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Bis[*N*-(9-anthrylmethyl)propylamino]methane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.061
wR factor = 0.198
Data-to-parameter ratio = 14.5

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

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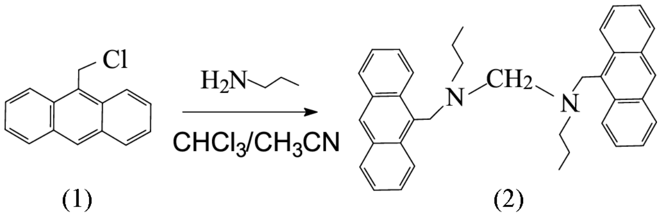
In the title compound, $C_{37}H_{38}N_2$, obtained by the reaction of 9-chloromethylanthracene and *n*-propylamine, two 9-anthracenemethylpropylamine moeties are linked through a methylene bridge. The two anthracene ring systems, and the two *n*-propyl groups, each lie in opposite directions.

Comment

The design of multicomponent fluorescent systems able to detect the presence and monitor concentration changes of protons is of considerable interest. Supramolecular systems based on the photochemical and photophysical properties of the anthracene ring have been investigated (de Silva *et al.*, 1997). As efficient fluorescent molecular sensors, amine compounds with anthracene chromophores are found to be sensitive in the detection of protons (Luigi & Antonio, 1995); therefore, this type of amine compound has attracted the attention of many researchers (Wang & Morawetz, 1976). We report here the synthesis and crystal structure of the title compound, (2).



(1) (2)

9-Chloromethylanthracene, when reacted with *n*-propylamine in $CHCl_3/CH_3CN$ solution, afforded a pale-yellow powder of (2). The molecular structure of (2) is illustrated in Fig. 1. The two 9-anthracenemethylpropylamine moieties are linked through a methylene bridge. The two anthracene ring systems, and the two *n*-propyl groups, lie in opposite directions, as shown in Fig. 1. The dihedral angle between the two anthracene ring systems is 0.9°, indicating that they lie in two nearly parallel planes. The N1—C1, N1—C2 and N1—C7 distances are 1.457 (4), 1.464 (4) and 1.485 (4) Å, respectively, and the C1—N1—C2, C1—N1—C7 and C2—N1—C7 bond angles are 113.2 (3), 110.0 (3) and 112.3 (3)°, respectively.

In the crystal structure of (2), the molecules are arranged in pairs, forming columns extending along the *c* axis (see Fig. 2).

Experimental

A $CHCl_3/CH_3CN$ suspension of 9-chloromethylanthracene (21.000 g, 0.091 mol) and *n*-propylamine (32.200 g, 0.546 mol), in the presence of K_2CO_3 (125.58 g, 0.910 mmol) and KI (4.550 g, 27.30 mmol), was stirred for 5 h at 303 K. After filtration, the solvent was removed with

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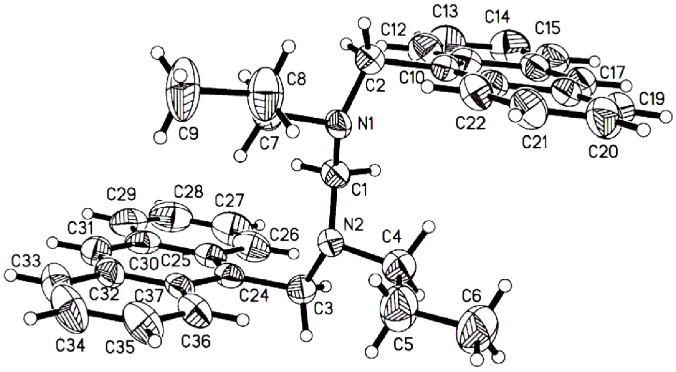

Figure 1
A view of (2), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

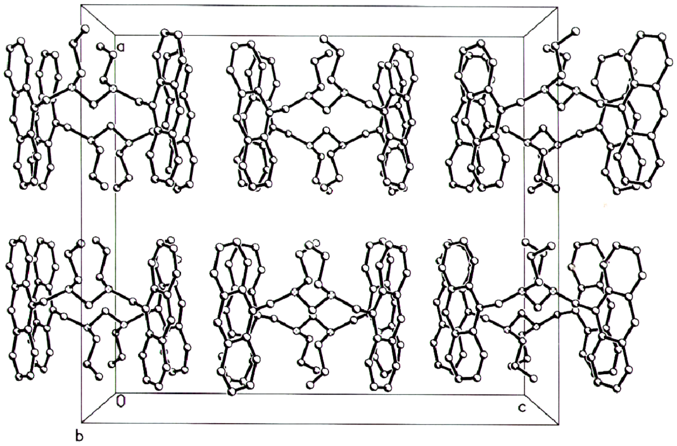

Figure 2
A view down the *b* axis of the packing arrangement in the crystal structure of (2). H atoms have been omitted for clarity.

a rotary evaporator and water (500 ml) was added. The mixture was extracted with CH_2Cl_2 (150 ml). The resulting solution was dried with anhydrous $MgSO_4$. After the solvent had been removed, an orange–yellow viscous liquid was obtained. The crude product was purified by column chromatography (SiO_2, acetone/petroleum ether 1:1) to give (2) as a yellow powder (3.318 g, 7%; m.p. 497–499 K). ^{1}H NMR (300 MHz, $CDCl_3$, p.p.m.): 0.59 (*t*, *J* = 7.2 Hz, 6H, CH_3), 1.77 (*m*, *J* = 7.2 Hz, 4H, CH_2), 2.60 (*t*, *J* = 7.2 Hz, 4H, CH_2), 4.57 (*s*, 4H, CH_2), 5.01 (*s*, 2H, CH_2), 7.24–8.35 (*m*, 18H, AnH) (An is anthracene). ^{13}C NMR (75 MHz, $CDCl_3$, p.p.m.): 1.90 (CH_3), 12.00 (CH_2), 20.33 (CH_2), 44.00 (CH_2), 50.85 (CH_2), 56.87 (CH_2), 123.4, 124.7, 125.3, 126.9, 128.9, 129.5, 130.6, 131.6 and 133.5 (AnC). Analysis calculated for $C_{37}H_{38}N_2$: C 87.02, H 7.50, N 5.49%; found: C 86.90, H 7.33, N 5.21%. Crystals suitable for X-ray analysis were obtained by slow evaporation of a CH_2Cl_2/CH_3CN solution at room temperature.

Crystal data

$C_{37}H_{38}N_2$
$M_r = 510.69$
Orthorhombic, *Pbca*
$a = 20.694$ (7) Å
$b = 12.031$ (4) Å
$c = 23.694$ (8) Å
$V = 5899$ (3) Å^3
$Z = 8$
$D_x = 1.150$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 625 reflections
$\theta = 2.1$–25.0°
$\mu = 0.07$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
22 761 measured reflections
5112 independent reflections

1878 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.132$
$\theta_{\rm max} = 25.0°$
$h = -24 \rightarrow 24$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.198$
$S = 0.99$
5112 reflections
352 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 2.0005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.002$
$\Delta\rho_{\rm max} = 0.13$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

All H atoms were initially located in difference Fourier maps. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in idealized positions and treated as riding atoms, with C—H distances in the range 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The prismatic crystal was of poor quality, leading to a rather high $R_{\rm int}$ value.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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