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9,10-Bis(dichloroethylaminomethyl)anthracene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.089
Data-to-parameter ratio = 15.3

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

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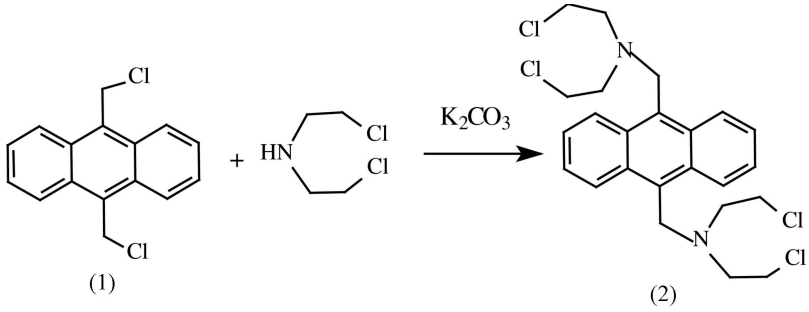
The title compound, $C_{24}H_{28}Cl_4N_2$, was obtained by the reaction of 9,10-dichloromethylanthracene and dichloroethylamine. The molecule is centrosymmetric, with the substituents above and below the anthracene plane.

Comment

Fluorescent chemosensors constitute an important aspect of supramolecular chemistry (de Silver *et al.*, 1997). Many of these fluorescent sensors with an anthracene ring system have been designed and investigated (Gunnlaugsson *et al.*, 2002). Amine compounds with anthracene chromophores have attracted considerable attention in the past decade owing to their capability to monitor acidic changes of water in rivers (Luigi & Antonio, 1995). We report here the synthesis and crystal structure of the title compound, (2).



The molecule of (2) is centrosymmetric, with the substituents above and below the anthracene ring plane (Fig. 1). The

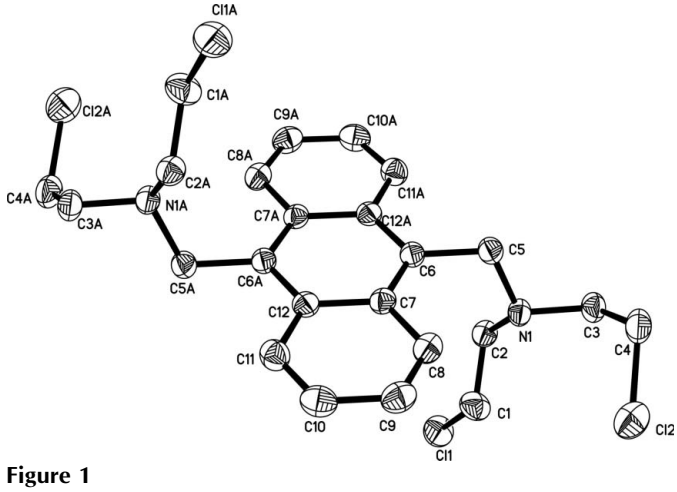


Figure 1
A view of (2), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry code: (A) $-x, 1-y, 1-z$.]

N—C bond lengths [1.459 (2), 1.452 (2) and 1.466 (2) Å] are similar to those [1.509 (6) and 1.494 (6) Å] of 9,10-dibenzylaminemethylanthracene (Chang *et al.*, 2000).

Experimental

To a toluene (100 ml) solution of 9,10-dichloromethylanthracene (5.00 g, 0.018 mol) were added dichloroethylamine (15.49 g, 0.109 mol) and K_2CO_3 (24.80 g, 0.180 mol) and the solution was stirred for 6 h at 353 K. The toluene solution was washed with water (150 ml) and dried with anhydrous $MgSO_4$, then concentrated to 40 ml; hexane (5 ml) was added to give a yellow solid (yield: 7.20 g, 81.4%; m.p. 535–537 K). Crystals of (2) suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature. Analysis calculated for $C_{24}H_{28}Cl_4N_2$: C 59.28, H 5.80, Cl 29.16, N 5.76%; found C 59.11, H 5.34, Cl 28.96, N 5.42%.

Crystal data

$C_{24}H_{28}Cl_4N_2$
M_r = 486.28
Monoclinic, $P2_1/c$
a = 13.3505 (12) Å
b = 10.6953 (10) Å
c = 8.3412 (8) Å
β = 92.879 (1)°
V = 1189.52 (19) Å^3
Z = 2
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 293 (2) K
Block, yellow
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.891, T_{max} = 0.921
6278 measured reflections
2093 independent reflections
1669 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.089
S = 1.07
2093 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.408P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0134 (15)

All H atoms were initially located in a difference Fourier map, but were then constrained to an ideal geometry, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and refined as riding on their parent atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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