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# 1,4-Di-9-anthrylbutane

Mustafa Arslan  
*Sakarya University, Adapazari, Turkey*

Erol Asker  
*Balikesir University, Balikesir, Turkey*

John Masnovi  
*Cleveland State University, j.masnovi@csuohio.edu*

Ronald J. Baker

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Mustafa Arslan,<sup>a\*</sup> Erol Asker,<sup>b</sup>  
John Masnovi<sup>c</sup> and Ronald J.  
Baker<sup>c</sup><sup>a</sup>Department of Chemistry, Faculty of Arts and Sciences, Sakarya University, 54140 Esentepe/Adapazari, Turkey, <sup>b</sup>Necatibey Faculty of Education, Balikesir University, 10100 Balikesir, Turkey, and <sup>c</sup>Department of Chemistry, Cleveland State University, Cleveland, OH 44115, USA

Correspondence e-mail: marslan@sakarya.edu.tr

## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  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>.

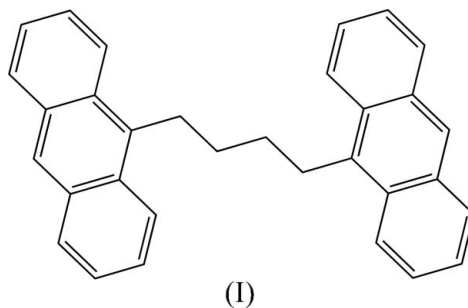
## 1,4-Di-9-anthrylbutane

In the title compound,  $\text{C}_{32}\text{H}_{26}$ , 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.

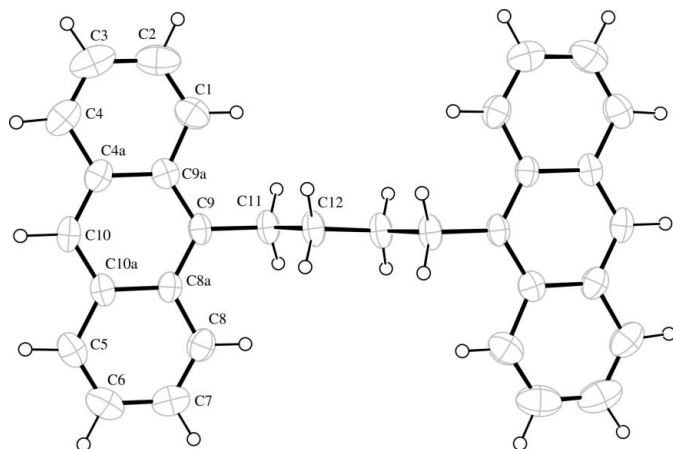


Compound (I) (Fig. 1) crystallizes in the monoclinic space group  $P2_1/n$ . The molecule has an inversion centre at the mid-point of the central C—C bond. Bond lengths and angles in the anthracene unit are in agreement with those in related compounds (Becker *et al.*, 1984; Becker *et al.*, 1992). The 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  $\pi$ – $\pi$  interactions are observed.

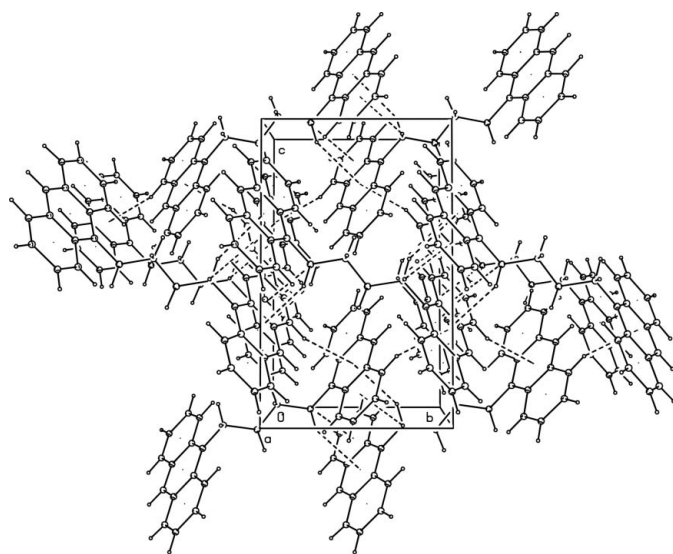
## Experimental

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<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 295$  (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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.1$  e Å<sup>-3</sup>

**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) Å<sup>2</sup>.

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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