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1,3-Bi-9-anthrylpropane

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1,3-Bi-9-anthrylpropane

The title compound, C_{31}H_{24}, with three molecules in the asymmetric unit. The crystal packing is mainly stabilized by weak C—H···π interactions in addition to van der Waals forces.

Comment

Bichromophoric model compounds of polyvinylanthracenes are extensively used in studies concerning the electrophotographic properties of polymers (Hayashi et al., 1976; Becker & Andersson, 1987; Becker et al., 1992). In pendant-type polymeric systems, photoconductivity depends largely on the spacing and orientation of the pendant units in the polymer backbone. The molecular geometries of 9,9′-bianthryl, bis-9-anthrylmethane (Becker et al., 1992) and 1,2-bis(9-anthryl)ethane (Becker et al., 1984) were determined in order to understand their photochemical and photophysical properties. We report here the crystal structure of the title compound, (I) (Fig. 1), as the third member of this family of bichromophoric model compounds of polyvinylanthracenes.

The crystal structure of compound (I) (Fig. 1) was solved in the non-centrosymmetric space group $P2_12_12_1$, with three independent molecules (A, B, and C) in the asymmetric unit. All six anthracene skeletons are essentially planar, the largest deviation from planarity of the fitted atoms being 0.088 (4) Å for atom C29b. The bond distances and angles of the anthracene rings in all three molecules are comparable with each other and with those of related molecules (Becker et al., 1984, 1992). The anthryl groups exhibit an anti–anti conformation along the connecting aliphatic chains. The dihedral angles formed by the anthracene planes are 61.00 (6)° in molecule A, 59.79 (6)° in molecule B and 69.85 (5)° in molecule C.

The crystal packing diagram (Fig. 2) reveals that the crystal structure of (I) is stabilized only by van der Waals forces and weak C—H···π interactions (Table 1). Although molecules with aromatic groups often pack in the solid state with parallel planar π systems, there are neither intra- nor intermolecular
The three independent molecules of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Experimental**

The title compound was prepared via LiAlH₄/AlCl₃ reduction of a mixture of 1,3-bis(9-anthryl)propan-1-one and 1,3-bis(9-anthryl)propan-1-ol, which were prepared according to the literature procedure (Becker & Andersson, 1983). First, AlCl₃ (3.3 g, 25 mmol) in propan-1-ol, which were prepared according to the literature procedure was added to a stirred solution of LiAlH₄ (0.95 g, 25 mmol) in diethyl ether (40 ml) in an ice bath, which was removed after the addition was complete. A mixture (2.15 g, 5.25 mmol) of 1,3-bis(9-anthryl)propan-1-ol and 1,3-bis(9-anthryl)propan-1-one (2:1 molar ratio) was dissolved in diethyl ether (50 ml) and a minimum amount of tetrahydrofuran (to increase solubility), and the solution was then added dropwise to the above LiAlH₄/AlCl₃ mixture and the reaction mixture refluxed for 2 h. After cooling, ethyl acetate (60 ml) and 20% H₂SO₄ (70 ml) were added to the reaction mixture to deactivate unreacted LiAlH₄. The mixture was extracted with dichloromethane and dried over sodium sulfate. The residue was obtained after vacuum evaporation of the solvents was purified by column chromatography on silica gel using hexane–dichloromethane (9:1 v/v) and crystallized from hexane–dichloromethane (1:1 v/v) to give 1.77 g (4.47 mmol, 82% yield) of (I) as yellow crystals (m.p. 468–469 K).

**Data collection**

Enraf–Nonius CAD-4 diffractometer

Absorption correction: none

6228 measured reflections

6228 independent reflections

Refinement

$R(F^2)$ = 0.044

wR(F²) = 0.103

S = 1.03

838 parameters

H-atom parameters constrained

$\Delta$ρ_{max} = 0.12 e Å⁻³

$\Delta$ρ_{min} = −0.10 e Å⁻³

### Table 1

<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>
<tbody>
<tr>
<td>C2α—H2α···Cg1</td>
<td>0.93</td>
<td>2.86</td>
<td>3.5722 (5)</td>
<td>135</td>
</tr>
<tr>
<td>C6c—H6c···Cg2</td>
<td>0.93</td>
<td>2.95</td>
<td>3.8708 (4)</td>
<td>170</td>
</tr>
<tr>
<td>C8b—H8b···Cg3β</td>
<td>0.93</td>
<td>2.82</td>
<td>3.7438 (6)</td>
<td>173</td>
</tr>
<tr>
<td>C8c—H8c···Cg4</td>
<td>0.93</td>
<td>2.80</td>
<td>3.6815 (5)</td>
<td>159</td>
</tr>
<tr>
<td>C17β—H17d···Cg5</td>
<td>0.97</td>
<td>2.90</td>
<td>3.8021 (4)</td>
<td>156</td>
</tr>
<tr>
<td>C17e—H17e···Cg6</td>
<td>0.97</td>
<td>2.90</td>
<td>3.8054 (4)</td>
<td>155</td>
</tr>
<tr>
<td>C23a—H23a···Cg7′′</td>
<td>0.93</td>
<td>2.59</td>
<td>3.5045 (5)</td>
<td>167</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) x + 1, y, z; (ii) x − 1/2, y + 1/2, −z; (iii) x − 1, y − 1/2, −z + 1/2; (iv) −x, y, z + 1/2.

All H atoms were positioned geometrically and allowed to ride on their corresponding parent atoms, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and with $U_{iso}$(H) = 1.2U_{eq}(C).

Data collection and cell refinement: CAD-4-PC Software (Enraf–Nonius, 1993); data reduction: DATR2 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 (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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**References**