

(4*R*,4*aS*,4*bS*,7*R*,10*aR*)-4-Hydroxy-4*a*,7-dimethyl-2-(propan-2-yl)-1,4,4*a*,4*b*,5,6,7,8,10,10*a*-decahydrophenanthren-1-one

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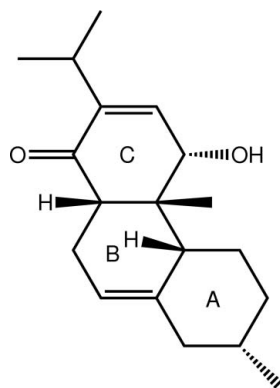
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Key indicators: single-crystal X-ray study; *T* = 290 K; mean $\sigma(\text{C}-\text{C})$ = 0.003 Å; *R* factor = 0.037; *wR* factor = 0.113; data-to-parameter ratio = 16.6.

In the title compound, C₁₉H₂₈O₂, the *A* ring adopts a chair conformation, and each of the *B* and *C* rings adopts a distorted half-chair conformation with the methine C atom in the CH₂C(H)C(=O) residue, common to both rings, lying 0.6397 (19) and 0.6328 (18) Å out of the approximate plane defined by the remaining five C atoms (r.m.s. deviations = 0.0791 and 0.0901 Å for rings *B* and *C*, respectively). Helical supramolecular chains along the *a* axis mediated by hydroxy-carbonyl O—H...O hydrogen bonds feature in the crystal packing.

Related literature

For background to the biological activity of some diterpene compounds, see: Guo *et al.* (2011); Slusarczyk *et al.* (2011). For the synthesis, see: Ferreira (2002). For conformational analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

C₁₉H₂₈O₂
M_r = 288.41
 Orthorhombic, *P*2₁2₁2₁
a = 7.3029 (9) Å
b = 13.211 (2) Å
c = 17.224 (3) Å
V = 1661.8 (4) Å³
Z = 4
 Mo *K*α radiation
 μ = 0.07 mm⁻¹
T = 290 K
 0.12 × 0.08 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 MACH 3 diffractometer
 3684 measured reflections
 3243 independent reflections
 2253 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.031
 3 standard reflections every 30 min
 intensity decay: 1.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
wR(*F*²) = 0.113
S = 1.04
 3243 reflections
 195 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}}$ = 0.15 e Å⁻³
 $\Delta\rho_{\text{min}}$ = -0.13 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2 <i>o</i> ...O1 ¹	0.82	2.01	2.805 (2)	162

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997), *DIAMOND* (Brandenburg, 2006) and *MarvinSketch* (Chemaxon, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5120).

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supplementary materials

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(4*R*,4*aS*,4*bS*,7*R*,10*aR*)-4-Hydroxy-4*a*,7-dimethyl-2-(propan-2-yl)-1,4,4*a*,4*b*,5,6,7,8,10,10*a*-decahydrophenanthren-1-one

I. Caracelli, J. Zukerman-Schpector, A. T. L. Machado, T. J. Brocksom, M. L. Ferreira and E. R. T. Tiekink

Comment

Natural diterpenes exhibit a wide range of biological activities such as neuroprotectives (Guo *et al.* 2011) and as antiplasmodials and antitrypanocidals (Slusarczyk *et al.* 2011). While aiming at the synthesis of some hydrophenanthrene diterpenes, a series of new intermediates were obtained and among them, was the title compound (Ferreira, 2002), (I), which has been characterized crystallographically.

The A ring has a chair conformation. Each of the B and C rings presents a distorted half-chair conformation with atom C7, common to both rings, lying 0.6397 (19) and 0.6328 (18) Å, for B and C, respectively, out of the approximate plane defined by the remaining five C atoms (r.m.s. deviations = 0.0791 and 0.0901, respectively). The ring puckering parameters are: $q_2 = 0.003$ (2), 0.360 (2), 0.363 (2) Å; $q_3 = 0.570$ (2), -0.315 (2), -0.332 (2) Å; $QT = 0.570$ (2), 0.478 (2), 0.492 (2) Å; and $\theta = 1.7$ (2), 131.1 (2), 132.5 (2)°, for rings A, B and C, respectively (Cremer & Pople, 1975).

In the crystal packing, the molecules are linked through O—H...O hydrogen bonds to form supramolecular helical chains along the *a* axis, Fig. 2 and Table 1.

Experimental

The detailed synthesis of the title compound is described in a Ph.D. thesis (Ferreira, 2002). Crystals were grown by slow evaporation from its hexane solution held at 293 K; *M*.pt: 466.2–468.1 K. ¹H-NMR (CDCl₃, 400 MHz): δ (p.p.m.): 6.44 (d, 1H, *J* = 3.8 Hz); 5.26 (s, 1H); 4.58 (s, 1H); 2.81–2.87 (m, 1H); 2.86–2.92 (m, 1H); 2.24 (d, 1H, *J* = 6.4 Hz); 2.10–2.26 (m, 2H); 1.90–2.10 (m, 2H); 1.82–2.10 (m, 1H); 1.37–1.54 (m, 4H); 1.27 (s, 3H); 1.04 (d, 3H, *J* = 6.8 Hz); 1.01 (d, 3H, *J* = 6.8 Hz); 0.73 (d, 3H, *J* = 6.8 Hz); δ (OH) not obs. ¹³C (CDCl₃, 100 MHz) δ (p.p.m.): 197.9; 144.4; 142.7; 135.5; 117.2; 76.1; 49.6; 49.5; 45.9; 44.6; 35.7; 35.6; 33.6; 23.6; 22.3; 21.7; 21.5; 20.2; 20.0. Analysis found: C 78.99, H 9.77%. C₁₉H₂₈O₂ requires: C 79.12, H 9.79%.

Refinement

The H atoms were geometrically placed (C—H = 0.93–0.98 Å; O—H = 0.82 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ and $U_{iso}(H) = 1.5U_{eq}(\text{methyl-C}, O)$. The absolute structure was based on that of a starting material used in the synthesis (Ferreira, 2002).

Figures

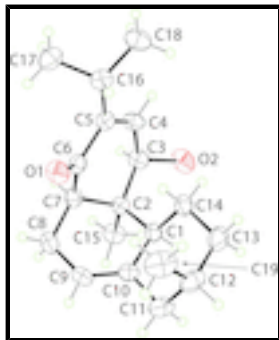


Fig. 1. The molecular structure of compound (I) showing atom labelling scheme and displacement ellipsoids at the 30% probability level (arbitrary spheres for the H atoms).

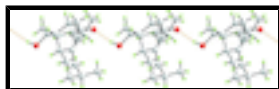


Fig. 2. A view of the helical supramolecular chain along the *a* axis in (I). The hydroxy-O—H...O(carbonyl) hydrogen bonds are represented by orange dashed lines.

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Crystal data

$C_{19}H_{28}O_2$

$M_r = 288.41$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.3029$ (9) Å

$b = 13.211$ (2) Å

$c = 17.224$ (3) Å

$V = 1661.8$ (4) Å³

$Z = 4$

$F(000) = 632$

$D_x = 1.153$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 9.2$ – 14.3°

$\mu = 0.07$ mm⁻¹

$T = 290$ K

Irregular, colourless

$0.12 \times 0.08 \times 0.07$ mm

Data collection

Enraf-Nonius CAD-4 MACH 3 diffractometer

Radiation source: fine-focus sealed tube graphite

$\omega/2\theta$ scans

3684 measured reflections

3243 independent reflections

2253 reflections with $I > 2\sigma(I)$

$R_{int} = 0.031$

$\theta_{max} = 26.0^\circ$, $\theta_{min} = 1.9^\circ$

$h = 0 \rightarrow 8$

$k = 0 \rightarrow 16$

$l = -21 \rightarrow 21$

3 standard reflections every 30 min

intensity decay: 1.1%

Refinement

Refinement on F^2

Least-squares matrix: full

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.037$$

$$wR(F^2) = 0.113$$

$$S = 1.04$$

3243 reflections

195 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.0421P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.13 \text{ e } \text{\AA}^{-3}$$

Special details

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6835 (3)	0.92045 (14)	0.83208 (11)	0.0386 (4)
H1	0.5721	0.9042	0.8613	0.046*
C2	0.6251 (2)	0.99993 (14)	0.77072 (11)	0.0378 (4)
C3	0.5391 (2)	0.95441 (16)	0.69613 (12)	0.0457 (5)
H3	0.4762	1.0096	0.6691	0.055*
C4	0.6752 (3)	0.91091 (16)	0.64072 (11)	0.0448 (5)
H4	0.6311	0.8659	0.6036	0.054*
C5	0.8545 (2)	0.93064 (15)	0.63955 (10)	0.0387 (4)
C6	0.9268 (2)	0.99737 (15)	0.70073 (11)	0.0382 (4)
C7	0.7918 (3)	1.06323 (13)	0.74402 (11)	0.0417 (5)
H7	0.7468	1.1144	0.7075	0.050*
C8	0.8794 (3)	1.11916 (16)	0.81222 (12)	0.0498 (5)
H8A	0.9985	1.1447	0.7967	0.060*
H8B	0.8036	1.1766	0.8263	0.060*
C9	0.9011 (3)	1.05182 (15)	0.88050 (12)	0.0471 (5)
H9	0.9814	1.0725	0.9193	0.056*
C10	0.8151 (3)	0.96451 (16)	0.89061 (11)	0.0415 (4)
C11	0.8553 (3)	0.89695 (17)	0.95906 (12)	0.0571 (6)
H11A	0.7435	0.8853	0.9881	0.068*
H11B	0.9424	0.9300	0.9932	0.068*
C12	0.9340 (4)	0.79528 (18)	0.93174 (14)	0.0613 (7)
H12	0.9403	0.7499	0.9767	0.074*
C13	0.8019 (4)	0.74886 (17)	0.87258 (13)	0.0626 (7)
H13A	0.8539	0.6862	0.8532	0.075*

supplementary materials

H13B	0.6878	0.7324	0.8985	0.075*
C14	0.7615 (3)	0.81779 (14)	0.80467 (12)	0.0462 (5)
H14A	0.6739	0.7852	0.7705	0.055*
H14B	0.8731	0.8292	0.7755	0.055*
C15	0.4816 (3)	1.06970 (16)	0.80839 (13)	0.0520 (5)
H15A	0.4561	1.1254	0.7743	0.078*
H15B	0.5282	1.0950	0.8568	0.078*
H15C	0.3711	1.0322	0.8176	0.078*
C16	0.9912 (3)	0.88187 (16)	0.58484 (11)	0.0439 (5)
H16	1.0830	0.8479	0.6172	0.053*
C17	1.0923 (3)	0.95967 (18)	0.53606 (13)	0.0618 (6)
H17A	1.1538	1.0067	0.5696	0.093*
H17B	1.0064	0.9954	0.5040	0.093*
H17C	1.1806	0.9260	0.5038	0.093*
C18	0.9070 (3)	0.80139 (17)	0.53282 (14)	0.0597 (6)
H18A	0.8167	0.8319	0.4998	0.090*
H18B	0.8501	0.7503	0.5643	0.090*
H18C	1.0009	0.7711	0.5015	0.090*
C19	1.1271 (4)	0.8076 (2)	0.89947 (16)	0.0762 (8)
H19A	1.1246	0.8534	0.8562	0.114*
H19B	1.1724	0.7430	0.8827	0.114*
H19C	1.2058	0.8343	0.9392	0.114*
O1	1.09041 (18)	1.00004 (12)	0.71585 (9)	0.0548 (4)
O2	0.4059 (2)	0.87899 (12)	0.71243 (11)	0.0637 (5)
H2o	0.3032	0.9036	0.7089	0.096*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0338 (9)	0.0390 (10)	0.0431 (10)	0.0005 (8)	0.0042 (8)	0.0009 (8)
C2	0.0291 (9)	0.0410 (10)	0.0433 (10)	0.0040 (8)	-0.0015 (8)	-0.0020 (9)
C3	0.0289 (9)	0.0551 (12)	0.0531 (11)	0.0041 (8)	-0.0081 (8)	-0.0028 (10)
C4	0.0362 (10)	0.0579 (13)	0.0403 (10)	0.0065 (9)	-0.0090 (8)	-0.0087 (10)
C5	0.0311 (10)	0.0456 (10)	0.0395 (10)	0.0037 (8)	-0.0032 (7)	0.0031 (9)
C6	0.0313 (9)	0.0415 (10)	0.0419 (10)	-0.0020 (8)	-0.0019 (8)	0.0072 (9)
C7	0.0419 (11)	0.0357 (10)	0.0476 (11)	0.0007 (9)	-0.0046 (8)	0.0046 (9)
C8	0.0495 (12)	0.0389 (10)	0.0611 (13)	-0.0058 (10)	-0.0002 (10)	-0.0079 (10)
C9	0.0450 (11)	0.0497 (12)	0.0465 (11)	0.0010 (10)	-0.0085 (9)	-0.0142 (9)
C10	0.0393 (10)	0.0458 (11)	0.0393 (10)	0.0087 (9)	0.0003 (8)	-0.0045 (9)
C11	0.0652 (15)	0.0656 (14)	0.0404 (11)	0.0150 (12)	0.0001 (10)	0.0004 (10)
C12	0.0764 (16)	0.0607 (14)	0.0467 (12)	0.0222 (13)	0.0046 (11)	0.0148 (11)
C13	0.0857 (18)	0.0395 (12)	0.0626 (14)	0.0097 (12)	0.0142 (13)	0.0084 (11)
C14	0.0527 (11)	0.0352 (10)	0.0507 (11)	-0.0007 (9)	-0.0008 (10)	-0.0012 (9)
C15	0.0426 (11)	0.0572 (12)	0.0563 (12)	0.0147 (10)	-0.0011 (10)	-0.0066 (11)
C16	0.0340 (10)	0.0536 (12)	0.0440 (11)	0.0109 (10)	-0.0015 (9)	-0.0001 (9)
C17	0.0585 (14)	0.0705 (15)	0.0565 (13)	0.0026 (13)	0.0138 (12)	0.0031 (12)
C18	0.0542 (13)	0.0635 (14)	0.0615 (14)	0.0150 (12)	-0.0001 (12)	-0.0155 (11)
C19	0.0692 (17)	0.0917 (19)	0.0677 (15)	0.0340 (16)	-0.0017 (13)	0.0006 (15)

O1	0.0310 (7)	0.0714 (10)	0.0622 (10)	-0.0043 (7)	-0.0035 (7)	-0.0086 (8)
O2	0.0282 (7)	0.0769 (11)	0.0861 (12)	-0.0086 (8)	-0.0018 (8)	-0.0182 (9)

Geometric parameters (Å, °)

C1—C10	1.510 (3)	C11—H11B	0.9700
C1—C14	1.545 (3)	C12—C19	1.524 (4)
C1—C2	1.550 (3)	C12—C13	1.532 (4)
C1—H1	0.9800	C12—H12	0.9800
C2—C15	1.539 (3)	C13—C14	1.511 (3)
C2—C7	1.547 (3)	C13—H13A	0.9700
C2—C3	1.551 (3)	C13—H13B	0.9700
C3—O2	1.421 (3)	C14—H14A	0.9700
C3—C4	1.493 (3)	C14—H14B	0.9700
C3—H3	0.9800	C15—H15A	0.9600
C4—C5	1.335 (3)	C15—H15B	0.9600
C4—H4	0.9300	C15—H15C	0.9600
C5—C6	1.472 (3)	C16—C17	1.519 (3)
C5—C16	1.517 (3)	C16—C18	1.520 (3)
C6—O1	1.223 (2)	C16—H16	0.9800
C6—C7	1.512 (3)	C17—H17A	0.9600
C7—C8	1.528 (3)	C17—H17B	0.9600
C7—H7	0.9800	C17—H17C	0.9600
C8—C9	1.483 (3)	C18—H18A	0.9600
C8—H8A	0.9700	C18—H18B	0.9600
C8—H8B	0.9700	C18—H18C	0.9600
C9—C10	1.325 (3)	C19—H19A	0.9600
C9—H9	0.9300	C19—H19B	0.9600
C10—C11	1.507 (3)	C19—H19C	0.9600
C11—C12	1.535 (3)	O2—H2o	0.8200
C11—H11A	0.9700		
C10—C1—C14	107.93 (16)	H11A—C11—H11B	108.1
C10—C1—C2	111.68 (15)	C19—C12—C13	112.5 (2)
C14—C1—C2	119.21 (15)	C19—C12—C11	111.4 (2)
C10—C1—H1	105.7	C13—C12—C11	108.6 (2)
C14—C1—H1	105.7	C19—C12—H12	108.1
C2—C1—H1	105.7	C13—C12—H12	108.1
C15—C2—C7	109.71 (16)	C11—C12—H12	108.1
C15—C2—C1	107.80 (15)	C14—C13—C12	113.36 (19)
C7—C2—C1	110.64 (15)	C14—C13—H13A	108.9
C15—C2—C3	107.81 (15)	C12—C13—H13A	108.9
C7—C2—C3	106.38 (15)	C14—C13—H13B	108.9
C1—C2—C3	114.42 (16)	C12—C13—H13B	108.9
O2—C3—C4	108.20 (17)	H13A—C13—H13B	107.7
O2—C3—C2	112.67 (17)	C13—C14—C1	111.38 (16)
C4—C3—C2	114.15 (15)	C13—C14—H14A	109.4
O2—C3—H3	107.1	C1—C14—H14A	109.4
C4—C3—H3	107.1	C13—C14—H14B	109.4
C2—C3—H3	107.1	C1—C14—H14B	109.4

supplementary materials

C5—C4—C3	125.97 (18)	H14A—C14—H14B	108.0
C5—C4—H4	117.0	C2—C15—H15A	109.5
C3—C4—H4	117.0	C2—C15—H15B	109.5
C4—C5—C6	117.27 (17)	H15A—C15—H15B	109.5
C4—C5—C16	124.90 (18)	C2—C15—H15C	109.5
C6—C5—C16	117.57 (16)	H15A—C15—H15C	109.5
O1—C6—C5	121.36 (18)	H15B—C15—H15C	109.5
O1—C6—C7	121.03 (18)	C5—C16—C17	112.10 (17)
C5—C6—C7	117.61 (15)	C5—C16—C18	113.38 (17)
C6—C7—C8	112.58 (17)	C17—C16—C18	110.12 (18)
C6—C7—C2	110.42 (15)	C5—C16—H16	107.0
C8—C7—C2	111.26 (16)	C17—C16—H16	107.0
C6—C7—H7	107.4	C18—C16—H16	107.0
C8—C7—H7	107.4	C16—C17—H17A	109.5
C2—C7—H7	107.4	C16—C17—H17B	109.5
C9—C8—C7	111.36 (16)	H17A—C17—H17B	109.5
C9—C8—H8A	109.4	C16—C17—H17C	109.5
C7—C8—H8A	109.4	H17A—C17—H17C	109.5
C9—C8—H8B	109.4	H17B—C17—H17C	109.5
C7—C8—H8B	109.4	C16—C18—H18A	109.5
H8A—C8—H8B	108.0	C16—C18—H18B	109.5
C10—C9—C8	125.16 (18)	H18A—C18—H18B	109.5
C10—C9—H9	117.4	C16—C18—H18C	109.5
C8—C9—H9	117.4	H18A—C18—H18C	109.5
C9—C10—C11	121.7 (2)	H18B—C18—H18C	109.5
C9—C10—C1	123.35 (18)	C12—C19—H19A	109.5
C11—C10—C1	114.70 (18)	C12—C19—H19B	109.5
C10—C11—C12	110.57 (17)	H19A—C19—H19B	109.5
C10—C11—H11A	109.5	C12—C19—H19C	109.5
C12—C11—H11A	109.5	H19A—C19—H19C	109.5
C10—C11—H11B	109.5	H19B—C19—H19C	109.5
C12—C11—H11B	109.5	C3—O2—H2o	109.5
C10—C1—C2—C15	-77.5 (2)	C3—C2—C7—C6	-58.80 (19)
C14—C1—C2—C15	155.54 (17)	C15—C2—C7—C8	59.1 (2)
C10—C1—C2—C7	42.5 (2)	C1—C2—C7—C8	-59.7 (2)
C14—C1—C2—C7	-84.5 (2)	C3—C2—C7—C8	175.44 (16)
C10—C1—C2—C3	162.63 (15)	C6—C7—C8—C9	-79.0 (2)
C14—C1—C2—C3	35.6 (2)	C2—C7—C8—C9	45.5 (2)
C15—C2—C3—O2	-73.6 (2)	C7—C8—C9—C10	-17.0 (3)
C7—C2—C3—O2	168.73 (15)	C8—C9—C10—C11	175.48 (19)
C1—C2—C3—O2	46.3 (2)	C8—C9—C10—C1	1.1 (3)
C15—C2—C3—C4	162.42 (17)	C14—C1—C10—C9	118.6 (2)
C7—C2—C3—C4	44.8 (2)	C2—C1—C10—C9	-14.3 (3)
C1—C2—C3—C4	-77.7 (2)	C14—C1—C10—C11	-56.2 (2)
O2—C3—C4—C5	-144.8 (2)	C2—C1—C10—C11	170.94 (16)
C2—C3—C4—C5	-18.5 (3)	C9—C10—C11—C12	-116.8 (2)
C3—C4—C5—C6	3.3 (3)	C1—C10—C11—C12	58.0 (3)
C3—C4—C5—C16	177.17 (19)	C10—C11—C12—C19	70.1 (3)
C4—C5—C6—O1	162.0 (2)	C10—C11—C12—C13	-54.3 (3)

C16—C5—C6—O1	-12.4 (3)	C19—C12—C13—C14	-68.0 (3)
C4—C5—C6—C7	-18.4 (3)	C11—C12—C13—C14	55.8 (3)
C16—C5—C6—C7	167.19 (17)	C12—C13—C14—C1	-56.9 (3)
O1—C6—C7—C8	-7.3 (3)	C10—C1—C14—C13	54.0 (2)
C5—C6—C7—C8	173.06 (16)	C2—C1—C14—C13	-177.28 (19)
O1—C6—C7—C2	-132.3 (2)	C4—C5—C16—C17	121.9 (2)
C5—C6—C7—C2	48.0 (2)	C6—C5—C16—C17	-64.2 (2)
C15—C2—C7—C6	-175.15 (16)	C4—C5—C16—C18	-3.5 (3)
C1—C2—C7—C6	66.04 (19)	C6—C5—C16—C18	170.39 (18)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2o \cdots O1 ⁱ	0.82	2.01	2.805 (2)	162

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

Fig. 1

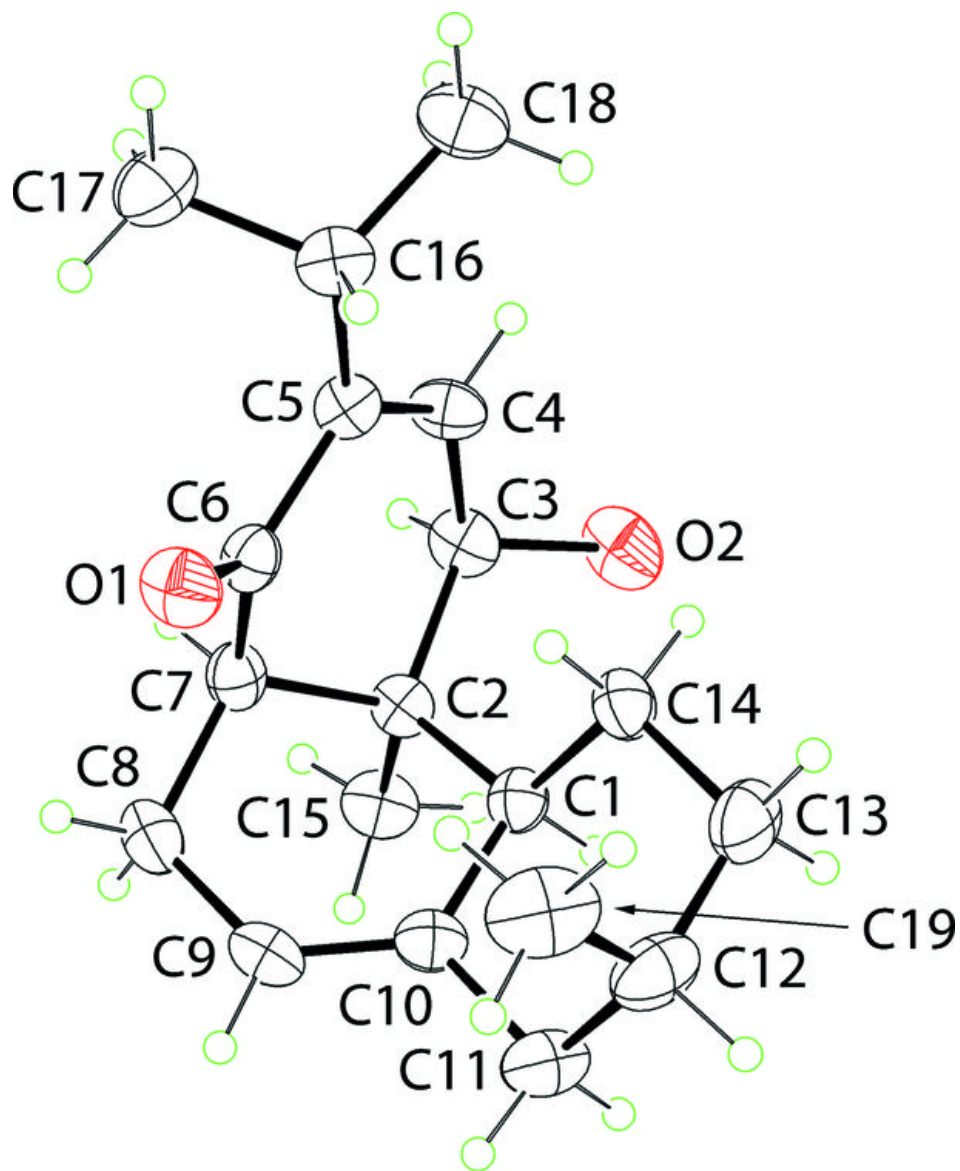


Fig. 2

