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1,4-Di-9-anthrylbutane

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Key indicators

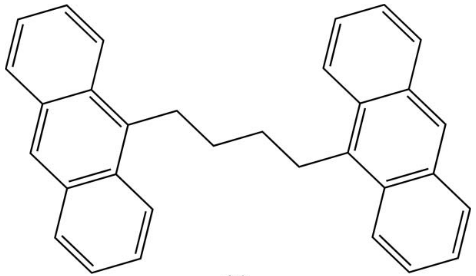
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.104
Data-to-parameter ratio = 10.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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.

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.



(I)

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

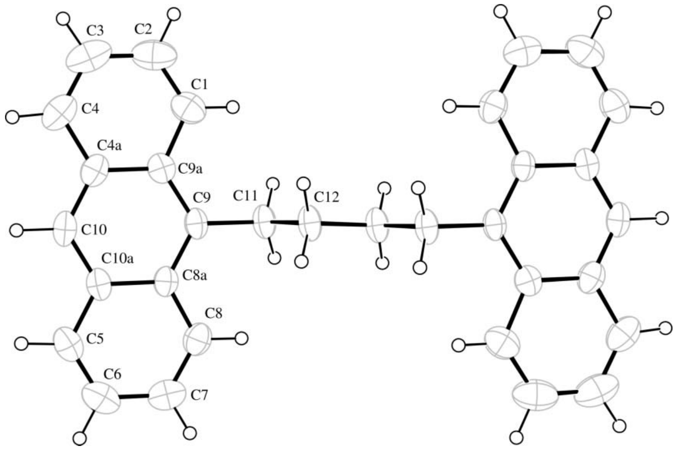


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator ($-x$, $-y + 1$, $-z + 1$).

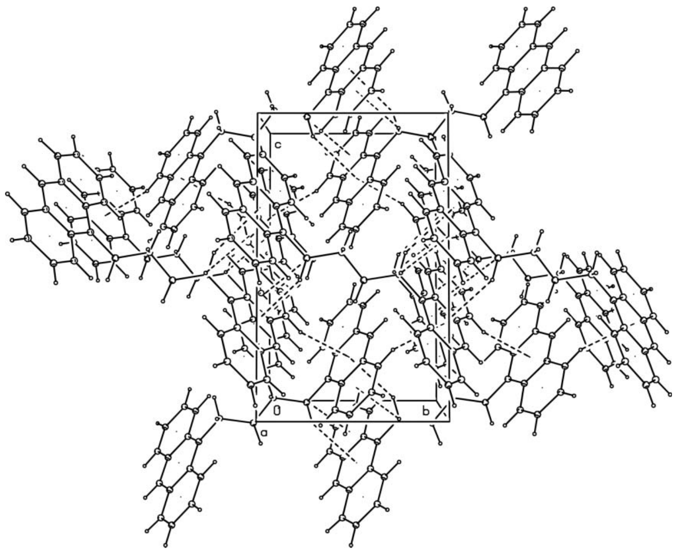


Figure 2
A packing diagram for (I), viewed down the *a* axis. Dashed lines represent C—H$\cdots\pi$ contacts.

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) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 295$ (2) K
0.5 × 0.4 × 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, °).

*Cg*1 is the centroid of the C4a/C9a/C9/C8a/C10a/C10 ring and *Cg*2 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$\cdots Cg1^{\rm i}$	0.98 (2)	2.57 (2)	3.496 (2)	160
C11—H11$A\cdots Cg2^{\rm ii}$	1.02 (2)	2.85 (2)	3.563 (2)	128
C11—H11$B\cdots Cg1^{\rm ii}$	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 $U_{\rm iso}$(H) values is 0.054 (4)–0.097 (7) Å^2.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC Software*; data reduction: *DATRD2* 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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References

Becker, H. D. & Andersson, K. (1987). *J. Org. Chem.* **52**, 5205–5213.
Becker, H. D., Langer, V., Sieler, J. & Becker, H. C. (1992). *J. Org. Chem.* **57**, 1883–1887.
Becker, H., Engelhardt, L. M., Hansen, L., Patrick, V. A. & White, A. H. (1984). *Aust. J. Chem.* **37**, 1329–1335.
Dunand, A., Ferguson, J., Puza, M. & Robertson, G. B. (1980). *J. Am. Chem. Soc.* **102**, 3524–3530.
Enraf–Nonius (1993). *CAD-4-PC* Software. Version 1.2. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

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Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.

Masnovi, J. M., Kochi, J. K., Hilinski, E. F. & Rentzepis, P. M. (1985). *J. Phys. Chem.* **89**, 5387–5395.

Rettig, W., Paeplow, B., Herbst, H., Müllen, K., Desvergne, J. P. & Bouas-Laurent, H. (1999). *New J. Chem.* **23**, 453–460.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

o2402 Arslan *et al.* • $C_{32}H_{26}$ *Acta Cryst.* (2007). E**63**, o2400–o2402