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5-[(9*H*-Fluoren-9-ylidene)methyl]furan-2-carbonitrileLucia Perašinová,^{a*} Anita Andicsová,^b Daniel Végh^b and Jozef Kožíšek^a

^aInstitute of Physical Chemistry and Chemical Physics, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, and ^bInstitute of Organic Chemistry, Catalysis and Petrochemistry, Faculty of Chemical Technology, Slovak Technical University, Radlinského 9, Bratislava 81237, Slovak Republic
Correspondence e-mail: lucia.perasinova@stuba.sk

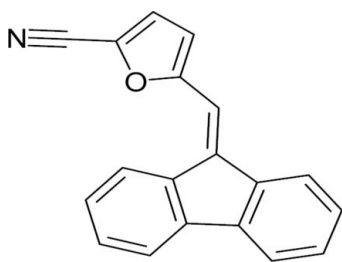
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.062; wR factor = 0.179; data-to-parameter ratio = 14.5.

The title compound, $\text{C}_{19}\text{H}_{11}\text{NO}$, is stabilized by one intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond. The compound can be synthesized in good yield (49%), by transformation of functional groups [starting with 5-(fluoren-9-ylidenemethyl)-furan-2-carbaldehyde]. The fluorene and furan ring systems are nearly coplanar, with a dihedral angle of 6.36 (7)°.

Related literature

For a related structure, see: Britten *et al.* (2001). For related literature, see: Allen (2002); Leclerc (2001).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{11}\text{NO}$
 $M_r = 269.29$

Monoclinic, $P2_1/n$
 $a = 15.899$ (3) Å

$b = 5.6109$ (11) Å
 $c = 15.664$ (3) Å
 $\beta = 103.69$ (3)°
 $V = 1357.6$ (5) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 293$ K
 $0.32 \times 0.07 \times 0.05$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
 $T_{\min} = 0.921$, $T_{\max} = 0.987$

27628 measured reflections
2746 independent reflections
1524 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$
 $wR(F^2) = 0.179$
 $S = 0.94$
2746 reflections

190 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{C11}-\text{H11A}\cdots\text{O1}$ | 0.93 | 2.27 | 3.034 (3) | 140 |

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2120).

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supplementary materials

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5-[(9*H*-Fluoren-9-ylidene)methyl]furan-2-carbonitrile

L. Perasínová, A. Andicsová, D. Végh and J. Kozísek

Comment

Our synthetic research efforts have been focused to a set of multi-ring monomer systems based on furan and fluorene. Fluorene containing oligomers are an important class of electroactive and photoactive materials. These compounds possess exceptional electrooptical properties for applications in polymer light emitting diodes (PLEDs) and nanocomposite materials with advanced anticorrosive properties (Leclerc, 2001).

In the title compound the O1—C15 [1.359 (2) Å] and O1—C18 [1.381 (2) Å] bond lengths, are in a quite good agreement with similar furan compounds in the Cambridge Structural Database (CSD; Version 5.27, 2006 release; Allen, 2002) 2-(1,2,3,5-Diselenadiazol-4-yl)-5-cyanofuran (Britten *et al.*, 2001; CSD refcode YIFHUQ) as representative example. The fluorene moiety is almost planar with maximum deviation of 0.030 (2) Å for C13. The fluorene and furan rings are nearly coplanar with a dihedral angle of 6.36 (7)°. In the crystal structure the molecular packing is stabilized by intramolecular hydrogen bond (Fig. 1).

Experimental

A solution of 5-fluoren-9-ylidenemethyl-furan-2-carbaldehyde (0.0033 mol, 0.91 g), NH₂OH·HCl (0.0039 mol, 0.3 g, 1.12 eq.) in *N*-Methyl-pyrrolidinone (5.5 ml) was heated at 110 – 115°C. Progress of the reaction was followed by TLC and after 8 h the mixture was poured into H₂O (100 ml) and extracted with EtOAc (2 x 50 ml). The combined layers EtOAc were dried (Na₂SO₄) and the solvent was evaporated *in vacuo*. Crude product could be purified by column chromatography using silikagel Merck 60 in toluene as eluent (40% yield) $R_f = 0,51$ (toluen). *M.p.*: 167–169°C.

¹H NMR (300 MHz, DMSO – d₆, p.p.m.): δ = 6.78 (d, 1H, J = 3.6 Hz), 7.15 (s, 1H), 7.31 – 7.29 (m, 1H), 7.45 – 7.33 (m, 4H), 7.72 – 7.66 (m, 3H), 8.51 (d, 1H, J = 7.65 Hz).

¹³C-NMR (75 MHz, DMSO – d₆, p.p.m.) δ = 109.99, 111.77, 114.62, 119.80, 119.87, 120.33, 123.91, 125.74, 125.82, 127.20, 127.69, 129.69, 129.23, 129.88, 135.25, 138.06, 139.37, 139.62, 141.75, 156.19.

IR (KBr, cm⁻¹): 3136 (w), 3120 (vw), 3053(w), 2221(s, νC≡N), 1716(s, ν(C=C)), 1633(m), 1611(m), 1600(m, ν(C=C) aromatic), 1494(s, ν(C=C) aromatic), 1469(w), 1448(s), 1354(m), 1297(m), 1290(m), 1274(m, ν_{as}(C—O—C)), 1263(m), 1198(w), 1180(m), 1152(m), 1138(w), 1111(m), 1098(w), 1029(s, ν_s(C—O—C)), 975(m), 966(m), 941(m), 917(m), 882(m), 871(m), 793(vs, γ(CCH)), 781(vs, γ(CCH)), 772(m, γ(CCH)), 737(m, γ(CCH)), 728(vs, γ(CCH)), 724(vs, γ(CCH)), 668(m), 645(m), 625(m), 580(w), 561(w), 524(w), 511(w), 473(m), 455(m), 442(vw), 432(vw), 401(m)

Refinement

H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 Å and $U_{iso}(H) = 1.2 U_{eq}(C)$.

Figures

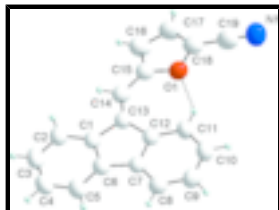


Fig. 1.
The numbering scheme of 5-[(9*H*-fluoren-9-ylidene) methyl] furan-2-carbonitrile. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen-bond interactions are indicated by dashed lines.

5-[(9*H*-Fluoren-9-ylidene)methyl]furan-2-carbonitrile

Crystal data

| | |
|--------------------------------|---|
| $C_{19}H_{11}NO$ | $F_{000} = 560$ |
| $M_r = 269.29$ | $D_x = 1.317 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| Hall symbol: $-P\ 2_1n$ | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 15.899 (3) \text{ \AA}$ | Cell parameters from 7057 reflections |
| $b = 5.6109 (11) \text{ \AA}$ | $\theta = 3.1\text{--}29.1^\circ$ |
| $c = 15.664 (3) \text{ \AA}$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $\beta = 103.69 (3)^\circ$ | $T = 293 \text{ K}$ |
| $V = 1357.6 (5) \text{ \AA}^3$ | Block, yellow |
| $Z = 4$ | $0.32 \times 0.07 \times 0.05 \text{ mm}$ |

Data collection

| | |
|---|--|
| Oxford Diffraction Gemini R CCD diffractometer | 2746 independent reflections |
| Radiation source: fine-focus sealed tube | 1524 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.043$ |
| $T = 293 \text{ K}$ | $\theta_{\text{max}} = 26.4^\circ$ |
| Rotation method data acquisition using ω and phi scans | $\theta_{\text{min}} = 4.2^\circ$ |
| Absorption correction: analytical (Clark & Reid, 1995) | $h = -19 \rightarrow 19$ |
| $T_{\text{min}} = 0.921$, $T_{\text{max}} = 0.987$ | $k = -7 \rightarrow 7$ |
| 27628 measured reflections | $l = -19 \rightarrow 19$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.062$ | H-atom parameters constrained |
| $wR(F^2) = 0.179$ | $w = 1/[\sigma^2(F_o^2) + (0.121P)^2]$ |
| | where $P = (F_o^2 + 2F_c^2)/3$ |

$S = 0.94$ $(\Delta/\sigma)_{\max} < 0.001$
 2746 reflections $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
 190 parameters $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

Special details

Experimental. face-indexed (*CrysAlis RED*; Oxford Diffraction, 2007)

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 $F^2 > 2\sigma(F^2)$ 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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|------------|--------------|----------------------------------|
| C1 | 0.17033 (14) | 0.6172 (3) | 0.88196 (13) | 0.0544 (5) |
| C2 | 0.23065 (15) | 0.6471 (4) | 0.96102 (15) | 0.0680 (6) |
| H2A | 0.2259 | 0.7739 | 0.9978 | 0.082* |
| C3 | 0.29834 (16) | 0.4852 (4) | 0.98462 (15) | 0.0737 (7) |
| H3A | 0.3385 | 0.5046 | 1.0380 | 0.088* |
| C4 | 0.30765 (16) | 0.2974 (4) | 0.93141 (16) | 0.0741 (7) |
| H4A | 0.3537 | 0.1919 | 0.9484 | 0.089* |
| C5 | 0.24829 (15) | 0.2672 (4) | 0.85303 (15) | 0.0651 (6) |
| H5A | 0.2536 | 0.1400 | 0.8166 | 0.078* |
| C6 | 0.17991 (13) | 0.4280 (3) | 0.82809 (13) | 0.0538 (5) |
| C7 | 0.10829 (13) | 0.4398 (3) | 0.75032 (13) | 0.0521 (5) |
| C8 | 0.08974 (15) | 0.2931 (4) | 0.67850 (14) | 0.0602 (6) |
| H8A | 0.1248 | 0.1626 | 0.6747 | 0.072* |
| C9 | 0.01799 (15) | 0.3426 (4) | 0.61169 (14) | 0.0660 (6) |
| H9A | 0.0044 | 0.2436 | 0.5627 | 0.079* |
| C10 | -0.03397 (15) | 0.5382 (4) | 0.61677 (14) | 0.0686 (6) |
| H10A | -0.0818 | 0.5685 | 0.5709 | 0.082* |
| C11 | -0.01619 (14) | 0.6875 (4) | 0.68787 (13) | 0.0605 (6) |
| H11A | -0.0512 | 0.8188 | 0.6904 | 0.073* |
| C12 | 0.05522 (13) | 0.6391 (3) | 0.75621 (12) | 0.0518 (5) |
| C13 | 0.09090 (13) | 0.7573 (3) | 0.84099 (13) | 0.0532 (5) |
| C14 | 0.06414 (15) | 0.9425 (3) | 0.88210 (14) | 0.0599 (6) |
| H14A | 0.1013 | 0.9725 | 0.9365 | 0.072* |
| C15 | -0.00743 (14) | 1.1057 (3) | 0.86312 (14) | 0.0577 (6) |
| C16 | -0.02863 (18) | 1.2789 (4) | 0.91496 (15) | 0.0737 (7) |
| H16A | 0.0017 | 1.3139 | 0.9720 | 0.088* |

supplementary materials

| | | | | |
|------|---------------|------------|--------------|------------|
| C17 | -0.10323 (17) | 1.3964 (4) | 0.86887 (16) | 0.0732 (7) |
| H17A | -0.1314 | 1.5227 | 0.8886 | 0.088* |
| C18 | -0.12551 (15) | 1.2896 (4) | 0.79073 (16) | 0.0647 (6) |
| C19 | -0.19420 (18) | 1.3303 (4) | 0.7165 (2) | 0.0743 (7) |
| N1 | -0.25096 (16) | 1.3660 (4) | 0.65689 (17) | 0.0953 (7) |
| O1 | -0.06784 (9) | 1.1091 (2) | 0.78554 (9) | 0.0624 (4) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.0575 (13) | 0.0541 (11) | 0.0489 (12) | -0.0072 (10) | 0.0075 (10) | 0.0027 (9) |
| C2 | 0.0730 (15) | 0.0716 (13) | 0.0545 (13) | -0.0084 (12) | 0.0054 (12) | -0.0022 (11) |
| C3 | 0.0701 (15) | 0.0820 (15) | 0.0601 (14) | -0.0014 (13) | -0.0021 (12) | 0.0087 (13) |
| C4 | 0.0673 (16) | 0.0750 (15) | 0.0735 (16) | 0.0064 (12) | 0.0036 (13) | 0.0144 (13) |
| C5 | 0.0609 (14) | 0.0672 (13) | 0.0650 (14) | 0.0063 (11) | 0.0102 (12) | 0.0039 (10) |
| C6 | 0.0540 (12) | 0.0550 (11) | 0.0524 (12) | -0.0026 (9) | 0.0126 (10) | 0.0015 (9) |
| C7 | 0.0565 (12) | 0.0515 (11) | 0.0487 (11) | -0.0040 (9) | 0.0130 (10) | 0.0011 (9) |
| C8 | 0.0649 (14) | 0.0590 (12) | 0.0572 (13) | -0.0001 (10) | 0.0156 (11) | -0.0064 (10) |
| C9 | 0.0745 (15) | 0.0676 (13) | 0.0534 (13) | -0.0045 (12) | 0.0101 (12) | -0.0116 (10) |
| C10 | 0.0710 (15) | 0.0762 (14) | 0.0521 (13) | 0.0013 (12) | 0.0015 (11) | -0.0044 (11) |
| C11 | 0.0613 (14) | 0.0601 (12) | 0.0542 (13) | 0.0058 (10) | 0.0020 (11) | -0.0042 (10) |
| C12 | 0.0540 (12) | 0.0518 (11) | 0.0485 (11) | -0.0052 (9) | 0.0099 (10) | 0.0009 (9) |
| C13 | 0.0578 (13) | 0.0519 (10) | 0.0478 (11) | -0.0054 (9) | 0.0083 (10) | -0.0021 (9) |
| C14 | 0.0685 (14) | 0.0564 (12) | 0.0536 (12) | -0.0046 (10) | 0.0119 (11) | -0.0030 (9) |
| C15 | 0.0656 (14) | 0.0555 (11) | 0.0526 (12) | -0.0046 (10) | 0.0154 (11) | -0.0029 (9) |
| C16 | 0.0938 (19) | 0.0651 (13) | 0.0619 (14) | 0.0079 (13) | 0.0179 (13) | -0.0055 (11) |
| C17 | 0.0869 (18) | 0.0621 (13) | 0.0746 (16) | 0.0074 (12) | 0.0272 (14) | -0.0099 (11) |
| C18 | 0.0620 (14) | 0.0586 (12) | 0.0759 (16) | 0.0016 (10) | 0.0211 (13) | -0.0007 (11) |
| C19 | 0.0684 (17) | 0.0674 (14) | 0.0895 (19) | 0.0048 (12) | 0.0233 (15) | -0.0074 (13) |
| N1 | 0.0808 (16) | 0.0981 (16) | 0.0986 (18) | 0.0118 (13) | 0.0047 (15) | -0.0131 (13) |
| O1 | 0.0625 (10) | 0.0616 (9) | 0.0637 (10) | 0.0017 (7) | 0.0162 (8) | -0.0079 (7) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|----------|-----------|
| C1—C2 | 1.386 (3) | C10—C11 | 1.368 (3) |
| C1—C6 | 1.386 (3) | C10—H10A | 0.9300 |
| C1—C13 | 1.497 (3) | C11—C12 | 1.390 (3) |
| C2—C3 | 1.390 (3) | C11—H11A | 0.9300 |
| C2—H2A | 0.9300 | C12—C13 | 1.473 (3) |
| C3—C4 | 1.373 (3) | C13—C14 | 1.344 (3) |
| C3—H3A | 0.9300 | C14—C15 | 1.436 (3) |
| C4—C5 | 1.370 (3) | C14—H14A | 0.9300 |
| C4—H4A | 0.9300 | C15—O1 | 1.359 (2) |
| C5—C6 | 1.396 (3) | C15—C16 | 1.359 (3) |
| C5—H5A | 0.9300 | C16—C17 | 1.399 (3) |
| C6—C7 | 1.459 (3) | C16—H16A | 0.9300 |
| C7—C8 | 1.369 (3) | C17—C18 | 1.333 (3) |
| C7—C12 | 1.417 (3) | C17—H17A | 0.9300 |
| C8—C9 | 1.381 (3) | C18—O1 | 1.381 (2) |

| | | | |
|--------------|--------------|-----------------|-------------|
| C8—H8A | 0.9300 | C18—C19 | 1.413 (4) |
| C9—C10 | 1.387 (3) | C19—N1 | 1.152 (3) |
| C9—H9A | 0.9300 | | |
| C2—C1—C6 | 119.0 (2) | C11—C10—H10A | 119.3 |
| C2—C1—C13 | 130.90 (19) | C9—C10—H10A | 119.3 |
| C6—C1—C13 | 110.13 (18) | C10—C11—C12 | 118.7 (2) |
| C1—C2—C3 | 119.1 (2) | C10—C11—H11A | 120.6 |
| C1—C2—H2A | 120.4 | C12—C11—H11A | 120.6 |
| C3—C2—H2A | 120.4 | C11—C12—C7 | 119.62 (18) |
| C4—C3—C2 | 121.9 (2) | C11—C12—C13 | 132.57 (18) |
| C4—C3—H3A | 119.1 | C7—C12—C13 | 107.81 (17) |
| C2—C3—H3A | 119.1 | C14—C13—C12 | 133.0 (2) |
| C5—C4—C3 | 119.2 (2) | C14—C13—C1 | 122.10 (19) |
| C5—C4—H4A | 120.4 | C12—C13—C1 | 104.83 (17) |
| C3—C4—H4A | 120.4 | C13—C14—C15 | 136.0 (2) |
| C4—C5—C6 | 119.8 (2) | C13—C14—H14A | 112.0 |
| C4—C5—H5A | 120.1 | C15—C14—H14A | 112.0 |
| C6—C5—H5A | 120.1 | O1—C15—C16 | 107.54 (19) |
| C1—C6—C5 | 121.0 (2) | O1—C15—C14 | 123.50 (18) |
| C1—C6—C7 | 107.29 (17) | C16—C15—C14 | 129.0 (2) |
| C5—C6—C7 | 131.70 (19) | C15—C16—C17 | 109.2 (2) |
| C8—C7—C12 | 120.82 (19) | C15—C16—H16A | 125.4 |
| C8—C7—C6 | 129.27 (19) | C17—C16—H16A | 125.4 |
| C12—C7—C6 | 109.90 (17) | C18—C17—C16 | 105.7 (2) |
| C7—C8—C9 | 118.7 (2) | C18—C17—H17A | 127.1 |
| C7—C8—H8A | 120.6 | C16—C17—H17A | 127.1 |
| C9—C8—H8A | 120.6 | C17—C18—O1 | 110.3 (2) |
| C8—C9—C10 | 120.78 (19) | C17—C18—C19 | 132.0 (2) |
| C8—C9—H9A | 119.6 | O1—C18—C19 | 117.7 (2) |
| C10—C9—H9A | 119.6 | N1—C19—C18 | 178.7 (3) |
| C11—C10—C9 | 121.3 (2) | C15—O1—C18 | 107.23 (16) |
| C6—C1—C2—C3 | -0.8 (3) | C8—C7—C12—C13 | 178.99 (18) |
| C13—C1—C2—C3 | 178.4 (2) | C6—C7—C12—C13 | -1.8 (2) |
| C1—C2—C3—C4 | 0.6 (3) | C11—C12—C13—C14 | 3.9 (4) |
| C2—C3—C4—C5 | -0.5 (4) | C7—C12—C13—C14 | -175.5 (2) |
| C3—C4—C5—C6 | 0.5 (3) | C11—C12—C13—C1 | -178.4 (2) |
| C2—C1—C6—C5 | 0.9 (3) | C7—C12—C13—C1 | 2.1 (2) |
| C13—C1—C6—C5 | -178.45 (18) | C2—C1—C13—C14 | -3.0 (3) |
| C2—C1—C6—C7 | -179.96 (18) | C6—C1—C13—C14 | 176.26 (18) |
| C13—C1—C6—C7 | 0.7 (2) | C2—C1—C13—C12 | 179.0 (2) |
| C4—C5—C6—C1 | -0.8 (3) | C6—C1—C13—C12 | -1.7 (2) |
| C4—C5—C6—C7 | -179.6 (2) | C12—C13—C14—C15 | -1.0 (4) |
| C1—C6—C7—C8 | 179.8 (2) | C1—C13—C14—C15 | -178.4 (2) |
| C5—C6—C7—C8 | -1.2 (4) | C13—C14—C15—O1 | -4.3 (4) |
| C1—C6—C7—C12 | 0.7 (2) | C13—C14—C15—C16 | 175.6 (2) |
| C5—C6—C7—C12 | 179.7 (2) | O1—C15—C16—C17 | -0.8 (3) |
| C12—C7—C8—C9 | -0.1 (3) | C14—C15—C16—C17 | 179.3 (2) |
| C6—C7—C8—C9 | -179.15 (19) | C15—C16—C17—C18 | 0.5 (3) |

supplementary materials

| | | | |
|-----------------|-------------|-----------------|--------------|
| C7—C8—C9—C10 | 0.5 (3) | C16—C17—C18—O1 | 0.0 (3) |
| C8—C9—C10—C11 | -0.2 (3) | C16—C17—C18—C19 | -179.5 (2) |
| C9—C10—C11—C12 | -0.5 (3) | C16—C15—O1—C18 | 0.8 (2) |
| C10—C11—C12—C7 | 0.8 (3) | C14—C15—O1—C18 | -179.31 (19) |
| C10—C11—C12—C13 | -178.6 (2) | C17—C18—O1—C15 | -0.5 (2) |
| C8—C7—C12—C11 | -0.5 (3) | C19—C18—O1—C15 | 179.08 (19) |
| C6—C7—C12—C11 | 178.63 (17) | | |

Hydrogen-bond geometry (Å, °)

| <i>D—H···A</i> | <i>D—H</i> | <i>H···A</i> | <i>D···A</i> | <i>D—H···A</i> |
|----------------|------------|--------------|--------------|----------------|
| C11—H11A···O1 | 0.93 | 2.27 | 3.034 (3) | 140 |

Fig. 1

