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

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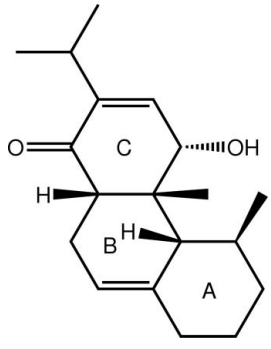
Key indicators: single-crystal X-ray study; $T$ = 290 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.037; $wR$ factor = 0.122; data-to-parameter ratio = 10.2.

In the title compound, $C_{19}H_{28}O_2$, the A ring adopts a chair conformation. Both the *B* and *C* rings adopt envelope conformations with the C atoms common to both rings and adjacent to the carbonyl and hydroxyl groups, respectively, lying 0.604 (3) and 0.634 (3) Å out of the mean planes defined by the remaining five C atoms of rings *B* and *C*, respectively (r.m.s. deviations = 0.0100 and 0.0157 Å, respectively). The formation of linear supramolecular *C*(7) chains along the *a* axis mediated by hydroxy-O—H···O(carbonyl) hydrogen bonds is the most prominent feature of 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

$C_{19}H_{28}O_2$
$M_r$ = 288.41
Orthorhombic, $P2_12_12_1$
$a$ = 6.5507 (9) Å
$b$ = 11.733 (1) Å
$c$ = 22.338 (3) Å
$V$ = 1716.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 290 K
0.15 × 0.12 × 0.09 mm

### Data collection

Enraf–Nonius CAD-4 Mach 3 diffractometer
2272 measured reflections
1945 independent reflections
1077 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038
3 standard reflections every 30 min
intensity decay: 2.0%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.122
$S$ = 1.02
1945 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 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···$A$ |
|---|---|---|---|---|
| O2—H2*o*···O1$^{i}$ | 0.82 | 2.02 | 2.804 (3) | 160 |

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).

We thank FAPESP, CNPq (306532/2009–3 to JZ-S; 308116/2010–0 to IC) and CAPES (808/2009 to JZ-S and IC) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6477).

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# supporting information

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

**Ignez Caracelli, Julio Zukerman-Schpector, André T. Lousada Machado, Timothy J. Brocksom, M. Lúcia Ferreira and Edward R. T. Tiekink**

### S1. Comment

Natural diterpenes exhibit a wide range of biological activities such as neuroprotectives (Guo *et al.*, 2011) and as anti-plasmodials and anti-trypanocidals (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 in (I), Fig. 1, has a chair conformation. Each of the B and C rings presents a half-chair conformation with atom C7 lying 0.604 (3) Å and C2 lying 0.634 (3) Å out of the approximate plane defined by the remaining five C atoms of rings B and C, respectively (r.m.s. deviation 0.0100 and 0.0157 Å for rings B and C, respectively). The ring puckering parameters are: $q_2$ = 0.040 (4), 0.348 (3), 0.367 (3) Å; $q_3$ = 0.530 (4), 0.265 (3), 0.269 (3) Å; QT = 0.531 (4), 0.438 (3), 0.455 (3) Å; and $\theta$ = 3.9 (4), 52.7 (4), 53.7 (4)°, 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 linear supramolecular chains along the *a* axis, Fig. 2 and Table 1. Chains pack in the crystal structure with no specific intermolecular interactions operating between them, Fig. 3.

### S2. 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. $^1$H-NMR ($CDCl_3$, 400 MHz): $\delta$ (p.p.m.): 6.47 (d, 1H, J = 5.4 Hz); 5.50 (d, 1H, J = 4.5 Hz); 4.4 (d, 1H, J = 5.4 Hz); 2.87 (heptet, 1H, J = 6.8 Hz); 2.39 (d, 1H, J = 3.7 Hz); 2.29–2.33 (m, 1H); 2.08–2.13 (m, 2H); 1.98–2.03 (m, 2H); 1.68–1.78 (m, 1H); 1.68–1.78 (m, 2H); 1.35 (dt, 2H, $J_1$ = 12.8 and $J_2$ = 3.6 Hz); 1.21 (d, 3H, J = 6.5 Hz); 1.16 (s, 3H); 1.06 (d, 3H, J = 6.9 Hz); 1.02 (d, 3H, J = 6.9 Hz); $\delta$(OH) not obs. $^{13}$C ($CDCl_3$, 100 MHz) $\delta$ (p.p.m.): 202.5; 142.2; 141.8; 136.0; 118.3; 71.0; 53.9; 53.1; 37.6; 36.7; 36.7; 33.6; 29.0; 27.5; 26.1; 26.0; 25.2; 21.4; 21.4 Analysis found: C 78.98, H 9.79%. $C_{19}H_{28}O_2$ requires: C 79.12, H 9.79%.

### S3. 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) = 1.2$U_{eq}$(C) and $U_{iso}$(H) = 1.5$U_{eq}$(methyl-C,*O*). The absolute structure was based on that of a starting material used in the synthesis (Ferreira, 2002). In the absence of significant anamolous dispersion effects, 287 Friedel pairs were merged in the final refinement cycles.

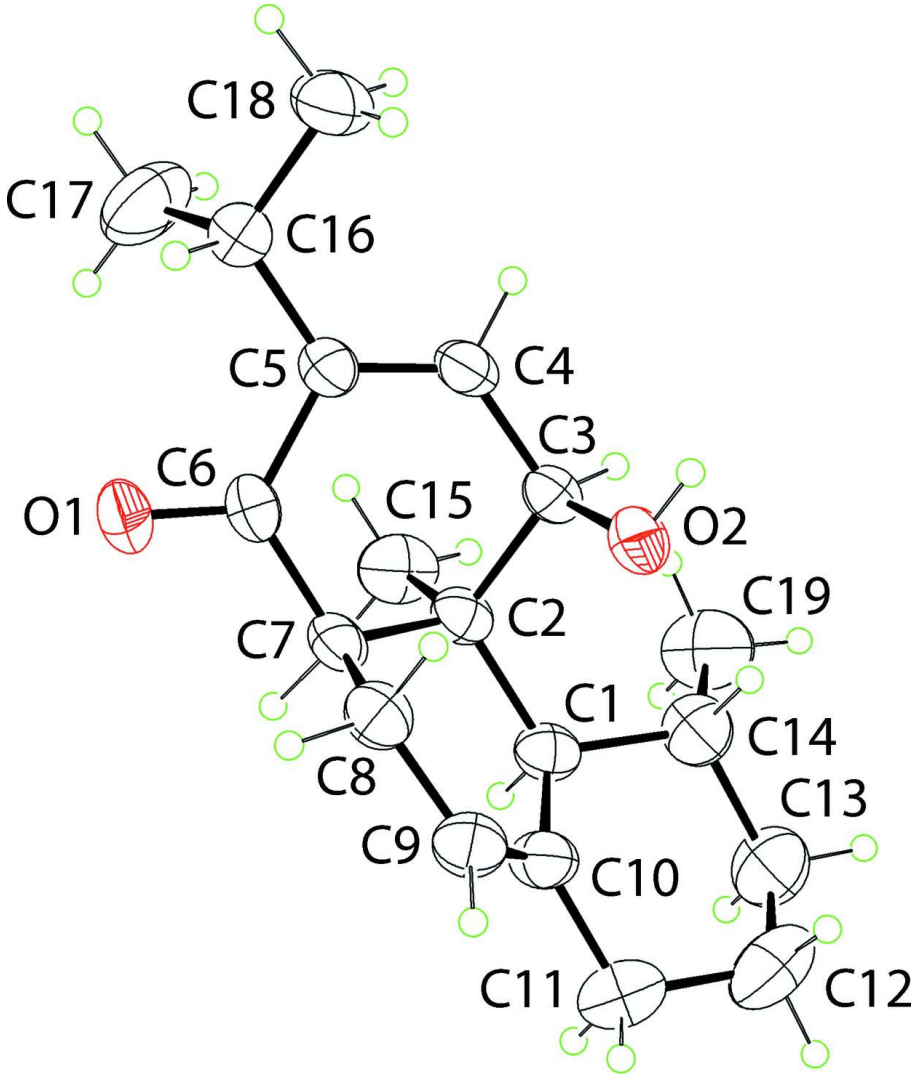


**Figure 1**

The molecular structure of compound (I) showing displacement ellipsoids at the 30% probability level (arbitrary spheres for the H atoms).

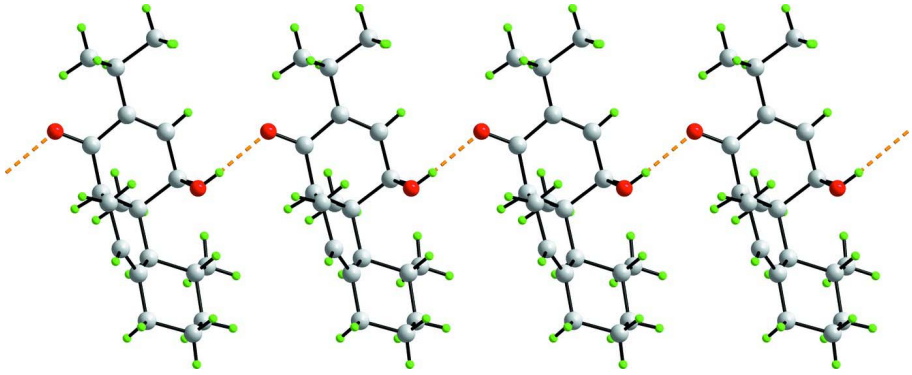

**Figure 2**

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

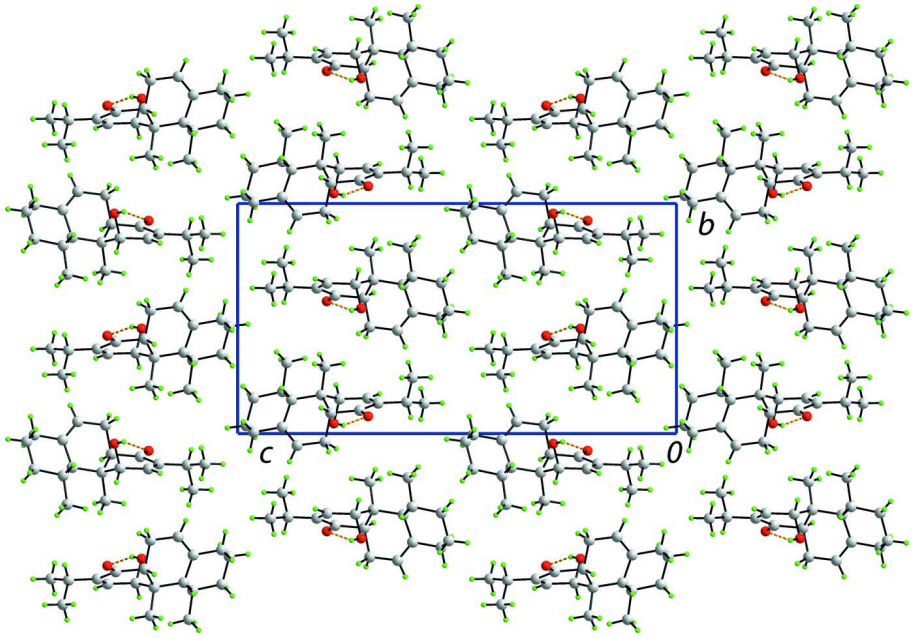


**Figure 3**

A view in projection down the *a* axis of the unit-cell contents of (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* = 6.5507 (9) Å
*b* = 11.733 (1) Å
*c* = 22.338 (3) Å
*V* = 1716.9 (4) Å$^3$
*Z* = 4
*F*(000) = 632
$D_x$ = 1.116 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 23 reflections
*θ* = 9.1–16.5°

$\mu$ = 0.07 mm$^{-1}$
$T$ = 290 K

Irregular, colourless
0.15 × 0.12 × 0.09 mm

*Data collection*

Enraf–Nonius CAD-4 Mach 3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$/–2$\theta$ scans
2272 measured reflections
1945 independent reflections
1077 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.038
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.0°
$h$ = −1→8
$k$ = −14→0
$l$ = −27→0
3 standard reflections every 30 min
intensity decay: 2.0%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.122
$S$ = 1.02
1945 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.0441P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.11 e Å$^{-3}$

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5700 (5) | 0.1474 (3) | 0.87731 (12) | 0.0536 (8) |
| H1 | 0.6626 | 0.1974 | 0.8996 | 0.064* |
| C2 | 0.6209 (4) | 0.1683 (2) | 0.80946 (13) | 0.0488 (8) |
| C3 | 0.4355 (4) | 0.1501 (3) | 0.76804 (12) | 0.0478 (7) |
| H3 | 0.3371 | 0.2113 | 0.7758 | 0.057* |
| C4 | 0.4904 (5) | 0.1535 (3) | 0.70352 (13) | 0.0527 (8) |
| H4 | 0.3867 | 0.1723 | 0.6769 | 0.063* |
| C5 | 0.6731 (5) | 0.1322 (3) | 0.68010 (13) | 0.0508 (7) |
| C6 | 0.8399 (5) | 0.1005 (3) | 0.72195 (15) | 0.0559 (8) |
| C7 | 0.7936 (4) | 0.0895 (2) | 0.78799 (14) | 0.0526 (8) |
| H7 | 0.9173 | 0.1121 | 0.8096 | 0.063* |
| C8 | 0.7588 (5) | −0.0363 (3) | 0.80105 (14) | 0.0616 (9) |
| H8A | 0.6508 | −0.0653 | 0.7755 | 0.074* |
| H8B | 0.8823 | −0.0789 | 0.7925 | 0.074* |

| | | | | |
|---|---|---|---|---|
| C9 | 0.7016 (6) | −0.0514 (3) | 0.86456 (15) | 0.0656 (9) |
| H9 | 0.7258 | −0.1223 | 0.8818 | 0.079* |
| C10 | 0.6191 (5) | 0.0279 (3) | 0.89854 (14) | 0.0592 (8) |
| C11 | 0.5787 (7) | 0.0058 (4) | 0.96343 (16) | 0.0875 (13) |
| H11A | 0.6721 | 0.0509 | 0.9874 | 0.105* |
| H11B | 0.6046 | −0.0739 | 0.9720 | 0.105* |
| C12 | 0.3627 (8) | 0.0344 (4) | 0.98085 (18) | 0.1012 (15) |
| H12A | 0.2688 | −0.0165 | 0.9606 | 0.121* |
| H12B | 0.3454 | 0.0245 | 1.0237 | 0.121* |
| C13 | 0.3167 (8) | 0.1551 (3) | 0.96402 (16) | 0.0900 (12) |
| H13A | 0.4014 | 0.2053 | 0.9880 | 0.108* |
| H13B | 0.1753 | 0.1712 | 0.9738 | 0.108* |
| C14 | 0.3521 (6) | 0.1821 (3) | 0.89755 (16) | 0.0699 (10) |
| H14 | 0.2546 | 0.1368 | 0.8743 | 0.084* |
| C15 | 0.6977 (6) | 0.2914 (3) | 0.80117 (15) | 0.0750 (11) |
| H15A | 0.5933 | 0.3438 | 0.8135 | 0.113* |
| H15B | 0.7300 | 0.3041 | 0.7598 | 0.113* |
| H15C | 0.8177 | 0.3030 | 0.8251 | 0.113* |
| C16 | 0.7253 (5) | 0.1371 (3) | 0.61470 (13) | 0.0627 (9) |
| H16 | 0.8109 | 0.0708 | 0.6056 | 0.075* |
| C17 | 0.8497 (8) | 0.2431 (4) | 0.60174 (17) | 0.1106 (16) |
| H17A | 0.8863 | 0.2445 | 0.5601 | 0.166* |
| H17B | 0.9713 | 0.2425 | 0.6257 | 0.166* |
| H17C | 0.7704 | 0.3095 | 0.6111 | 0.166* |
| C18 | 0.5396 (6) | 0.1315 (4) | 0.57472 (15) | 0.0879 (13) |
| H18A | 0.5818 | 0.1327 | 0.5336 | 0.132* |
| H18B | 0.4530 | 0.1958 | 0.5826 | 0.132* |
| H18C | 0.4659 | 0.0624 | 0.5826 | 0.132* |
| C19 | 0.2980 (9) | 0.3082 (3) | 0.88848 (17) | 0.1022 (16) |
| H19A | 0.1605 | 0.3215 | 0.9015 | 0.153* |
| H19B | 0.3100 | 0.3272 | 0.8468 | 0.153* |
| H19C | 0.3898 | 0.3547 | 0.9114 | 0.153* |
| O1 | 1.0090 (3) | 0.0749 (2) | 0.70292 (10) | 0.0824 (8) |
| O2 | 0.3390 (3) | 0.04403 (17) | 0.78121 (9) | 0.0563 (6) |
| H2o | 0.2390 | 0.0359 | 0.7595 | 0.085* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0577 (17) | 0.0556 (18) | 0.0474 (17) | −0.0035 (17) | −0.0097 (15) | −0.0039 (15) |
| C2 | 0.0480 (18) | 0.0450 (17) | 0.0533 (17) | −0.0047 (15) | −0.0104 (15) | 0.0007 (13) |
| C3 | 0.0434 (16) | 0.0470 (17) | 0.0529 (17) | 0.0061 (15) | −0.0055 (13) | 0.0023 (14) |
| C4 | 0.0456 (16) | 0.0577 (19) | 0.0546 (18) | 0.0020 (16) | −0.0140 (15) | 0.0068 (15) |
| C5 | 0.0432 (16) | 0.0584 (19) | 0.0509 (16) | −0.0044 (16) | −0.0060 (15) | 0.0036 (15) |
| C6 | 0.0357 (15) | 0.068 (2) | 0.064 (2) | −0.0068 (16) | −0.0025 (16) | 0.0015 (16) |
| C7 | 0.0381 (16) | 0.0631 (19) | 0.0566 (19) | −0.0061 (15) | −0.0127 (15) | 0.0056 (16) |
| C8 | 0.0565 (18) | 0.060 (2) | 0.068 (2) | 0.0132 (17) | −0.0010 (17) | 0.0056 (17) |
| C9 | 0.069 (2) | 0.057 (2) | 0.071 (2) | 0.0115 (19) | −0.0020 (18) | 0.0172 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0614 (19) | 0.062 (2) | 0.0543 (19) | 0.0002 (18) | −0.0080 (17) | 0.0110 (17) |
| C11 | 0.112 (3) | 0.089 (3) | 0.062 (2) | −0.001 (3) | 0.001 (2) | 0.012 (2) |
| C12 | 0.127 (4) | 0.109 (3) | 0.068 (2) | −0.018 (3) | 0.028 (3) | 0.005 (2) |
| C13 | 0.094 (3) | 0.108 (3) | 0.068 (2) | 0.009 (3) | 0.014 (2) | −0.017 (2) |
| C14 | 0.072 (2) | 0.074 (2) | 0.064 (2) | 0.007 (2) | 0.002 (2) | −0.0152 (17) |
| C15 | 0.092 (3) | 0.054 (2) | 0.079 (2) | −0.018 (2) | −0.014 (2) | 0.0031 (17) |
| C16 | 0.0524 (18) | 0.082 (2) | 0.0536 (19) | −0.0020 (19) | −0.0015 (16) | 0.0041 (17) |
| C17 | 0.129 (4) | 0.126 (4) | 0.077 (3) | −0.042 (4) | 0.018 (3) | 0.021 (3) |
| C18 | 0.077 (2) | 0.130 (3) | 0.057 (2) | 0.019 (3) | −0.017 (2) | −0.009 (2) |
| C19 | 0.129 (4) | 0.091 (3) | 0.087 (3) | 0.044 (3) | 0.007 (3) | −0.018 (2) |
| O1 | 0.0360 (11) | 0.143 (2) | 0.0685 (15) | 0.0035 (15) | 0.0004 (12) | 0.0002 (15) |
| O2 | 0.0438 (11) | 0.0629 (13) | 0.0623 (13) | −0.0109 (12) | −0.0077 (11) | −0.0014 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C10 | 1.514 (4) | C11—H11B | 0.9700 |
| C1—C14 | 1.552 (5) | C12—C13 | 1.495 (6) |
| C1—C2 | 1.571 (4) | C12—H12A | 0.9700 |
| C1—H1 | 0.9800 | C12—H12B | 0.9700 |
| C2—C7 | 1.538 (4) | C13—C14 | 1.536 (5) |
| C2—C15 | 1.541 (4) | C13—H13A | 0.9700 |
| C2—C3 | 1.542 (4) | C13—H13B | 0.9700 |
| C3—O2 | 1.427 (3) | C14—C19 | 1.535 (5) |
| C3—C4 | 1.486 (4) | C14—H14 | 0.9800 |
| C3—H3 | 0.9800 | C15—H15A | 0.9600 |
| C4—C5 | 1.330 (4) | C15—H15B | 0.9600 |
| C4—H4 | 0.9300 | C15—H15C | 0.9600 |
| C5—C6 | 1.485 (4) | C16—C18 | 1.511 (5) |
| C5—C16 | 1.501 (4) | C16—C17 | 1.515 (5) |
| C6—O1 | 1.224 (4) | C16—H16 | 0.9800 |
| C6—C7 | 1.512 (5) | C17—H17A | 0.9600 |
| C7—C8 | 1.522 (4) | C17—H17B | 0.9600 |
| C7—H7 | 0.9800 | C17—H17C | 0.9600 |
| C8—C9 | 1.478 (4) | C18—H18A | 0.9600 |
| C8—H8A | 0.9700 | C18—H18B | 0.9600 |
| C8—H8B | 0.9700 | C18—H18C | 0.9600 |
| C9—C10 | 1.317 (4) | C19—H19A | 0.9600 |
| C9—H9 | 0.9300 | C19—H19B | 0.9600 |
| C10—C11 | 1.496 (5) | C19—H19C | 0.9600 |
| C11—C12 | 1.505 (6) | O2—H2o | 0.8200 |
| C11—H11A | 0.9700 | | |
| | | | |
| C10—C1—C14 | 110.3 (3) | H11A—C11—H11B | 107.9 |
| C10—C1—C2 | 113.7 (2) | C13—C12—C11 | 109.6 (4) |
| C14—C1—C2 | 115.8 (3) | C13—C12—H12A | 109.7 |
| C10—C1—H1 | 105.3 | C11—C12—H12A | 109.7 |
| C14—C1—H1 | 105.3 | C13—C12—H12B | 109.7 |
| C2—C1—H1 | 105.3 | C11—C12—H12B | 109.7 |

| | | | |
|---|---|---|---|
| C7—C2—C15 | 106.6 (3) | H12A—C12—H12B | 108.2 |
| C7—C2—C3 | 108.0 (2) | C12—C13—C14 | 114.1 (3) |
| C15—C2—C3 | 108.3 (2) | C12—C13—H13A | 108.7 |
| C7—C2—C1 | 111.3 (2) | C14—C13—H13A | 108.7 |
| C15—C2—C1 | 109.4 (2) | C12—C13—H13B | 108.7 |
| C3—C2—C1 | 113.0 (2) | C14—C13—H13B | 108.7 |
| O2—C3—C4 | 109.3 (2) | H13A—C13—H13B | 107.6 |
| O2—C3—C2 | 110.2 (2) | C19—C14—C13 | 106.9 (3) |
| C4—C3—C2 | 112.8 (2) | C19—C14—C1 | 115.2 (4) |
| O2—C3—H3 | 108.1 | C13—C14—C1 | 111.5 (3) |
| C4—C3—H3 | 108.1 | C19—C14—H14 | 107.6 |
| C2—C3—H3 | 108.1 | C13—C14—H14 | 107.6 |
| C5—C4—C3 | 126.5 (3) | C1—C14—H14 | 107.6 |
| C5—C4—H4 | 116.8 | C2—C15—H15A | 109.5 |
| C3—C4—H4 | 116.8 | C2—C15—H15B | 109.5 |
| C4—C5—C6 | 117.5 (3) | H15A—C15—H15B | 109.5 |
| C4—C5—C16 | 125.5 (3) | C2—C15—H15C | 109.5 |
| C6—C5—C16 | 117.0 (3) | H15A—C15—H15C | 109.5 |
| O1—C6—C5 | 120.6 (3) | H15B—C15—H15C | 109.5 |
| O1—C6—C7 | 120.0 (3) | C5—C16—C18 | 113.0 (3) |
| C5—C6—C7 | 119.2 (3) | C5—C16—C17 | 109.8 (3) |
| C6—C7—C8 | 107.5 (3) | C18—C16—C17 | 110.9 (3) |
| C6—C7—C2 | 113.6 (2) | C5—C16—H16 | 107.6 |
| C8—C7—C2 | 114.4 (3) | C18—C16—H16 | 107.6 |
| C6—C7—H7 | 107.0 | C17—C16—H16 | 107.6 |
| C8—C7—H7 | 107.0 | C16—C17—H17A | 109.5 |
| C2—C7—H7 | 107.0 | C16—C17—H17B | 109.5 |
| C9—C8—C7 | 109.8 (3) | H17A—C17—H17B | 109.5 |
| C9—C8—H8A | 109.7 | C16—C17—H17C | 109.5 |
| C7—C8—H8A | 109.7 | H17A—C17—H17C | 109.5 |
| C9—C8—H8B | 109.7 | H17B—C17—H17C | 109.5 |
| C7—C8—H8B | 109.7 | C16—C18—H18A | 109.5 |
| H8A—C8—H8B | 108.2 | C16—C18—H18B | 109.5 |
| C10—C9—C8 | 124.9 (3) | H18A—C18—H18B | 109.5 |
| C10—C9—H9 | 117.6 | C16—C18—H18C | 109.5 |
| C8—C9—H9 | 117.6 | H18A—C18—H18C | 109.5 |
| C9—C10—C11 | 120.5 (3) | H18B—C18—H18C | 109.5 |
| C9—C10—C1 | 124.1 (3) | C14—C19—H19A | 109.5 |
| C11—C10—C1 | 115.2 (3) | C14—C19—H19B | 109.5 |
| C10—C11—C12 | 112.2 (4) | H19A—C19—H19B | 109.5 |
| C10—C11—H11A | 109.2 | C14—C19—H19C | 109.5 |
| C12—C11—H11A | 109.2 | H19A—C19—H19C | 109.5 |
| C10—C11—H11B | 109.2 | H19B—C19—H19C | 109.5 |
| C12—C11—H11B | 109.2 | C3—O2—H2o | 109.5 |

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| C10—C1—C2—C7 | −26.9 (3) | C15—C2—C7—C8 | 171.6 (3) |
| C14—C1—C2—C7 | −156.1 (3) | C3—C2—C7—C8 | −72.2 (3) |
| C10—C1—C2—C15 | −144.5 (3) | C1—C2—C7—C8 | 52.4 (3) |

| | | | |
|---|---|---|---|
| C14—C1—C2—C15 | 86.3 (4) | C6—C7—C8—C9 | −176.9 (3) |
| C10—C1—C2—C3 | 94.8 (3) | C2—C7—C8—C9 | −49.8 (4) |
| C14—C1—C2—C3 | −34.5 (4) | C7—C8—C9—C10 | 23.6 (5) |
| C7—C2—C3—O2 | 74.3 (3) | C8—C9—C10—C11 | −176.3 (3) |
| C15—C2—C3—O2 | −170.6 (3) | C8—C9—C10—C1 | 0.0 (6) |
| C1—C2—C3—O2 | −49.2 (3) | C14—C1—C10—C9 | 133.7 (4) |
| C7—C2—C3—C4 | −48.2 (3) | C2—C1—C10—C9 | 1.7 (5) |
| C15—C2—C3—C4 | 67.0 (3) | C14—C1—C10—C11 | −49.8 (4) |
| C1—C2—C3—C4 | −171.7 (3) | C2—C1—C10—C11 | 178.2 (3) |
| O2—C3—C4—C5 | −99.1 (4) | C9—C10—C11—C12 | −128.9 (4) |
| C2—C3—C4—C5 | 23.9 (4) | C1—C10—C11—C12 | 54.5 (5) |
| C3—C4—C5—C6 | 0.8 (5) | C10—C11—C12—C13 | −55.1 (5) |
| C3—C4—C5—C16 | −179.5 (3) | C11—C12—C13—C14 | 55.9 (5) |
| C4—C5—C6—O1 | 176.7 (3) | C12—C13—C14—C19 | −179.9 (4) |
| C16—C5—C6—O1 | −3.1 (5) | C12—C13—C14—C1 | −53.1 (5) |
| C4—C5—C6—C7 | 2.3 (4) | C10—C1—C14—C19 | 169.7 (3) |
| C16—C5—C6—C7 | −177.4 (3) | C2—C1—C14—C19 | −59.4 (4) |
| O1—C6—C7—C8 | −77.0 (4) | C10—C1—C14—C13 | 47.6 (4) |
| C5—C6—C7—C8 | 97.4 (3) | C2—C1—C14—C13 | 178.5 (3) |
| O1—C6—C7—C2 | 155.4 (3) | C4—C5—C16—C18 | −18.6 (5) |
| C5—C6—C7—C2 | −30.2 (4) | C6—C5—C16—C18 | 161.2 (3) |
| C15—C2—C7—C6 | −64.5 (3) | C4—C5—C16—C17 | 105.8 (4) |
| C3—C2—C7—C6 | 51.7 (3) | C6—C5—C16—C17 | −74.5 (4) |
| C1—C2—C7—C6 | 176.3 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*o*···O1$^{i}$ | 0.82 | 2.02 | 2.804 (3) | 160 |

Symmetry code: (i) *x*−1, *y*, *z*.