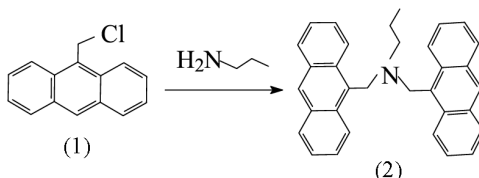# N,N-Bis(anthracen-9-ylmethyl)propylamine

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Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.077
wR factor = 0.208
Data-to-parameter ratio = 16.3

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

The title compound, $C_{33}H_{29}N$, was obtained by the reaction of 9-chloromethylanthracene and *n*-propylamine. Two anthracenylmethyl units are linked to the N atom of *n*-propylamine and the dihedral angle between the two anthracene systems is 64.3 (2)°.

Comment

Fluorescent sensors and switch systems play an important part in supramolecular chemistry, and the study of fluorescent sensors and switches of proton guests has been developing rapidly in recent years (de Silva *et al.*, 1997). The fluorescent intensity of amine compounds with anthracene chromophores can be effectively modulated by protonation (Luigi & Antonio, 1995). As a result, such amine compounds can be used to monitor acidic changes of water in rivers or lakes; this is of importance in the protection of the environment (Wang & Morawetz, 1976). We report here the synthesis and crystal structure of bis(9-anthracenemethyl)propylamine, (2).

9-Chloromethylanthracene reacted with *n*-propylamine in benzene solution to afford a pale-yellow powder of (2). In (2), two anthracenylmethyl units are linked to the N atom of *n*-propylamine, and the dihedral angle between the two anthracene systems is 64.3 (2)° (Fig. 1). Selected bond lengths and angles are given in Table 1.

Experimental

A benzene suspension of 9-chloromethylanthracene (21.000 g, 0.091 mol), (1), and *n*-propylamine (2.685 g, 0.046 mol) in the presence of K_2CO_3 (125.580 g, 0.910 mmol) and KI (4.550 g, 27.300 mmol) was stirred for 5 h at 303 K. After filtering, the solvent was removed using a rotary evaporator, and water (500 ml) was added, then the mixture was extracted with CH_2Cl_2 (150 ml). The extracted solution was dried with anhydrous $MgSO_4$. After the solvent was 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 a pale-yellow powder, (2) [16.304 g, 40%; m.p. 555–557 K (decomposition)]. Crystals of (2) suitable for X-ray diffraction were obtained by evaporating slowly a CH_3CN solution at room temperature. ^{1}H NMR (300 MHZ, CDCl$_3$): δ 0.50 (*t*, *J* = 7.2 Hz, 3H, CH$_3$), 1.63 (*m*, *J* = 7.2 Hz, 2H, CH$_2$), 2.53 (*t*, *J* = 7.2 Hz, 2H, CH$_2$), 4.58 (*s*, 2H, CH$_2$), 7.29 (*t*, *J* = 7.5 Hz, 4H, AnH),
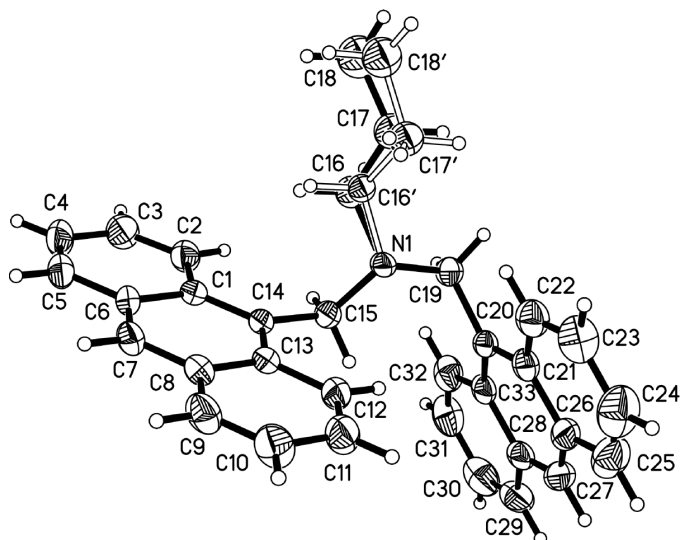
Figure 1
A view of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Both disorder components are shown.
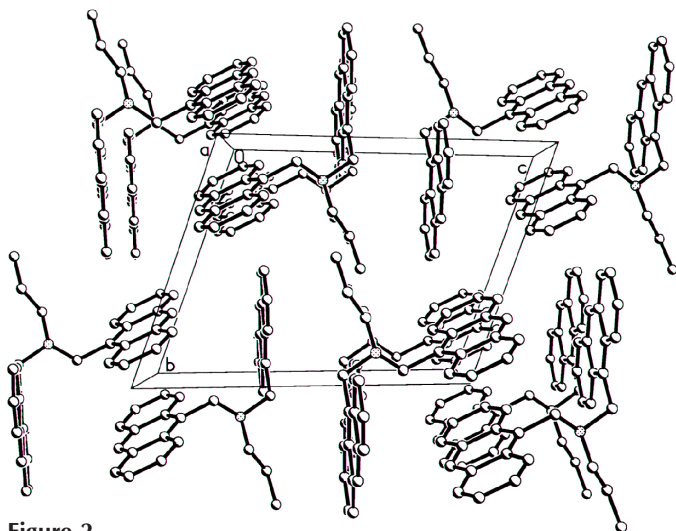

Figure 2
A view, down the *b* axis, of the packing arrangement in the crystal structure. H atoms have been omitted.

7.47 (*t*, *J* = 7.5 Hz, 4H, AnH), 8.06 (*d*, *J* = 7.5 Hz, 4H, AnH), 8.36 (*d*, *J* = 7.5 Hz, 4H, AnH), 8.56 (*s*, 2H, AnH); ^{13}C NMR (75 MHz, CDCl$_3$): δ 1.94 (CH$_3$), 12.00 (CH$_2$), 20.31(CH$_2$), 50.81(CH$_2$), 56.80(CH$_2$), 124.8, 125.2, 125.4, 127.4, 128.9, 130.5, 131.4 and 131.5 (AnC). Analysis calculated for C$_{33}$H$_{29}$N: C 90.17, H 6.65, N 3.19%; found: C 89.80, H 6.85, N 3.29%.

Crystal data

C$_{33}$H$_{29}$N	$Z = 2$
$M_r = 439.57$	$D_x = 1.193$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.891\ (4)$ Å	Cell parameters from 689
$b = 10.188\ (4)$ Å	reflections
$c = 13.592\ (5)$ Å	$\theta = 2.3$–22.3°
$\alpha = 106.179\ (7)°$	$\mu = 0.07$ mm^{-1}
$\beta = 106.822\ (7)°$	$T = 293\ (2)$ K
$\gamma = 97.750\ (7)°$	Block, yellow
$V = 1224.1\ (7)$ Å^3	$0.32 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer	4975 independent reflections
	2036 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan	$\theta_{max} = 26.5°$
(*SADABS*; Sheldrick, 1996)	$h = -10 \rightarrow 12$
$T_{min} = 0.881$, $T_{max} = 0.990$	$k = -12 \rightarrow 9$
7130 measured reflections	$l = -15 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0803P)^2]$
$wR(F^2) = 0.208$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4975 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
305 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C15	1.465 (4)	N1—C16	1.508 (7)
N1—C19	1.469 (3)		
C15—N1—C19	111.0 (2)	C19—N1—C16	106.5 (5)
C15—N1—C16	102.2 (5)		

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). The *n*-Pr group showed disorder and was modelled over two sites, with occupancies of 0.621 (14) and 0.379 (14). The partially occupied C atoms were refined with isotropic displacement parameters and the C—C distances were restrained to 1.52 (1) Å.

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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