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9-(Methoxymethyl)anthracene

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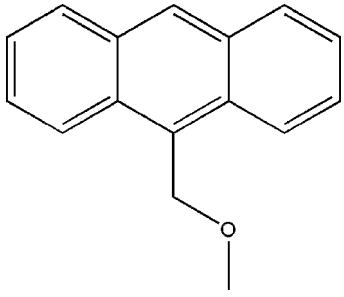
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 7.3.

The title compound, $C_{16}H_{14}O$, crystallizes with two independent molecules in the asymmetric unit, one of which lies on a crystallographic mirror plane. Intermolecular C—H···O hydrogen bonds link the molecules into infinite one-dimensional chains.

Related literature

For related literature, see: Stevenson (1911); Park *et al.* (2007); Zimmermann *et al.* (1999); Ramos Silva *et al.* (2000); Desiraju (1996).



Experimental

Crystal data

$C_{16}H_{14}O$
M_r = 222.27
Orthorhombic, $Cmc2_1$
a = 41.2360 (16) Å
b = 10.1110 (8) Å
c = 8.6930 (6) Å
V = 3624.4 (4) Å^3
Z = 12
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.854, T_{max} = 0.982
8859 measured reflections
1746 independent reflections
1313 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.08
1746 reflections
239 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···O1^{i}	0.97	2.58	3.436 (5)	148

Symmetry code: (i) $x, -y+1, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2058).

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supplementary materials

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9-(Methoxymethyl)anthracene

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Comment

Many organic substances possess the property of fluorescence, when exposed to light of a suitable wavelength, and they emit light of a different wavelength. Anthracene itself fluoresces both as solid and vapor as well as in solution (Stevenson, 1911). This phenomenon has been of interest to the chemist. In order to establish some relation between the structure and the fluorescence of the substances, new series of anthracene derivatives have been prepared (Park *et al.*, 2007; Zimmermann *et al.*, 1999). In this paper, an anthracene derivative has been synthesized, and its structure (I) is reported.

The title compound, $C_{16}H_{14}O$, crystallizes with two independent molecules in the asymmetric unit. As shown in Fig. 1, the dihedral angle between the two methylanthracene plane is 74.8°. Each $C_{16}H_{14}O$ molecule consists of a methyl group linked to an anthracene moiety through an ether linkage. The C—C bonds and C—C—C angles in the anthracene fragment are comparable with reported values (Ramos Silva *et al.*, 2000). The C15—O1, C16–O1, C25—O2 and C26—O2 bond lengths are 1.406 (4), 1.427 (4), 1.420 (6) and 1.408 (6) Å, respectively, which are typical of ether bonds. Intermolecular C—H···O hydrogen bonds link the molecules into infinite one-dimensional chains.

Previous studies (Desiraju, 1996) have revealed that the C···O distances in C—H···O hydrogen bonds are in the range of 3.0–4.0 Å. The C—H···O angles θ in the range of 110–180° are acceptable. As shown in Fig. 2, the C(15)···O(1) distance of 3.436 Å and C(15)—H(15*a*)···O(1) angle of 147.7° indicate a weak C—H···O hydrogen bond, which links the molecules into an infinite one-dimensional chain. All the chains are parallel along the *c* axis in the crystal.

Experimental

The title compound was prepared according to the reported procedure (Zimmermann *et al.*, 1999). Crystals suitable for X-ray analysis were obtained by recrystallization from methanol solution of the compound.

Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for aromatic, 0.96 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH_3 atoms and 0.97 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH_2 atoms. The absolute structure could not be determined from the diffraction data. Friedel pairs have been merged, and the configuration shown is arbitary.

Figures

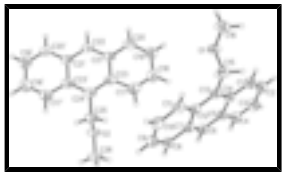

Fig. 1. A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level.

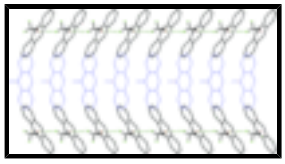

Fig. 2. Packing diagram showing the C—H···O hydrogen bonds.

9-(Methoxymethyl)anthracene

Crystal data

$C_{16}H_{14}O$	F_{000} = 1416
M_r = 222.27	D_x = 1.222 Mg m^{-3}
Orthorhombic, *Cmc*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2c -2	Cell parameters from 1313 reflections
a = 41.2360 (16) Å	θ = 1.0–25.0º
b = 10.1110 (8) Å	μ = 0.08 mm^{-1}
c = 8.6930 (6) Å	*T* = 293 (2) K
V = 3624.4 (4) Å^3	Block, yellow
Z = 12	0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer	1746 independent reflections
Radiation source: fine-focus sealed tube	1313 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 293(2) K	θ_{max} = 25.1º
ω scans	θ_{min} = 1.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −46→48
T_{min} = 0.854, T_{max} = 0.982	*k* = −12→9
8859 measured reflections	*l* = −10→10

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.5696P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.102	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
S = 1.08	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
1746 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
239 parameters	Extinction coefficient: 0.0033 (5)
1 restraint	

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
C1	0.78219 (8)	0.7300 (3)	0.5267 (4)	0.0695 (9)	
H1	0.7759	0.6462	0.5594	0.083*	
C2	0.76281 (8)	0.7976 (4)	0.4294 (5)	0.0794 (11)	
H2	0.7433	0.7601	0.3978	0.095*	
C3	0.77155 (8)	0.9240 (4)	0.3749 (5)	0.0813 (10)	
H3	0.7579	0.9691	0.3077	0.098*	
C4	0.79948 (7)	0.9787 (4)	0.4200 (4)	0.0694 (9)	
H4	0.8051	1.0618	0.3826	0.083*	
C5	0.82076 (7)	0.9132 (3)	0.5239 (4)	0.0552 (7)	
C6	0.84968 (7)	0.9698 (3)	0.5729 (4)	0.0577 (8)	
H6	0.8554	1.0527	0.5353	0.069*	
C7	0.87030 (7)	0.9072 (3)	0.6757 (3)	0.0526 (7)	
C8	0.89975 (7)	0.9686 (3)	0.7243 (4)	0.0622 (8)	
H8	0.9050	1.0523	0.6876	0.075*	
C9	0.92012 (8)	0.9072 (3)	0.8225 (4)	0.0690 (9)	
H9	0.9392	0.9483	0.8528	0.083*	
C10	0.91236 (8)	0.7810 (3)	0.8789 (4)	0.0712 (9)	
H10	0.9266	0.7391	0.9462	0.085*	
C11	0.88455 (8)	0.7190 (3)	0.8374 (4)	0.0663 (9)	
H11	0.8799	0.6360	0.8781	0.080*	
C12	0.86212 (7)	0.7782 (3)	0.7323 (3)	0.0531 (7)	
C13	0.83312 (8)	0.7169 (3)	0.6835 (3)	0.0544 (8)	
C14	0.81206 (7)	0.7842 (3)	0.5805 (3)	0.0549 (7)	
C15	0.82409 (8)	0.5802 (3)	0.7375 (4)	0.0626 (8)	
H15A	0.8356	0.5596	0.8319	0.075*	
H15B	0.8010	0.5761	0.7580	0.075*	
C16	0.82168 (10)	0.3581 (3)	0.6614 (5)	0.0868 (12)	
H16A	0.8274	0.2981	0.5803	0.130*	

H16B	0.7986	0.3582	0.6744	0.130*	
H16C	0.8319	0.3306	0.7554	0.130*	
C17	0.93912 (9)	0.7459 (3)	0.4267 (4)	0.0703 (9)	
H17	0.9381	0.8111	0.5020	0.084*	
C18	0.91127 (9)	0.6979 (3)	0.3669 (5)	0.0777 (10)	
H18	0.8915	0.7301	0.4023	0.093*	
C19	0.91169 (9)	0.5998 (3)	0.2517 (5)	0.0788 (10)	
H19	0.8924	0.5690	0.2095	0.095*	
C20	0.94047 (8)	0.5509 (3)	0.2030 (5)	0.0761 (10)	
H20	0.9406	0.4845	0.1289	0.091*	
C21	0.97045 (8)	0.5984 (3)	0.2621 (4)	0.0610 (8)	
C22	1.0000	0.5506 (4)	0.2086 (6)	0.0689 (13)	
H22	1.0000	0.4844	0.1344	0.083*	
C23	0.97033 (8)	0.6990 (3)	0.3772 (3)	0.0570 (7)	
C24	1.0000	0.7484 (4)	0.4348 (5)	0.0594 (11)	
C25	1.0000	0.8575 (4)	0.5519 (5)	0.0709 (13)	
H25A	0.9809	0.8510	0.6166	0.085*	0.50
H25B	1.0191	0.8510	0.6166	0.085*	0.50
C26	1.0000	1.0899 (5)	0.5704 (7)	0.098 (2)	
H26A	1.0000	1.1697	0.5104	0.147*	
H26B	1.0190	1.0876	0.6341	0.147*	0.50
H26C	0.9810	1.0876	0.6341	0.147*	0.50
O1	0.83235 (5)	0.4882 (2)	0.6226 (3)	0.0661 (6)	
O2	1.0000	0.9797 (3)	0.4714 (4)	0.0749 (9)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.071 (2)	0.069 (2)	0.068 (2)	−0.0136 (18)	0.0117 (19)	−0.0047 (18)
C2	0.061 (2)	0.093 (3)	0.084 (3)	−0.0089 (19)	−0.0028 (19)	−0.006 (2)
C3	0.072 (2)	0.087 (2)	0.085 (3)	0.0065 (19)	−0.014 (2)	0.007 (2)
C4	0.073 (2)	0.067 (2)	0.068 (2)	0.0038 (17)	−0.0019 (18)	0.0076 (18)
C5	0.0606 (18)	0.0549 (17)	0.0503 (17)	0.0017 (15)	0.0070 (15)	0.0016 (14)
C6	0.0679 (18)	0.0496 (17)	0.0555 (19)	−0.0034 (15)	0.0098 (15)	0.0028 (15)
C7	0.0614 (17)	0.0498 (16)	0.0466 (16)	0.0032 (14)	0.0054 (14)	−0.0039 (13)
C8	0.0687 (18)	0.0616 (19)	0.0563 (19)	−0.0041 (15)	0.0070 (18)	−0.0049 (17)
C9	0.0639 (19)	0.080 (2)	0.063 (2)	−0.0002 (17)	−0.0013 (17)	−0.0102 (19)
C10	0.077 (2)	0.075 (2)	0.062 (2)	0.0132 (18)	−0.006 (2)	−0.0040 (19)
C11	0.084 (2)	0.0537 (18)	0.061 (2)	0.0091 (17)	0.0070 (18)	−0.0006 (16)
C12	0.0672 (18)	0.0486 (16)	0.0434 (16)	0.0065 (13)	0.0070 (15)	−0.0039 (14)
C13	0.0705 (19)	0.0474 (16)	0.0454 (17)	−0.0012 (15)	0.0124 (15)	−0.0031 (13)
C14	0.0637 (17)	0.0543 (17)	0.0466 (17)	−0.0039 (14)	0.0119 (15)	−0.0052 (14)
C15	0.081 (2)	0.0584 (18)	0.0481 (17)	−0.0064 (15)	0.0123 (17)	0.0001 (16)
C16	0.120 (3)	0.055 (2)	0.085 (3)	−0.022 (2)	0.020 (2)	0.0004 (19)
C17	0.097 (3)	0.0559 (19)	0.058 (2)	0.0103 (19)	0.0110 (19)	0.0044 (16)
C18	0.085 (2)	0.072 (2)	0.077 (2)	0.005 (2)	0.011 (2)	0.017 (2)
C19	0.080 (2)	0.067 (2)	0.089 (3)	−0.0058 (18)	−0.001 (2)	0.011 (2)
C20	0.092 (3)	0.055 (2)	0.082 (2)	−0.0099 (18)	−0.008 (2)	−0.0077 (19)

C21	0.082 (2)	0.0411 (15)	0.0599 (19)	−0.0034 (15)	−0.0012 (18)	0.0001 (14)
C22	0.089 (3)	0.045 (2)	0.072 (3)	0.000	0.000	−0.014 (2)
C23	0.086 (2)	0.0409 (14)	0.0437 (16)	0.0030 (15)	0.0037 (18)	0.0062 (13)
C24	0.094 (3)	0.043 (2)	0.041 (2)	0.000	0.000	0.0061 (18)
C25	0.101 (4)	0.065 (3)	0.047 (3)	0.000	0.000	−0.008 (2)
C26	0.126 (5)	0.070 (3)	0.096 (5)	0.000	0.000	−0.039 (3)
O1	0.0944 (14)	0.0447 (10)	0.0593 (12)	−0.0068 (11)	0.0160 (12)	0.0000 (10)
O2	0.109 (2)	0.0506 (18)	0.065 (2)	0.000	0.000	−0.0179 (16)

Geometric parameters (Å, °)

C1—C2	1.349 (5)	C15—H15B	0.9700
C1—C14	1.427 (4)	C16—O1	1.427 (4)
C1—H1	0.9300	C16—H16A	0.9600
C2—C3	1.410 (5)	C16—H16B	0.9600
C2—H2	0.9300	C16—H16C	0.9600
C3—C4	1.337 (4)	C17—C18	1.351 (5)
C3—H3	0.9300	C17—C23	1.438 (4)
C4—C5	1.423 (4)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.411 (5)
C5—C6	1.389 (4)	C18—H18	0.9300
C5—C14	1.440 (4)	C19—C20	1.353 (5)
C6—C7	1.387 (4)	C19—H19	0.9300
C6—H6	0.9300	C20—C21	1.423 (4)
C7—C8	1.428 (4)	C20—H20	0.9300
C7—C12	1.434 (4)	C21—C22	1.391 (4)
C8—C9	1.349 (4)	C21—C23	1.427 (4)
C8—H8	0.9300	C22—C21^{i}	1.391 (4)
C9—C10	1.404 (5)	C22—H22	0.9300
C9—H9	0.9300	C23—C24	1.413 (4)
C10—C11	1.356 (4)	C24—C23^{i}	1.413 (4)
C10—H10	0.9300	C24—C25	1.501 (6)
C11—C12	1.431 (4)	C25—O2	1.420 (6)
C11—H11	0.9300	C25—H25A	0.9700
C12—C13	1.412 (4)	C25—H25B	0.9700
C13—C14	1.421 (4)	C26—O2	1.408 (6)
C13—C15	1.506 (4)	C26—H26A	0.9600
C15—O1	1.406 (4)	C26—H26B	0.9600
C15—H15A	0.9700	C26—H26C	0.9600
C2—C1—C14	121.5 (3)	C13—C15—H15B	109.9
C2—C1—H1	119.3	H15A—C15—H15B	108.3
C14—C1—H1	119.3	O1—C16—H16A	109.5
C1—C2—C3	121.2 (3)	O1—C16—H16B	109.5
C1—C2—H2	119.4	H16A—C16—H16B	109.5
C3—C2—H2	119.4	O1—C16—H16C	109.5
C4—C3—C2	119.8 (3)	H16A—C16—H16C	109.5
C4—C3—H3	120.1	H16B—C16—H16C	109.5
C2—C3—H3	120.1	C18—C17—C23	121.8 (3)

C3—C4—C5	121.6 (3)	C18—C17—H17	119.1
C3—C4—H4	119.2	C23—C17—H17	119.1
C5—C4—H4	119.2	C17—C18—C19	121.1 (4)
C6—C5—C4	122.1 (3)	C17—C18—H18	119.5
C6—C5—C14	118.8 (3)	C19—C18—H18	119.5
C4—C5—C14	119.0 (3)	C20—C19—C18	119.3 (4)
C7—C6—C5	122.4 (3)	C20—C19—H19	120.3
C7—C6—H6	118.8	C18—C19—H19	120.3
C5—C6—H6	118.8	C19—C20—C21	121.7 (3)
C6—C7—C8	120.9 (3)	C19—C20—H20	119.1
C6—C7—C12	119.5 (3)	C21—C20—H20	119.1
C8—C7—C12	119.6 (3)	C22—C21—C20	121.6 (3)
C9—C8—C7	121.1 (3)	C22—C21—C23	119.0 (3)
C9—C8—H8	119.4	C20—C21—C23	119.4 (3)
C7—C8—H8	119.4	C21^{i}—C22—C21	122.3 (4)
C8—C9—C10	119.8 (3)	C21^{i}—C22—H22	118.8
C8—C9—H9	120.1	C21—C22—H22	118.8
C10—C9—H9	120.1	C24—C23—C21	119.8 (3)
C11—C10—C9	121.3 (3)	C24—C23—C17	123.5 (3)
C11—C10—H10	119.3	C21—C23—C17	116.6 (3)
C9—C10—H10	119.3	C23^{i}—C24—C23	120.0 (4)
C10—C11—C12	121.5 (3)	C23^{i}—C24—C25	120.0 (2)
C10—C11—H11	119.2	C23—C24—C25	120.0 (2)
C12—C11—H11	119.2	O2—C25—C24	107.8 (3)
C13—C12—C11	123.7 (3)	O2—C25—H25A	110.1
C13—C12—C7	119.7 (3)	C24—C25—H25A	110.1
C11—C12—C7	116.6 (3)	O2—C25—H25B	110.1
C12—C13—C14	119.8 (3)	C24—C25—H25B	110.1
C12—C13—C15	121.2 (3)	H25A—C25—H25B	108.5
C14—C13—C15	119.0 (3)	O2—C26—H26A	109.5
C13—C14—C1	123.4 (3)	O2—C26—H26B	109.5
C13—C14—C5	119.8 (3)	H26A—C26—H26B	109.5
C1—C14—C5	116.8 (3)	O2—C26—H26C	109.5
O1—C15—C13	109.0 (2)	H26A—C26—H26C	109.5
O1—C15—H15A	109.9	H26B—C26—H26C	109.5
C13—C15—H15A	109.9	C15—O1—C16	111.6 (2)
O1—C15—H15B	109.9	C26—O2—C25	112.8 (4)
C14—C1—C2—C3	1.0 (5)	C2—C1—C14—C5	−1.1 (5)
C1—C2—C3—C4	−0.2 (6)	C6—C5—C14—C13	−0.5 (4)
C2—C3—C4—C5	−0.6 (6)	C4—C5—C14—C13	179.6 (3)
C3—C4—C5—C6	−179.3 (3)	C6—C5—C14—C1	−179.9 (3)
C3—C4—C5—C14	0.6 (5)	C4—C5—C14—C1	0.3 (4)
C4—C5—C6—C7	179.1 (3)	C12—C13—C15—O1	−99.2 (3)
C14—C5—C6—C7	−0.8 (4)	C14—C13—C15—O1	80.2 (3)
C5—C6—C7—C8	−179.6 (3)	C23—C17—C18—C19	−0.5 (5)
C5—C6—C7—C12	1.2 (4)	C17—C18—C19—C20	1.6 (5)
C6—C7—C8—C9	−179.0 (3)	C18—C19—C20—C21	−1.7 (5)
C12—C7—C8—C9	0.2 (4)	C19—C20—C21—C22	−178.1 (4)

C7—C8—C9—C10	−0.2 (5)	C19—C20—C21—C23	0.8 (5)
C8—C9—C10—C11	−0.4 (5)	C20—C21—C22—C21^{i}	178.3 (3)
C9—C10—C11—C12	1.0 (5)	C23—C21—C22—C21^{i}	−0.7 (7)
C10—C11—C12—C13	178.9 (3)	C22—C21—C23—C24	0.0 (5)
C10—C11—C12—C7	−1.1 (4)	C20—C21—C23—C24	−178.9 (3)
C6—C7—C12—C13	−0.4 (4)	C22—C21—C23—C17	179.2 (3)
C8—C7—C12—C13	−179.5 (3)	C20—C21—C23—C17	0.2 (4)
C6—C7—C12—C11	179.7 (3)	C18—C17—C23—C24	178.8 (3)
C8—C7—C12—C11	0.5 (4)	C18—C17—C23—C21	−0.4 (4)
C11—C12—C13—C14	179.1 (3)	C21—C23—C24—C23^{i}	0.6 (5)
C7—C12—C13—C14	−0.9 (4)	C17—C23—C24—C23^{i}	−178.5 (2)
C11—C12—C13—C15	−1.5 (4)	C21—C23—C24—C25	177.9 (3)
C7—C12—C13—C15	178.5 (3)	C17—C23—C24—C25	−1.2 (5)
C12—C13—C14—C1	−179.4 (3)	C23^{i}—C24—C25—O2	88.7 (3)
C15—C13—C14—C1	1.2 (4)	C23—C24—C25—O2	−88.7 (3)
C12—C13—C14—C5	1.4 (4)	C13—C15—O1—C16	−174.7 (3)
C15—C13—C14—C5	−178.1 (3)	C24—C25—O2—C26	180.000 (2)
C2—C1—C14—C13	179.6 (3)		

Symmetry codes: (i) −*x*+2, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15A···O1^{ii}	0.97	2.58	3.436 (5)	148

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

Fig. 1

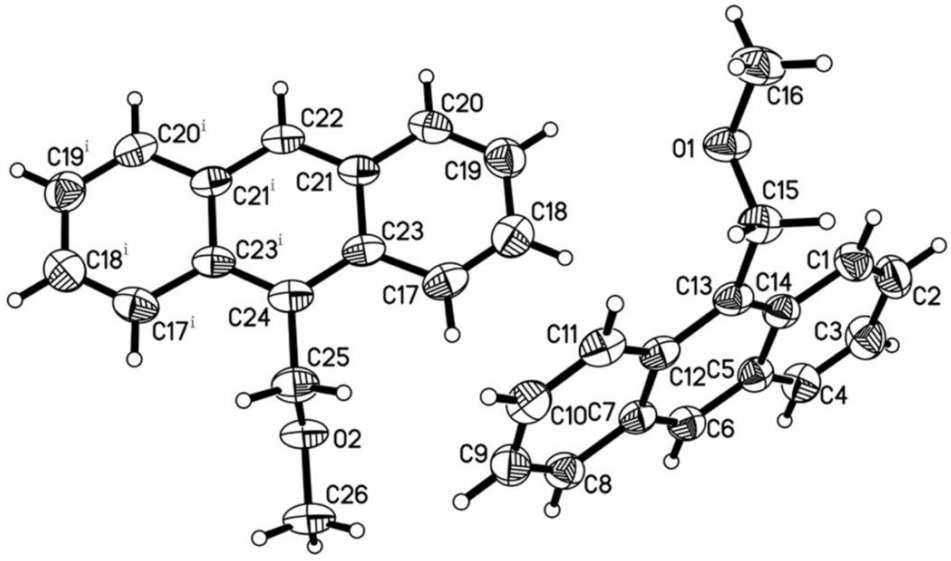
C16
O1
C15
C1
C2
C13
C14
C3
C11
C12
C5
C4
C10
C7
C6
C9
C8
C20
C22
C20i
C19i
C21i
C21
C19
C18
C23
C23i
C18i
C17
C24
C17i
C25
O2
C26

Fig. 2