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1,4-Di-9-anthrylbutane

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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.002$ Å
 R factor = 0.040
 wR factor = 0.104
Data-to-parameter ratio = 10.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

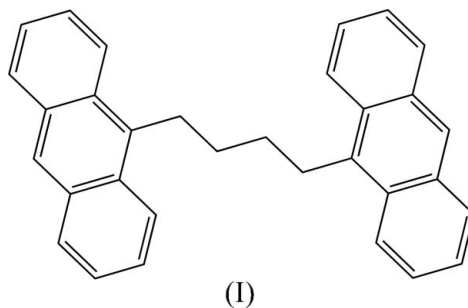
1,4-Di-9-anthrylbutane

In the title compound, $C_{32}H_{26}$, the molecule has an inversion centre at the mid-point of the central C—C bond. Weak intermolecular C—H $\cdots\pi$ interactions help to stabilize the crystal structure.

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Comment

Bisanthrylalkanes are extensively used in studies aimed at gaining information on the photophysical properties and electron donor–acceptor complexations of the related photoconductive polymers (Masnovi *et al.*, 1985; Becker & Andersson, 1987; Becker *et al.*, 1992; Rettig *et al.*, 1999). The spacing and orientation of the chromophore groups are determining factors in the photophysical and photochemical features of these dimers. For the complexation studies of a series of bis-9-anthrylalkanes with a number of electron acceptors, we have prepared the title compound, (I), and carried out a single-crystal X-ray analysis to establish its structure.



Compound (I) (Fig. 1) crystallizes in the monoclinic space group $P2_1/n$. The molecule has an inversion centre at the mid-point of the central C—C bond. Bond lengths and angles in the anthracene unit are in agreement with those in related compounds (Becker *et al.*, 1984; Becker *et al.*, 1992). The 14 atoms of the anthracene skeleton are coplanar to within 0.019 (2) Å. The methylene chain connecting the two ring systems adopts an *anti-anti-anti* conformation. The two anthracene ring systems are parallel to each other.

The crystal packing of (I) is mainly determined by weak intermolecular C—H $\cdots\pi$ interactions (Table 1), together with van der Waals forces. No intermolecular π – π interactions are observed.

Experimental

The title compound was prepared according to the literature procedure of Dunand *et al.* (1980) *via* the formation of a di-Grignard

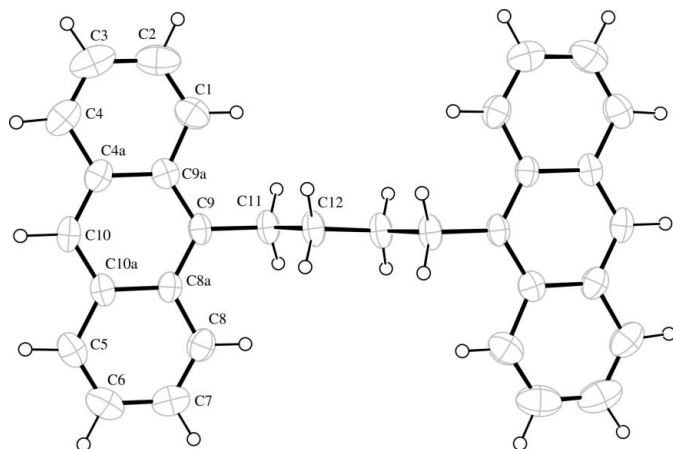


Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x, -y + 1, -z + 1)$.

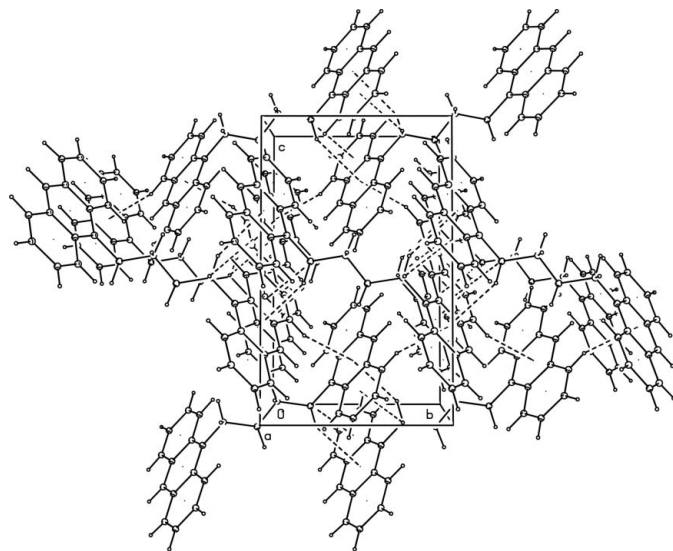


Figure 2

A packing diagram for (I), viewed down the a axis. Dashed lines represent $C-H \cdots \pi$ contacts.

reagent from 1,4-dibromobutane followed by its reaction with anthrone. The di-Grignard reagent was prepared by stirring magnesium (0.50 g, 20 mmol) (washed twice with acetone and dried) and 1,4-dibromobutane (1.0 ml, 8.2 mmol) in anhydrous diethyl ether (20 ml) with a small chunk of iodine. The mixture was stirred under a nitrogen atmosphere for 24 h under ambient conditions. A hot solution of anthrone (0.01 mol) in anhydrous benzene (40 ml) was then added. The reaction mixture was stirred and refluxed under a nitrogen atmosphere for 5 h, until the colour of the mixture turned green. The green mixture was cooled and decomposed with ice and dilute hydrochloric acid; the organic solvents were extracted and evaporated. The residue was washed eight times with hot 20% NaOH solution to remove unreacted anthrone. Column chromatography of the crude product on basic alumina using hexane–dichloromethane (9:1 v/v) as the eluting solvents gave 1.19 g (2.90 mmol, 29% yield) of the title compound as pale-yellow needles [m.p. 527–528 K; literature value 527 K (Dunand *et al.*, 1980)]. Single crystals of (I) suitable for

X-ray diffraction analysis were grown from a chloroform–hexane (1:1 v/v) solvent mixture using the slow evaporation technique.

Crystal data

$C_{32}H_{26}$
 $M_r = 410.53$
 Monoclinic, $P2_1/n$
 $a = 11.3964$ (8) Å
 $b = 7.9000$ (10) Å
 $c = 12.7887$ (6) Å
 $\beta = 94.747$ (5)°

$V = 1147.44$ (17) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 295$ (2) K
 $0.5 \times 0.4 \times 0.3$ mm

Data collection

Enraf–Nonius CAD-4
 diffractometer
 Absorption correction: none
 2015 measured reflections
 2015 independent reflections

1396 reflections with $I > 2\sigma(I)$
 3 standard reflections
 frequency: 120 min
 intensity decay: 0.1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.104$
 $S = 1.03$
 2015 reflections

197 parameters
 All H-atom parameters refined
 $\Delta\rho_{\max} = 0.13$ e Å⁻³
 $\Delta\rho_{\min} = -0.1$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$ is the centroid of the $C4a/C9a/C9/C8a/C10a/C10$ ring and $Cg2$ is the centroid of the $C5/C6/C7/C8/C8a/C10a$ ring.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C5-H5 \cdots Cg1^i$	0.98 (2)	2.57 (2)	3.496 (2)	160
$C11-H11A \cdots Cg2^{ii}$	1.02 (2)	2.85 (2)	3.563 (2)	128
$C11-H11B \cdots Cg1^{ii}$	1.01 (2)	2.82 (2)	3.550 (2)	130

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

All H atoms were located in difference Fourier maps and refined freely. The range of refined C–H distances is 0.96 (2)–1.02 (2) Å and the range of $U_{\text{iso}}(\text{H})$ values is 0.054 (4)–0.097 (7) Å².

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC Software*; data reduction: *DATRED2* in *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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