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# 9-(Pent-4-enyl)anthracene

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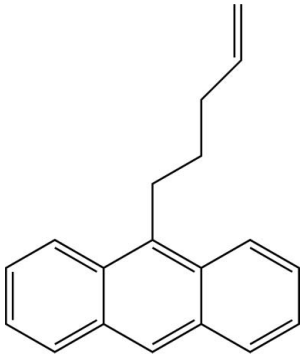
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.001 Å; $R$ factor = 0.049; $wR$ factor = 0.151; data-to-parameter ratio = 30.6.

In the title compound, $C_{19}H_{18}$, the anthracene system is almost planar, with a maximum deviation of −0.039 (1) Å. The structure is stabilized by C—H$\cdots\pi$ interactions. The pentene moiety is not planar and is twisted away from the attached anthracene system with a maximum torsion angle of 91.2 (1)°.

## Related literature

For background to anthracene, see: de Silva *et al.* (1997); Klarner *et al.* (1998); Han *et al.* (2009).



## Experimental

### Crystal data

$C_{19}H_{18}$
$M_r$ = 246.33
Monoclinic, $P2_1/c$
$a$ = 11.1555 (2) Å
$b$ = 7.2678 (1) Å
$c$ = 19.7129 (3) Å
$\beta$ = 119.096 (1)°
$V$ = 1396.55 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 100 K
0.73 × 0.38 × 0.26 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.953, $T_{max}$ = 0.983
20185 measured reflections
5271 independent reflections
3948 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.151
$S$ = 1.05
5271 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

**Table 1**
C—H$\cdots\pi$ interactions (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C1/C6–C8/C13/C14 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C5—H5$A\cdots Cg2^{i}$ | 0.95 | 2.63 | 3.5729 (9) | 175 |
| C7—H7$A\cdots Cg1^{i}$ | 0.95 | 2.74 | 3.6851 (9) | 177 |
| C17—H17$A\cdots Cg2^{ii}$ | 0.99 | 2.58 | 3.4643 (9) | 149 |
| C18—H18$A\cdots Cg1^{ii}$ | 0.95 | 2.90 | 3.6553 (11) | 138 |

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5202).

## References

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§ Thomson Reuters ResearcherID: A-5599-2009.

# supporting information

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## 9-(Pent-4-enyl)anthracene

**Natarajan Arumugam, Abdulrahman I. Almansour, Usama Karama, Mohd Mustaqim Rosli and Ibrahim Abdul Razak**

### S1. Comment

Anthracene is an attractive material in its photochemical and electrochemical properties as well as used as a potential medium for photoconductive (de Silva *et al.*, 1997) and electroluminescence (Klarner *et al.*, 1998) devices. Furthermore, anthracene derivatives exhibited anticancer activity has also been reported recently (Han *et al.*, 2009). As part of an ongoing study on such compounds, in this paper, we present the crystal structure of the title compound, which was synthesized as an intermediate.

All parameters in (I) within normal ranges. The anthracene is planar with maximum deviation of -0.039 (1)Å from atom C11. In the crystal, C—H···$\pi$ (Table 1) interactions contribute in stabilizing the crystal structure involving *Cg*1 = C1—C6 and *Cg*2 = C1/C6–8/C13—C14.

### S2. Experimental

A solution of anthrone (1 g, 5.1 mmol) in anhydrous THF (20 ml) was slowly added to pent-4-enylmagnesium bromide (0.47 g, 6.5 mmol). The mixture was stirred for 8 h at room temperature. The reaction mixture was subsequently acidified with 10% HCl, the organic layer was separated, and the aqueous layer was extracted with ether (2 *X* 10 ml). The combined organic layer was washed with water, dried over $MgSO_4$ and the solvent was evaporated under reduced pressure and the crude product was added 5 ml benzene, 1.2 g $P_2O_5$ and stirred for 6 h at room temperature. The $P_2O_5$ was filtered off and the benzene was removed under vacuum. The crude product was purified by column chromatography (hexane-dichloromethene 1:1). The product was recrystallized from EtOAc to yield title compound as colourless crystals.

### S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 and 0.99 Å, and with $U_{iso}$ = 1.2$U_{eq}$(C).

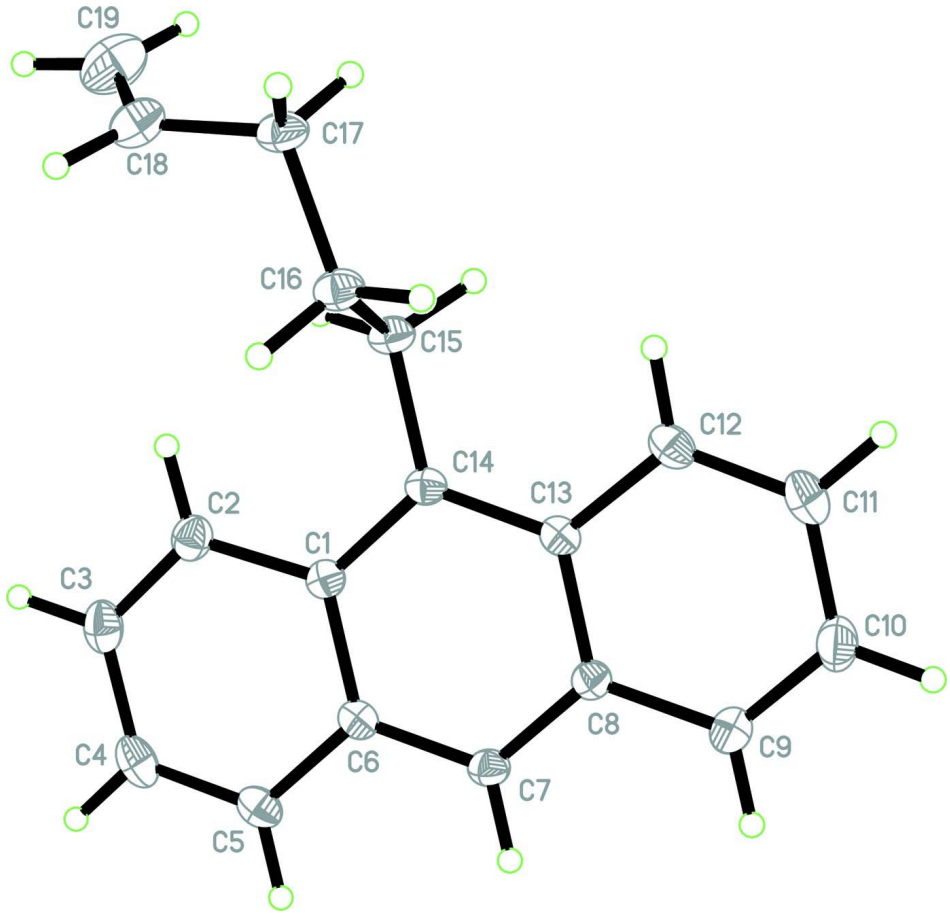


**Figure 1**

The molecular structure, showing 50% probability displacement ellipsoids. Hydrogen atoms are shown as spheres of arbitrary radius.

### 9-(Pent-4-enyl)anthracene

*Crystal data*

$C_{19}H_{18}$
$M_r = 246.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.1555$ (2) Å
$b = 7.2678$ (1) Å
$c = 19.7129$ (3) Å
$\beta = 119.096$ (1)°
$V = 1396.55$ (4) Å$^3$
$Z = 4$
$F(000) = 528$
$D_x = 1.172$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5794 reflections
$\theta = 2.4$–33.0°
$\mu = 0.07$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.73 × 0.38 × 0.26 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.953$, $T_{max} = 0.983$
20185 measured reflections
5271 independent reflections

3948 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 33.1°$, $\theta_{min} = 2.1°$
$h = -17 \rightarrow 16$
$k = -9 \rightarrow 11$
$l = -30 \rightarrow 30$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.151$
$S = 1.05$
5271 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 0.1778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.12149 (8) | 0.51562 (11) | 0.87949 (5) | 0.01455 (16) |
| C2 | 0.03754 (9) | 0.45215 (12) | 0.91135 (5) | 0.01904 (17) |
| H2A | 0.0693 | 0.3540 | 0.9478 | 0.023* |
| C3 | −0.08723 (9) | 0.53006 (14) | 0.89033 (5) | 0.02260 (19) |
| H3A | −0.1405 | 0.4860 | 0.9126 | 0.027* |
| C4 | −0.13826 (9) | 0.67610 (14) | 0.83556 (6) | 0.02333 (19) |
| H4A | −0.2250 | 0.7294 | 0.8216 | 0.028* |
| C5 | −0.06301 (9) | 0.73990 (12) | 0.80296 (5) | 0.01996 (18) |
| H5A | −0.0981 | 0.8372 | 0.7662 | 0.024* |
| C6 | 0.06813 (8) | 0.66222 (11) | 0.82341 (5) | 0.01545 (16) |
| C7 | 0.14534 (8) | 0.72875 (11) | 0.79022 (5) | 0.01635 (16) |
| H7A | 0.1101 | 0.8263 | 0.7536 | 0.020* |
| C8 | 0.27345 (8) | 0.65400 (11) | 0.81012 (5) | 0.01535 (16) |
| C9 | 0.35206 (9) | 0.72202 (13) | 0.77582 (5) | 0.02136 (18) |
| H9A | 0.3178 | 0.8221 | 0.7404 | 0.026* |
| C10 | 0.47518 (9) | 0.64570 (14) | 0.79301 (6) | 0.0248 (2) |
| H10A | 0.5258 | 0.6919 | 0.7695 | 0.030* |
| C11 | 0.52754 (9) | 0.49685 (14) | 0.84623 (6) | 0.02274 (19) |
| H11A | 0.6129 | 0.4430 | 0.8575 | 0.027* |
| C12 | 0.45707 (8) | 0.43008 (12) | 0.88137 (5) | 0.01865 (17) |

| | | | | |
|---|---|---|---|---|
| H12A | 0.4948 | 0.3312 | 0.9172 | 0.022* |
| C13 | 0.32723 (8) | 0.50604 (11) | 0.86544 (5) | 0.01458 (15) |
| C14 | 0.25201 (8) | 0.43960 (11) | 0.90096 (5) | 0.01431 (15) |
| C15 | 0.30778 (9) | 0.28354 (11) | 0.95877 (5) | 0.01744 (17) |
| H15A | 0.2711 | 0.2941 | 0.9953 | 0.021* |
| H15B | 0.4089 | 0.2943 | 0.9891 | 0.021* |
| C16 | 0.27031 (9) | 0.09379 (11) | 0.91969 (5) | 0.01856 (17) |
| H16A | 0.3180 | 0.0757 | 0.8890 | 0.022* |
| H16B | 0.1703 | 0.0887 | 0.8836 | 0.022* |
| C17 | 0.31046 (9) | −0.06170 (12) | 0.97964 (5) | 0.01997 (18) |
| H17A | 0.3154 | −0.1789 | 0.9555 | 0.024* |
| H17B | 0.4028 | −0.0361 | 1.0238 | 0.024* |
| C18 | 0.21099 (11) | −0.08229 (13) | 1.00944 (6) | 0.0254 (2) |
| H18A | 0.1204 | −0.1198 | 0.9734 | 0.031* |
| C19 | 0.23850 (14) | −0.05277 (16) | 1.08162 (7) | 0.0363 (3) |
| H19A | 0.3279 | −0.0151 | 1.1195 | 0.044* |
| H19C | 0.1689 | −0.0692 | 1.0957 | 0.044* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0157 (3) | 0.0131 (3) | 0.0142 (3) | −0.0012 (2) | 0.0068 (3) | −0.0018 (3) |
| C2 | 0.0204 (4) | 0.0205 (4) | 0.0175 (4) | −0.0032 (3) | 0.0101 (3) | −0.0017 (3) |
| C3 | 0.0200 (4) | 0.0287 (4) | 0.0226 (4) | −0.0048 (3) | 0.0131 (3) | −0.0049 (4) |
| C4 | 0.0156 (4) | 0.0283 (4) | 0.0260 (4) | 0.0005 (3) | 0.0100 (3) | −0.0056 (4) |
| C5 | 0.0165 (3) | 0.0199 (4) | 0.0207 (4) | 0.0034 (3) | 0.0069 (3) | −0.0005 (3) |
| C6 | 0.0146 (3) | 0.0147 (3) | 0.0157 (3) | 0.0005 (3) | 0.0063 (3) | −0.0014 (3) |
| C7 | 0.0170 (3) | 0.0144 (3) | 0.0164 (4) | 0.0015 (3) | 0.0071 (3) | 0.0018 (3) |
| C8 | 0.0159 (3) | 0.0150 (3) | 0.0151 (3) | −0.0003 (3) | 0.0075 (3) | 0.0001 (3) |
| C9 | 0.0208 (4) | 0.0235 (4) | 0.0215 (4) | −0.0012 (3) | 0.0116 (3) | 0.0027 (3) |
| C10 | 0.0209 (4) | 0.0321 (5) | 0.0253 (4) | −0.0029 (3) | 0.0144 (4) | 0.0003 (4) |
| C11 | 0.0165 (4) | 0.0276 (4) | 0.0245 (4) | 0.0010 (3) | 0.0103 (3) | −0.0046 (4) |
| C12 | 0.0162 (3) | 0.0173 (4) | 0.0203 (4) | 0.0020 (3) | 0.0071 (3) | −0.0017 (3) |
| C13 | 0.0141 (3) | 0.0132 (3) | 0.0152 (3) | 0.0003 (2) | 0.0061 (3) | −0.0022 (3) |
| C14 | 0.0159 (3) | 0.0115 (3) | 0.0139 (3) | 0.0000 (2) | 0.0060 (3) | −0.0008 (3) |
| C15 | 0.0201 (4) | 0.0139 (3) | 0.0155 (3) | 0.0004 (3) | 0.0065 (3) | 0.0009 (3) |
| C16 | 0.0220 (4) | 0.0140 (3) | 0.0171 (4) | 0.0002 (3) | 0.0074 (3) | 0.0004 (3) |
| C17 | 0.0230 (4) | 0.0135 (3) | 0.0200 (4) | 0.0013 (3) | 0.0078 (3) | 0.0019 (3) |
| C18 | 0.0320 (5) | 0.0180 (4) | 0.0272 (5) | −0.0009 (3) | 0.0151 (4) | 0.0021 (3) |
| C19 | 0.0531 (7) | 0.0295 (5) | 0.0336 (6) | 0.0003 (5) | 0.0267 (5) | 0.0015 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C14 | 1.4159 (11) | C11—C12 | 1.3650 (13) |
| C1—C2 | 1.4340 (11) | C11—H11A | 0.9500 |
| C1—C6 | 1.4393 (11) | C12—C13 | 1.4349 (11) |
| C2—C3 | 1.3670 (12) | C12—H12A | 0.9500 |
| C2—H2A | 0.9500 | C13—C14 | 1.4139 (11) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.4208 (14) | C14—C15 | 1.5108 (11) |
| C3—H3A | 0.9500 | C15—C16 | 1.5352 (11) |
| C4—C5 | 1.3628 (13) | C15—H15A | 0.9900 |
| C4—H4A | 0.9500 | C15—H15B | 0.9900 |
| C5—C6 | 1.4311 (11) | C16—C17 | 1.5361 (12) |
| C5—H5A | 0.9500 | C16—H16A | 0.9900 |
| C6—C7 | 1.3971 (12) | C16—H16B | 0.9900 |
| C7—C8 | 1.3950 (11) | C17—C18 | 1.4941 (14) |
| C7—H7A | 0.9500 | C17—H17A | 0.9900 |
| C8—C9 | 1.4309 (12) | C17—H17B | 0.9900 |
| C8—C13 | 1.4385 (11) | C18—C19 | 1.3193 (15) |
| C9—C10 | 1.3625 (13) | C18—H18A | 0.9500 |
| C9—H9A | 0.9500 | C19—H19A | 0.9500 |
| C10—C11 | 1.4199 (14) | C19—H19C | 0.9500 |
| C10—H10A | 0.9500 | | |

| | | | |
|---|---|---|---|
| C14—C1—C2 | 122.63 (7) | C11—C12—C13 | 121.42 (8) |
| C14—C1—C6 | 119.97 (7) | C11—C12—H12A | 119.3 |
| C2—C1—C6 | 117.40 (7) | C13—C12—H12A | 119.3 |
| C3—C2—C1 | 121.30 (8) | C14—C13—C12 | 122.63 (7) |
| C3—C2—H2A | 119.3 | C14—C13—C8 | 120.10 (7) |
| C1—C2—H2A | 119.3 | C12—C13—C8 | 117.26 (7) |
| C2—C3—C4 | 120.83 (8) | C13—C14—C1 | 119.36 (7) |
| C2—C3—H3A | 119.6 | C13—C14—C15 | 120.27 (7) |
| C4—C3—H3A | 119.6 | C1—C14—C15 | 120.32 (7) |
| C5—C4—C3 | 120.09 (8) | C14—C15—C16 | 112.59 (7) |
| C5—C4—H4A | 120.0 | C14—C15—H15A | 109.1 |
| C3—C4—H4A | 120.0 | C16—C15—H15A | 109.1 |
| C4—C5—C6 | 120.84 (8) | C14—C15—H15B | 109.1 |
| C4—C5—H5A | 119.6 | C16—C15—H15B | 109.1 |
| C6—C5—H5A | 119.6 | H15A—C15—H15B | 107.8 |
| C7—C6—C5 | 120.67 (8) | C15—C16—C17 | 111.62 (7) |
| C7—C6—C1 | 119.80 (7) | C15—C16—H16A | 109.3 |
| C5—C6—C1 | 119.52 (8) | C17—C16—H16A | 109.3 |
| C8—C7—C6 | 120.93 (7) | C15—C16—H16B | 109.3 |
| C8—C7—H7A | 119.5 | C17—C16—H16B | 109.3 |
| C6—C7—H7A | 119.5 | H16A—C16—H16B | 108.0 |
| C7—C8—C9 | 120.79 (8) | C18—C17—C16 | 112.44 (7) |
| C7—C8—C13 | 119.79 (7) | C18—C17—H17A | 109.1 |
| C9—C8—C13 | 119.41 (7) | C16—C17—H17A | 109.1 |
| C10—C9—C8 | 121.14 (8) | C18—C17—H17B | 109.1 |
| C10—C9—H9A | 119.4 | C16—C17—H17B | 109.1 |
| C8—C9—H9A | 119.4 | H17A—C17—H17B | 107.8 |
| C9—C10—C11 | 119.78 (8) | C19—C18—C17 | 125.45 (10) |
| C9—C10—H10A | 120.1 | C19—C18—H18A | 117.3 |
| C11—C10—H10A | 120.1 | C17—C18—H18A | 117.3 |
| C12—C11—C10 | 120.96 (8) | C18—C19—H19A | 120.0 |
| C12—C11—H11A | 119.5 | C18—C19—H19C | 120.0 |

| | | | |
|---|---|---|---|
| C10—C11—H11A | 119.5 | H19A—C19—H19C | 120.0 |
| | | | |
| C14—C1—C2—C3 | 179.04 (8) | C11—C12—C13—C14 | 179.98 (8) |
| C6—C1—C2—C3 | −1.14 (12) | C11—C12—C13—C8 | 0.79 (12) |
| C1—C2—C3—C4 | 0.48 (14) | C7—C8—C13—C14 | −1.54 (12) |
| C2—C3—C4—C5 | 0.28 (14) | C9—C8—C13—C14 | 178.80 (8) |
| C3—C4—C5—C6 | −0.31 (14) | C7—C8—C13—C12 | 177.67 (7) |
| C4—C5—C6—C7 | −179.61 (8) | C9—C8—C13—C12 | −1.98 (11) |
| C4—C5—C6—C1 | −0.39 (13) | C12—C13—C14—C1 | −176.95 (7) |
| C14—C1—C6—C7 | 0.14 (12) | C8—C13—C14—C1 | 2.22 (12) |
| C2—C1—C6—C7 | −179.68 (7) | C12—C13—C14—C15 | 0.50 (12) |
| C14—C1—C6—C5 | −179.09 (7) | C8—C13—C14—C15 | 179.67 (7) |
| C2—C1—C6—C5 | 1.09 (12) | C2—C1—C14—C13 | 178.29 (7) |
| C5—C6—C7—C8 | 179.78 (8) | C6—C1—C14—C13 | −1.52 (12) |
| C1—C6—C7—C8 | 0.56 (12) | C2—C1—C14—C15 | 0.84 (12) |
| C6—C7—C8—C9 | 179.78 (8) | C6—C1—C14—C15 | −178.97 (7) |
| C6—C7—C8—C13 | 0.13 (12) | C13—C14—C15—C16 | −86.19 (9) |
| C7—C8—C9—C10 | −177.80 (8) | C1—C14—C15—C16 | 91.23 (9) |
| C13—C8—C9—C10 | 1.85 (13) | C14—C15—C16—C17 | −172.08 (7) |
| C8—C9—C10—C11 | −0.43 (14) | C15—C16—C17—C18 | 78.26 (9) |
| C9—C10—C11—C12 | −0.83 (15) | C16—C17—C18—C19 | −114.87 (11) |
| C10—C11—C12—C13 | 0.63 (14) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the C1–C6 and C1/C6–C8/C13/C14 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5*A*···*Cg*2$^{i}$ | 0.95 | 2.63 | 3.5729 (9) | 175 |
| C7—H7*A*···*Cg*1$^{i}$ | 0.95 | 2.74 | 3.6851 (9) | 177 |
| C17—H17*A*···*Cg*2$^{ii}$ | 0.99 | 2.58 | 3.4643 (9) | 149 |
| C18—H18*A*···*Cg*1$^{ii}$ | 0.95 | 2.90 | 3.6553 (11) | 138 |

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+3/2; (ii) *x*, *y*−1, *z*.