1,4-Di-9-anthrylbutane

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In the title compound, \( \text{C}_{32}\text{H}_{26} \), the molecule has an inversion centre at the mid-point of the central \( \text{C}—\text{C} \) bond. Weak intermolecular \( \text{C}—\text{H} \cdots \pi \) 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.

Experimental

The title compound was prepared according to the literature procedure of Dunand et al. (1980) via the formation of a di-Grignard...
X-ray diffraction analysis were grown from a chloroform–hexane (1:1 v/v) solvent mixture using the slow evaporation technique.

**Crystal data**

\[ \text{C}_{32}\text{H}_{26} \quad V = 1147.44 (17) \text{ Å}^3 \]

\[ m = 410.53 \quad Z = 2 \]

Monoclinic, \( P2_1/n \)

\[ a = 11.3964 (8) \text{ Å} \quad \text{Mo } K\alpha \text{ radiation} \]

\[ b = 7.9000 (10) \text{ Å} \quad \mu = 0.07 \text{ mm}^{-1} \]

\[ c = 12.7887 (6) \text{ Å} \quad T = 295 (2) \text{ K} \]

\[ \beta = 94.747 (5) ^\circ \]

\[ 0.5 \times 0.4 \times 0.3 \text{ mm} \]

**Data collection**

Enraf–Nonius CAD-4

diffraconeter

Absorption correction: none

1396 reflections with \( I > 2\sigma (I) \)

3 standard reflections

frequency: 120 min

intensity decay: 0.1%

2015 independent reflections

2015 measured reflections

**Refinement**

\[ R(F^2 > 2\sigma(F^2)) = 0.040 \]

\[ wR(F^2) = 0.104 \]

\[ S = 1.03 \]

\[ 197 \text{ parameters} \]

All H-atom parameters refined

\( \Delta \rho_{\text{max}} = 0.13 \text{ e Å}^{-3} \)

\( \Delta \rho_{\text{min}} = -0.1 \text{ e Å}^{-3} \)

**Table 1**

Hydrogen-bond geometry (Å, º).

\[ \text{Cg}1 \text{ is the centroid of the C4a/C9a/C9/C8a/C10a/C110 ring and Cg2 is the centroid of the C5/C6/C7/C8/C8a/C10a ring.} \]

\[ \begin{array}{cccc}
\text{D} & \text{H} & \cdot & \text{A} \\
\text{C5} & -\text{H}^5 & \cdot & \text{Cg1}^i \\
\text{C11} & -\text{H11A} & \cdots & \text{Cg2}^a \\
\text{C11} & -\text{H11B} & \cdots & \text{Cg1}^ii \\
\end{array} \]

\[ \begin{array}{cccc}
\text{D} & \text{H} & \cdot & \text{A} \\
0.98 (2) & 2.57 (2) & 3.496 (2) & 160 \\
1.02 (2) & 2.85 (2) & 3.563 (2) & 128 \\
1.01 (2) & 2.82 (2) & 3.550 (2) & 130 \\
\end{array} \]

Symmetry codes: (i) \(-x+2, y+\frac{1}{2}, -z+\frac{1}{2}\); (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 \( U_{	ext{iso}}(H) \) 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 \textit{Windows} (Farrugia, 1997); software used to prepare material for publication: \textit{WinGX} (Farrugia, 1999).

The authors thank the Turkish Ministry of Education and the CSU College of Graduate Studies for their support of this work.

**References**


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