 (8)	C13—C14—C15—C16	−32.9 (7)
C2—C1—C10—C9	164.4 (6)	C14—C15—C16—O1	−177.1 (9)
C2—C1—C10—C20	−72.0 (7)	C14—C15—C16—C17	6.5 (7)
C6—C5—C10—C1	173.3 (7)	C21—C13—C17—O2	−42.2 (7)
C4—C5—C10—C1	−60.9 (7)	C12—C13—C17—O2	84.6 (6)
C6—C5—C10—C9	56.3 (7)	C14—C13—C17—O2	−162.0 (5)
C4—C5—C10—C9	−177.9 (5)	C21—C13—C17—C16	78.5 (6)
C6—C5—C10—C20	−66.6 (8)	C12—C13—C17—C16	−154.6 (6)
C4—C5—C10—C20	59.2 (8)	C14—C13—C17—C16	−41.3 (6)
C11—C9—C10—C1	63.0 (6)	O1—C16—C17—O2	−31.4 (11)
C8—C9—C10—C1	−170.6 (5)	C15—C16—C17—O2	145.2 (6)
C11—C9—C10—C5	177.9 (5)	O1—C16—C17—C13	−154.4 (8)
C8—C9—C10—C5	−55.7 (6)	C15—C16—C17—C13	22.2 (7)
C11—C9—C10—C20	−59.4 (7)	O3—C18—O2—C17	−0.9 (11)
C8—C9—C10—C20	67.0 (6)	C19—C18—O2—C17	−176.8 (6)
C10—C9—C11—C12	−178.9 (6)	C13—C17—O2—C18	−127.4 (6)
C8—C9—C11—C12	53.0 (7)	C16—C17—O2—C18	116.5 (7)
C9—C11—C12—C13	−56.0 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19*C*···O1^{i}	0.96	2.55	3.496 (11)	170

Symmetry code: (i) *x*−1, *y*, *z*.