1,4-Di-9-anthrylbutane

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Key indicators

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-crystal X-ray study</td>
<td></td>
</tr>
<tr>
<td>$T = 295$ K</td>
<td></td>
</tr>
<tr>
<td>Mean σ(C–C) = 0.002 Å</td>
<td></td>
</tr>
<tr>
<td>$R$ factor = 0.040</td>
<td></td>
</tr>
<tr>
<td>$wR$ factor = 0.104</td>
<td></td>
</tr>
<tr>
<td>Data-to-parameter ratio = 10.2</td>
<td></td>
</tr>
</tbody>
</table>

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⋯π 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.

![Structure of 1,4-Di-9-anthrylbutane](image)

Compound (I) (Fig. 1) crystallizes in the monoclinic space group $P2_1/n$. The molecule has an inversion centre at the midpoint 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⋯π 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.

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

Crystal data

\[
\begin{align*}
\text{C}_{32}\text{H}_{26} & \\
M_r & = 410.53 \\
\text{Monoclinic, } P2_1/n & \\
a & = 11.3964 (8) \, \text{Å} \\
b & = 7.9000 (10) \, \text{Å} \\
c & = 12.7887 (6) \, \text{Å} \\
\beta & = 94.747 (5) ^\circ \\
V & = 1147.44 (17) \, \text{Å}^3 \\
Z & = 2 \\
\text{Mo K}\alpha \text{ radiation} & \\
\mu & = 0.07 \, \text{mm}^{-1} \\
T & = 295 (2) \, \text{K} \\
\delta &= 0.5 \times 0.4 \times 0.3 \, \text{mm}
\end{align*}
\]

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2015 measured reflections
1396 reflections with \(I > 2\sigma(I)\)
3 standard reflections
frequency: 120 min
intensity decay: 0.1%

Refinement

\[
\begin{align*}
R[F^2 > 2\sigma(F^2)] &= 0.040 \\
wR(F^2) & = 0.104 \\
S & = 1.03 \\
197 \text{ parameters} \\
\text{All H-atom parameters refined} \\
\Delta\rho_{\text{max}} & = 0.13 \, \text{e Å}^{-3} \\
\Delta\rho_{\text{min}} & = -0.1 \, \text{e Å}^{-3}
\end{align*}
\]

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

<table>
<thead>
<tr>
<th>D—H ⋅⋅⋅A</th>
<th>D—H</th>
<th>H ⋅⋅⋅A</th>
<th>D⋯A</th>
<th>D—H ⋅⋅⋅A</th>
</tr>
</thead>
</table>
| C5—H5⋯Cg1
\(i\) & 0.98 (2) & 2.57 (2) & 3.496 (2) & 160
| C11—H11A⋯Cg2
\(ii\) & 1.02 (2) & 2.85 (2) & 3.563 (2) & 128
| C11—H11B⋯Cg1
\(ii\) & 1.01 (2) & 2.82 (2) & 3.550 (2) & 130

Symmetry codes: (i) \(-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}\) (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 \(U_{eq}(H)\) values is 0.054 (4)–0.097 (7) Å².

Data collection: \textit{CAD-4-PC Software} (Enraf–Nonius, 1993); cell refinement: \textit{CAD-4-PC Software}; data reduction: \textit{DATR2D} in \textit{NRCVAX} (Gabe et al., 1989); program(s) used to solve structure: \textit{SHELXS97} (Sheldrick, 1997); program(s) used to refine structure: \textit{SHELXL97} (Sheldrick, 1997); molecular graphics: \textit{ORTEP-3 for Windows} (Farrugia, 1997); software used to prepare material for publication: \textit{WinGX} (Farrugia, 1999).

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References