# organic compounds

# 5α-Androst-3-en-17β-yl acetate

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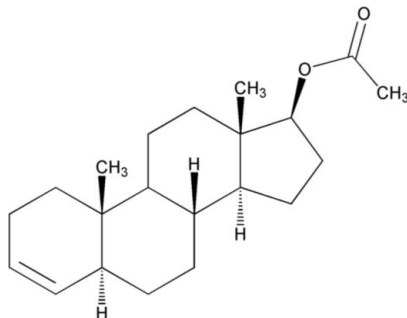
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In the crystal structure of the title compound, $C_{21}H_{32}O_2$, ring $A$ is highly distorted, with a conformation intermediate between 10β-sofa and 1α,10β-half chair; rings $B$ and $C$ have slightly flattened chair conformations. Ring $D$ assumes an unusual 13β-envelope conformation, probably induced by the acetoxy substituent. Cohesion of the crystal structure is due only to weak van der Waals interactions.

## Related literature

For structure–activity relationships (SAR) of steroids with modified $A$ and $D$ rings as aromatase inhibitors, see: Cepa *et al.* (2005, 2008). For the synthesis and assignment of the absolute configuration, see: Cepa *et al.* (2008). For a related structure, see Paixão *et al.* (2001). For reference bond-length data, see: Allen *et al.* 1987. For conformational details, see: Duax & Norton (1975); Cremer & Pople (1975); Altona *et al.* (1968).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{21}H_{32}O_2$ | $V$ = 1847.21 (7) Å$^3$ |
| $M_r$ = 316.47 | $Z$ = 4 |
| Monoclinic, $C2$ | Mo $K\alpha$ radiation |
| $a$ = 14.7728 (3) Å | $\mu$ = 0.07 mm$^{-1}$ |
| $b$ = 6.2673 (1) Å | $T$ = 293 K |
| $c$ = 20.2514 (5) Å | 0.41 × 0.39 × 0.10 mm |
| $\beta$ = 99.874 (1)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 22420 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000) | 2292 independent reflections |
| | 1554 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.971, $T_{max}$ = 0.993 | $R_{int}$ = 0.030 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | 1 restraint |
| $wR(F^2)$ = 0.102 | H-atom parameters constrained |
| $S$ = 1.08 | $\Delta\rho_{max}$ = 0.13 e Å$^{-3}$ |
| 2292 reflections | $\Delta\rho_{min}$ = −0.17 e Å$^{-3}$ |
| 211 parameters | |

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

## References

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# supporting information

## 5*α*-Androst-3-en-17*β*-yl acetate

## L. C. R. Andrade, J. A. Paixão, M. J. M. de Almeida, E. J. Tavares da Silva and F. M. Fernandes Roleira

### S1. Comment

Following our interest in the study of structure-activity relationships (SAR) of steroids with modified A- and D-rings as aromatase inhibitors (Cepa *et al.*, 2005), we have recently prepared and evaluated the title compound (Cepa *et al.*, 2008), the 17-acetyl derivative of a potent aromatase inhibitor previously studied by X-ray diffraction (Paixão *et al.*, 2001). In order to understand the role of specific D-ring substitution patterns in this inhibition process, its crystal structure was determined by single-crystal X-ray diffractometry.
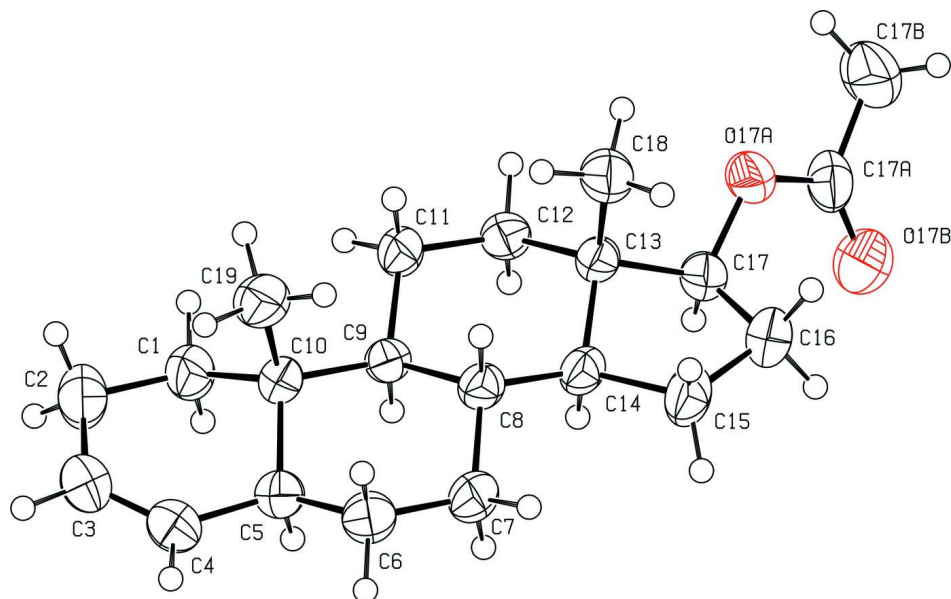
   Apart from the C6—C7 bond length, which is slightly shorter [1.511 (3) Å] than the average $Csp^3$—$Csp^3$ bond length in the molecule [1.53 (1) Å], bond lengths are well within reported values (Allen *et al.*, 1987). Due to the C3=C4 double bond, ring A is highly distorted with a conformation intermediate between 10*β*-sofa and 1*α*,10*β*-half chair [(asymmetry parameters (Duax & Norton, 1975): $\Delta C_s(3)$=8.9 (3), $\Delta C_2(3,4)$=16.8 (4) and $\Delta C_2(1,2)$=52.2 (4)°]. Rings B and C have slightly flattened chair conformations. Ring D assumes an unusual 13*β*-envelope conformation [puckering parameters (Cremer & Pople, 1975) $q_2$=0.477 (3)Å and $\varphi_2$=188.6 (4)°; pseudo-rotation (Altona *et al.*, 1968) and asymmetry parameters (Duax & Norton, 1975): $\Delta$=25.0 (4), $\varphi_m$=49.3 (2), $\Delta C_s(13)$=5.8 (3), $\Delta C_2(13,14)$=17.0 (3) and $\Delta C_s(14)$=30.5 (3)°]. The distance C3—O17B is 11.087 (3) Å. A pseudo-torsion C19—C10···C13—C18 angle of 3.3 (2)° indicates a slight twist of the molecule. The dihedral angle between the least-squares plane of ring D (C14···C17) and that of the four non-H atoms of the 17*β* acetate group is 69.2 (1)°. The structure lacks any strong hydrogen-bond donor; only weak van der Waals interactions can be responsible for the cohesion of the crystal structure.

### S2. Experimental

The title steroid was prepared according to the procedure previously reported (Cepa *et al.*, 2008), yielding 95% of the pure compound as a white solid. Crystals suitable for X-ray studies were grown by slow evaporation from absolute ethanol. Mp 389–392 K.

### S3. Refinement

All hydrogen atoms were refined as riding on their parent atoms, with C—H = 0.96, 0.97 and 0.98 Å for methyl, methylene and methine hydrogen atoms; $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H atoms and 1.2 for all other H atoms. The absolute configuration was known from the synthetic route. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

**Figure 1**

*ORTEPII* (Johnson, 1976) plot of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

**5α-Androst-3-en-17β-yl acetate**

*Crystal data*

| | |
|---|---|
| $C_{21}H_{32}O_2$ | $F(000) = 696$ |
| $M_r = 316.47$ | $D_x = 1.138$ Mg m$^{-3}$ |
| Monoclinic, $C2$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 14.7728$ (3) Å | Cell parameters from 7585 reflections |
| $b = 6.2673$ (1) Å | $\theta = 2.8–21.5°$ |
| $c = 20.2514$ (5) Å | $\mu = 0.07$ mm$^{-1}$ |
| $\beta = 99.874$ (1)° | $T = 293$ K |
| $V = 1847.21$ (7) Å$^3$ | Prism, colourless |
| $Z = 4$ | $0.41 \times 0.39 \times 0.10$ mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 22420 measured reflections |
| | 2292 independent reflections |
| Radiation source: fine-focus sealed tube | 1554 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.030$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 27.9°$, $\theta_{min} = 2.0°$ |
| Absorption correction: multi-scan | $h = -18 \rightarrow 18$ |
| (*SADABS*; Sheldrick, 2000) | $k = -8 \rightarrow 8$ |
| $T_{min} = 0.971$, $T_{max} = 0.993$ | $l = -26 \rightarrow 25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | 211 parameters |
| Least-squares matrix: full | 1 restraint |
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | Primary atom site location: structure-invariant direct methods |
| $wR(F^2) = 0.102$ | |
| $S = 1.08$ | Secondary atom site location: difference Fourier map |
| 2292 reflections | |

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.3162P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$

*Special details*

**Experimental**. IR $\nu_{max}$(KBr) cm$^{-1}$: 3015 (=C–H), 1733 (C=O); $^1$H NMR (300 MHz, CDCl$_3$) $\delta$: 0.77 (3$H$, s, 18-H$_3$)\*, 0.79 (3$H$, s, 19-H$_3$)\*, 2.03 (3$H$, s, CH$_3$COO), 4.59 (1$H$, dd, $J_{17\alpha,16\alpha}$=7.9, $J_{17\alpha,16\beta}$=7.9, 17$\alpha$-H), 5.27 (1$H$, ddd, $J_{4,3}$=9.8, $J_{4,5\alpha}$=4.5, $J_{4,2\alpha}$=2.5, 4-H), 5.54 (1$H$, ddd, $J_{3,4}$=9.8, $J_{3,2\beta}$=6.3, $J_{3,2\alpha}$=3.2, 3-H); $^{13}$C NMR (75.6 MHz, DMSO-d$_6$) $\delta$: 11.8 (C-19)\*\*, 12.2 (C-18)\*\*, 20.5, 21.1, 23.4, 23.5, 27.2, 27.5, 31.5, 34.1, 34.9, 35.3, 36.9, 42.7, 45.8 (C-5), 50.7, 53.3, 82.9 (C-17), 125.4 (C-3), 131.2 (C-4); 171.2 (C=O); EIMS *m/z* 316 ($M^+$, 100%). \*,\*\* Signals may be interchangeable.

**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* | $U_{iso}$\*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.19131 (17) | 0.6621 (5) | 0.62336 (12) | 0.0534 (7) |
| H1A | 0.1677 | 0.7480 | 0.6565 | 0.064\* |
| H1B | 0.2252 | 0.7558 | 0.5983 | 0.064\* |
| C2 | 0.11018 (18) | 0.5657 (6) | 0.57530 (14) | 0.0724 (9) |
| H2A | 0.0626 | 0.5259 | 0.6006 | 0.087\* |
| H2B | 0.0848 | 0.6733 | 0.5429 | 0.087\* |
| C3 | 0.13589 (19) | 0.3740 (5) | 0.53863 (13) | 0.0633 (8) |
| H3 | 0.0923 | 0.3151 | 0.5050 | 0.076\* |
| C4 | 0.21769 (18) | 0.2854 (5) | 0.55206 (12) | 0.0525 (7) |
| H4 | 0.2288 | 0.1648 | 0.5279 | 0.063\* |
| C5 | 0.29364 (15) | 0.3678 (4) | 0.60392 (11) | 0.0428 (6) |
| H5 | 0.3265 | 0.4721 | 0.5808 | 0.051\* |
| C6 | 0.36450 (17) | 0.2002 (4) | 0.63145 (13) | 0.0508 (7) |
| H6A | 0.3366 | 0.0950 | 0.6568 | 0.061\* |
| H6B | 0.3858 | 0.1278 | 0.5946 | 0.061\* |
| C7 | 0.44506 (15) | 0.3031 (4) | 0.67622 (12) | 0.0480 (7) |
| H7A | 0.4773 | 0.3944 | 0.6493 | 0.058\* |
| H7B | 0.4873 | 0.1928 | 0.6958 | 0.058\* |
| C8 | 0.41595 (15) | 0.4351 (4) | 0.73221 (11) | 0.0385 (6) |
| H8 | 0.3911 | 0.3380 | 0.7626 | 0.046\* |
| C9 | 0.34047 (14) | 0.5989 (4) | 0.70474 (10) | 0.0353 (5) |
| H9 | 0.3681 | 0.6951 | 0.6756 | 0.042\* |
| C10 | 0.25731 (14) | 0.4943 (4) | 0.65963 (11) | 0.0394 (6) |
| C11 | 0.31613 (15) | 0.7380 (4) | 0.76137 (11) | 0.0434 (6) |
| H11A | 0.2728 | 0.8468 | 0.7421 | 0.052\* |
| H11B | 0.2860 | 0.6500 | 0.7905 | 0.052\* |

| C12 | 0.39942 (15) | 0.8466 (4) | 0.80345 (11) | 0.0429 (6) |
| H12A | 0.4253 | 0.9487 | 0.7759 | 0.052* |
| H12B | 0.3800 | 0.9237 | 0.8401 | 0.052* |
| C13 | 0.47280 (15) | 0.6831 (4) | 0.83163 (11) | 0.0378 (6) |
| C14 | 0.49663 (14) | 0.5547 (4) | 0.77246 (11) | 0.0399 (6) |
| H14 | 0.5161 | 0.6592 | 0.7417 | 0.048* |
| C15 | 0.58350 (16) | 0.4311 (5) | 0.80303 (13) | 0.0599 (8) |
| H15A | 0.6212 | 0.4002 | 0.7694 | 0.072* |
| H15B | 0.5679 | 0.2981 | 0.8229 | 0.072* |
| C16 | 0.63351 (16) | 0.5840 (5) | 0.85708 (13) | 0.0572 (7) |
| H16A | 0.6450 | 0.5148 | 0.9006 | 0.069* |
| H16B | 0.6917 | 0.6301 | 0.8458 | 0.069* |
| C17 | 0.56810 (15) | 0.7744 (4) | 0.85757 (12) | 0.0447 (6) |
| H17 | 0.5826 | 0.8834 | 0.8263 | 0.054* |
| C18 | 0.44041 (17) | 0.5428 (5) | 0.88509 (12) | 0.0530 (7) |
| H18A | 0.4859 | 0.4358 | 0.8998 | 0.080* |
| H18B | 0.3835 | 0.4751 | 0.8664 | 0.080* |
| H18C | 0.4316 | 0.6296 | 0.9225 | 0.080* |
| C19 | 0.20421 (17) | 0.3490 (5) | 0.70079 (13) | 0.0562 (7) |
| H19A | 0.1693 | 0.4350 | 0.7265 | 0.084* |
| H19B | 0.2468 | 0.2625 | 0.7305 | 0.084* |
| H19C | 0.1634 | 0.2587 | 0.6711 | 0.084* |
| C17A | 0.64397 (18) | 0.9967 (5) | 0.94474 (13) | 0.0538 (7) |
| C17B | 0.6399 (2) | 1.0837 (7) | 1.01266 (14) | 0.0876 (11) |
| H17B | 0.5804 | 1.0557 | 1.0238 | 0.131* |
| H17C | 0.6505 | 1.2348 | 1.0129 | 0.131* |
| H17D | 0.6862 | 1.0165 | 1.0450 | 0.131* |
| O17A | 0.57234 (11) | 0.8688 (3) | 0.92319 (8) | 0.0531 (5) |
| O17B | 0.70289 (13) | 1.0344 (4) | 0.91272 (10) | 0.0760 (7) |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| --- | --- | --- | --- | --- | --- | --- |
| C1 | 0.0468 (15) | 0.0607 (18) | 0.0501 (15) | 0.0143 (13) | 0.0005 (13) | −0.0053 (14) |
| C2 | 0.0503 (16) | 0.094 (2) | 0.0664 (19) | 0.0145 (18) | −0.0084 (15) | −0.021 (2) |
| C3 | 0.0517 (17) | 0.085 (2) | 0.0500 (16) | −0.0041 (17) | −0.0007 (13) | −0.0134 (17) |
| C4 | 0.0549 (16) | 0.0559 (16) | 0.0456 (15) | −0.0013 (14) | 0.0061 (13) | −0.0085 (13) |
| C5 | 0.0421 (13) | 0.0468 (14) | 0.0400 (13) | 0.0028 (13) | 0.0082 (11) | 0.0007 (12) |
| C6 | 0.0507 (16) | 0.0492 (15) | 0.0520 (15) | 0.0099 (13) | 0.0074 (13) | −0.0120 (13) |
| C7 | 0.0422 (14) | 0.0486 (15) | 0.0530 (15) | 0.0155 (12) | 0.0072 (12) | −0.0062 (13) |
| C8 | 0.0365 (12) | 0.0400 (13) | 0.0394 (13) | 0.0057 (11) | 0.0079 (10) | 0.0030 (11) |
| C9 | 0.0356 (12) | 0.0359 (13) | 0.0354 (12) | 0.0034 (11) | 0.0085 (10) | 0.0034 (11) |
| C10 | 0.0324 (12) | 0.0456 (14) | 0.0399 (13) | 0.0033 (11) | 0.0059 (10) | 0.0007 (11) |
| C11 | 0.0379 (13) | 0.0472 (16) | 0.0437 (14) | 0.0117 (12) | 0.0028 (11) | −0.0036 (12) |
| C12 | 0.0437 (14) | 0.0432 (14) | 0.0421 (13) | 0.0076 (12) | 0.0079 (11) | −0.0051 (12) |
| C13 | 0.0327 (12) | 0.0441 (14) | 0.0367 (13) | 0.0037 (10) | 0.0063 (10) | 0.0037 (11) |
| C14 | 0.0325 (12) | 0.0421 (14) | 0.0452 (13) | 0.0073 (11) | 0.0074 (10) | 0.0029 (12) |
| C15 | 0.0391 (14) | 0.070 (2) | 0.0666 (18) | 0.0160 (14) | −0.0019 (13) | −0.0073 (16) |

| C16 | 0.0378 (13) | 0.073 (2) | 0.0582 (16) | 0.0059 (15) | 0.0001 (12) | 0.0014 (16) |
|---|---|---|---|---|---|---|
| C17 | 0.0382 (13) | 0.0567 (15) | 0.0389 (14) | −0.0024 (12) | 0.0059 (11) | 0.0019 (12) |
| C18 | 0.0490 (15) | 0.0644 (17) | 0.0459 (15) | −0.0046 (14) | 0.0087 (12) | 0.0078 (14) |
| C19 | 0.0474 (14) | 0.0678 (18) | 0.0556 (15) | −0.0138 (14) | 0.0148 (12) | −0.0053 (15) |
| C17A | 0.0412 (15) | 0.0629 (18) | 0.0527 (17) | −0.0044 (14) | −0.0049 (13) | 0.0013 (14) |
| C17B | 0.070 (2) | 0.124 (3) | 0.0644 (19) | −0.028 (2) | 0.0012 (15) | −0.027 (2) |
| O17A | 0.0442 (10) | 0.0721 (12) | 0.0418 (9) | −0.0114 (10) | 0.0045 (7) | −0.0088 (10) |
| O17B | 0.0516 (11) | 0.1011 (17) | 0.0758 (14) | −0.0238 (13) | 0.0125 (10) | −0.0063 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.533 (3) | C11—H11B | 0.9700 |
| C1—C10 | 1.533 (3) | C12—C13 | 1.529 (3) |
| C1—H1A | 0.9700 | C12—H12A | 0.9700 |
| C1—H1B | 0.9700 | C12—H12B | 0.9700 |
| C2—C3 | 1.495 (4) | C13—C17 | 1.527 (3) |
| C2—H2A | 0.9700 | C13—C18 | 1.534 (3) |
| C2—H2B | 0.9700 | C13—C14 | 1.534 (3) |
| C3—C4 | 1.315 (3) | C14—C15 | 1.536 (3) |
| C3—H3 | 0.9300 | C14—H14 | 0.9800 |
| C4—C5 | 1.491 (3) | C15—C16 | 1.545 (4) |
| C4—H4 | 0.9300 | C15—H15A | 0.9700 |
| C5—C6 | 1.520 (3) | C15—H15B | 0.9700 |
| C5—C10 | 1.548 (3) | C16—C17 | 1.536 (4) |
| C5—H5 | 0.9800 | C16—H16A | 0.9700 |
| C6—C7 | 1.511 (3) | C16—H16B | 0.9700 |
| C6—H6A | 0.9700 | C17—O17A | 1.446 (3) |
| C6—H6B | 0.9700 | C17—H17 | 0.9800 |
| C7—C8 | 1.524 (3) | C18—H18A | 0.9600 |
| C7—H7A | 0.9700 | C18—H18B | 0.9600 |
| C7—H7B | 0.9700 | C18—H18C | 0.9600 |
| C8—C14 | 1.521 (3) | C19—H19A | 0.9600 |
| C8—C9 | 1.547 (3) | C19—H19B | 0.9600 |
| C8—H8 | 0.9800 | C19—H19C | 0.9600 |
| C9—C11 | 1.532 (3) | C17A—O17B | 1.195 (3) |
| C9—C10 | 1.546 (3) | C17A—O17A | 1.340 (3) |
| C9—H9 | 0.9800 | C17A—C17B | 1.490 (4) |
| C10—C19 | 1.538 (3) | C17B—H17B | 0.9600 |
| C11—C12 | 1.531 (3) | C17B—H17C | 0.9600 |
| C11—H11A | 0.9700 | C17B—H17D | 0.9600 |
| | | | |
| C2—C1—C10 | 113.4 (2) | H11A—C11—H11B | 107.7 |
| C2—C1—H1A | 108.9 | C13—C12—C11 | 111.2 (2) |
| C10—C1—H1A | 108.9 | C13—C12—H12A | 109.4 |
| C2—C1—H1B | 108.9 | C11—C12—H12A | 109.4 |
| C10—C1—H1B | 108.9 | C13—C12—H12B | 109.4 |
| H1A—C1—H1B | 107.7 | C11—C12—H12B | 109.4 |
| C3—C2—C1 | 113.2 (2) | H12A—C12—H12B | 108.0 |

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| C3—C2—H2A | 108.9 | C17—C13—C12 | 115.5 (2) |
| C1—C2—H2A | 108.9 | C17—C13—C18 | 110.66 (18) |
| C3—C2—H2B | 108.9 | C12—C13—C18 | 111.13 (19) |
| C1—C2—H2B | 108.9 | C17—C13—C14 | 98.27 (17) |
| H2A—C2—H2B | 107.7 | C12—C13—C14 | 107.64 (17) |
| C4—C3—C2 | 122.6 (3) | C18—C13—C14 | 113.1 (2) |
| C4—C3—H3 | 118.7 | C8—C14—C13 | 114.43 (17) |
| C2—C3—H3 | 118.7 | C8—C14—C15 | 119.4 (2) |
| C3—C4—C5 | 123.6 (3) | C13—C14—C15 | 103.75 (18) |
| C3—C4—H4 | 118.2 | C8—C14—H14 | 106.1 |
| C5—C4—H4 | 118.2 | C13—C14—H14 | 106.1 |
| C4—C5—C6 | 114.0 (2) | C15—C14—H14 | 106.1 |
| C4—C5—C10 | 112.18 (18) | C14—C15—C16 | 103.8 (2) |
| C6—C5—C10 | 112.93 (18) | C14—C15—H15A | 111.0 |
| C4—C5—H5 | 105.6 | C16—C15—H15A | 111.0 |
| C6—C5—H5 | 105.6 | C14—C15—H15B | 111.0 |
| C10—C5—H5 | 105.6 | C16—C15—H15B | 111.0 |
| C7—C6—C5 | 110.3 (2) | H15A—C15—H15B | 109.0 |
| C7—C6—H6A | 109.6 | C17—C16—C15 | 105.17 (18) |
| C5—C6—H6A | 109.6 | C17—C16—H16A | 110.7 |
| C7—C6—H6B | 109.6 | C15—C16—H16A | 110.7 |
| C5—C6—H6B | 109.6 | C17—C16—H16B | 110.7 |
| H6A—C6—H6B | 108.1 | C15—C16—H16B | 110.7 |
| C6—C7—C8 | 112.61 (19) | H16A—C16—H16B | 108.8 |
| C6—C7—H7A | 109.1 | O17A—C17—C13 | 111.19 (17) |
| C8—C7—H7A | 109.1 | O17A—C17—C16 | 113.30 (19) |
| C6—C7—H7B | 109.1 | C13—C17—C16 | 104.5 (2) |
| C8—C7—H7B | 109.1 | O17A—C17—H17 | 109.2 |
| H7A—C7—H7B | 107.8 | C13—C17—H17 | 109.2 |
| C14—C8—C7 | 111.78 (18) | C16—C17—H17 | 109.2 |
| C14—C8—C9 | 108.42 (18) | C13—C18—H18A | 109.5 |
| C7—C8—C9 | 111.75 (17) | C13—C18—H18B | 109.5 |
| C14—C8—H8 | 108.3 | H18A—C18—H18B | 109.5 |
| C7—C8—H8 | 108.3 | C13—C18—H18C | 109.5 |
| C9—C8—H8 | 108.3 | H18A—C18—H18C | 109.5 |
| C11—C9—C10 | 114.78 (17) | H18B—C18—H18C | 109.5 |
| C11—C9—C8 | 110.83 (16) | C10—C19—H19A | 109.5 |
| C10—C9—C8 | 112.44 (17) | C10—C19—H19B | 109.5 |
| C11—C9—H9 | 106.0 | H19A—C19—H19B | 109.5 |
| C10—C9—H9 | 106.0 | C10—C19—H19C | 109.5 |
| C8—C9—H9 | 106.0 | H19A—C19—H19C | 109.5 |
| C1—C10—C19 | 108.93 (19) | H19B—C19—H19C | 109.5 |
| C1—C10—C9 | 111.59 (19) | O17B—C17A—O17A | 123.3 (3) |
| C19—C10—C9 | 111.01 (18) | O17B—C17A—C17B | 125.3 (3) |
| C1—C10—C5 | 105.87 (18) | O17A—C17A—C17B | 111.4 (2) |
| C19—C10—C5 | 111.4 (2) | C17A—C17B—H17B | 109.5 |
| C9—C10—C5 | 107.95 (16) | C17A—C17B—H17C | 109.5 |
| C12—C11—C9 | 113.60 (18) | H17B—C17B—H17C | 109.5 |

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| C12—C11—H11A | 108.8 | C17A—C17B—H17D | 109.5 |
| C9—C11—H11A | 108.8 | H17B—C17B—H17D | 109.5 |
| C12—C11—H11B | 108.8 | H17C—C17B—H17D | 109.5 |
| C9—C11—H11B | 108.8 | C17A—O17A—C17 | 116.84 (19) |
| | | | |
| C10—C1—C2—C3 | −37.9 (3) | C9—C11—C12—C13 | −55.1 (3) |
| C1—C2—C3—C4 | 6.9 (4) | C11—C12—C13—C17 | 163.78 (18) |
| C2—C3—C4—C5 | −1.2 (5) | C11—C12—C13—C18 | −69.1 (2) |
| C3—C4—C5—C6 | 155.6 (3) | C11—C12—C13—C14 | 55.2 (2) |
| C3—C4—C5—C10 | 25.7 (4) | C7—C8—C14—C13 | −177.5 (2) |
| C4—C5—C6—C7 | 172.2 (2) | C9—C8—C14—C13 | 58.9 (2) |
| C10—C5—C6—C7 | −58.2 (3) | C7—C8—C14—C15 | −53.7 (3) |
| C5—C6—C7—C8 | 54.7 (3) | C9—C8—C14—C15 | −177.28 (19) |
| C6—C7—C8—C14 | −174.4 (2) | C17—C13—C14—C8 | 179.97 (19) |
| C6—C7—C8—C9 | −52.7 (3) | C12—C13—C14—C8 | −59.9 (2) |
| C14—C8—C9—C11 | −53.2 (2) | C18—C13—C14—C8 | 63.3 (2) |
| C7—C8—C9—C11 | −176.8 (2) | C17—C13—C14—C15 | 48.1 (2) |
| C14—C8—C9—C10 | 176.82 (17) | C12—C13—C14—C15 | 168.3 (2) |
| C7—C8—C9—C10 | 53.2 (2) | C18—C13—C14—C15 | −68.6 (2) |
| C2—C1—C10—C19 | −60.0 (3) | C8—C14—C15—C16 | −162.0 (2) |
| C2—C1—C10—C9 | 177.1 (2) | C13—C14—C15—C16 | −33.2 (2) |
| C2—C1—C10—C5 | 59.9 (3) | C14—C15—C16—C17 | 4.6 (3) |
| C11—C9—C10—C1 | 61.9 (2) | C12—C13—C17—O17A | 78.3 (3) |
| C8—C9—C10—C1 | −170.18 (18) | C18—C13—C17—O17A | −49.0 (3) |
| C11—C9—C10—C19 | −59.8 (3) | C14—C13—C17—O17A | −167.57 (19) |
| C8—C9—C10—C19 | 68.1 (2) | C12—C13—C17—C16 | −159.1 (2) |
| C11—C9—C10—C5 | 177.85 (19) | C18—C13—C17—C16 | 73.6 (2) |
| C8—C9—C10—C5 | −54.2 (2) | C14—C13—C17—C16 | −45.0 (2) |
| C4—C5—C10—C1 | −52.5 (3) | C15—C16—C17—O17A | 146.8 (2) |
| C6—C5—C10—C1 | 177.1 (2) | C15—C16—C17—C13 | 25.6 (3) |
| C4—C5—C10—C19 | 65.8 (3) | O17B—C17A—O17A—C17 | −0.1 (4) |
| C6—C5—C10—C19 | −64.7 (2) | C17B—C17A—O17A—C17 | 179.8 (2) |
| C4—C5—C10—C9 | −172.1 (2) | C13—C17—O17A—C17A | −164.9 (2) |
| C6—C5—C10—C9 | 57.5 (2) | C16—C17—O17A—C17A | 77.7 (3) |
| C10—C9—C11—C12 | −177.70 (18) | C19—C10—C13—C18 | 3.33 (19) |
| C8—C9—C11—C12 | 53.6 (2) | | |