# (9-Anthrylmethyl)trimethylammonium chloride monohydrate

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Key indicators

Single-crystal X-ray study

T = 148 K

Mean σ(C–C) = 0.008 Å

R factor = 0.044

wR factor = 0.054

Data-to-parameter ratio = 8.3

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

The title compound, $C_{18}H_{20}N^+\cdot Cl^-\cdot H_2O$, contains a tetra-alkylammonium chloride functionality bound to an anthryl moiety. There are two formula units in the asymmetric unit of the crystal structure, with a dihedral angle of 22.55 (1)° between the anthryl planes.

Comment

The behavior of anthracene and its derivatives plays a large role in many areas of chemistry including nanoscience (Zhang *et al.*, 2003), organometallic chemistry (Carano *et al.*, 2001), asymmetric organic synthesis (Corey *et al.*, 1997), and biochemical probes (Ihmels *et al.*, 2000; Becker & Norden, 2000). The title compound, (I), has been synthesized from the substitution reaction of trimethylamine and 9-(chloromethyl)anthracene (Takagi *et al.*, 1983) and recrystallized from acetonitrile.

(I)
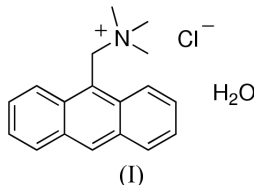
The compound crystallizes with two cations, two anions, and two water molecules in the asymmetric unit. The cationic N atoms have tetrahedral geometry and form ion pairs with the chloride counter-ions. The N···Cl distances [N1···Cl1 = 3.99 (1) Å and N2···Cl2 = 4.03 (1) Å] are consistent with reported values in similar compounds (for a recent example, see Corey *et al.*, 1997). Each chloride ion is hydrogen bonded to two water molecules, one in the asymmetric unit and one symmetry-related water molecule, with distances Cl1···O1 = 3.190 (5) Å, Cl1···O1′ = 3.178 (6) Å, Cl2···O2 = 3.191 (5) Å and Cl2···O2″ = 3.158 (4) Å.

The closest contact between the two anthryl moieties within the asymmetric unit is C3···C29, 3.427 (8) Å. The dihedral angle between the anthracene planes is 22.55 (1)°, indicative of little or no π-stacking. A similar anthracene derivative has been reported (Le Magueres *et al.*, 2000). This previously reported structure exhibits a dihedral angle between layers (23°) that is similar to that observed here between cations.

Experimental

The synthesis of (I) has been described in the literature (Takagi *et al.*, 1983). Suitable crystals were obtained by slow evaporation of a saturated solution of (I) in wet acetonitrile.

Crystal data

$C_{18}H_{20}N^+·Cl^-·H_2O$
$M_r = 303.83$
Monoclinic, $P2_1$
$a = 8.1368 (6)$ Å
$b = 10.2645 (8)$ Å
$c = 19.351 (2)$ Å
$\beta = 92.088 (1)°$
$V = 1615.1 (2)$ Å^3
$Z = 4$

$D_x = 1.249$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3212
  reflections
$\theta = 2.5–24.3°$
$\mu = 0.24$ mm^{-1}
$T = 148.2$ K
Tablet, yellow
$0.23 \times 0.15 \times 0.12$ mm

Data collection

SMART 1K CCD diffractometer
ω scans
Absorption correction: multi-scan
  (Blessing, 1995)
  $T_{min} = 0.80$, $T_{max} = 0.97$
7199 measured reflections
4282 independent reflections

3143 reflections with $F^2 > 3\sigma(F^2)$
$R_{int} = 0.057$
$\theta_{max} = 24.7°$
$h = -9 \rightarrow 8$
$k = -11 \rightarrow 10$
$l = -22 \rightarrow 22$

Refinement

Refinement on F
$R = 0.044$
$wR = 0.054$
$S = 1.54$
3143 reflections
378 parameters
H atoms treated by a mixture of
  independent and constrained
  refinement

$(\Delta/\sigma)_{max} = 0.007$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Absolute structure: Flack (1983),
  4282 Friedel pairs
Flack parameter = 0.18 (8)

Table 1
Selected geometric parameters (Å, °).

N1—C15	1.539 (6)	N2—C33	1.535 (6)
N1—C16	1.488 (6)	N2—C34	1.492 (7)
N1—C17	1.495 (6)	N2—C35	1.503 (6)
N1—C18	1.503 (6)	N2—C36	1.490 (7)
C15—N1—C16	113.4 (3)	C33—N2—C35	107.5 (4)
C15—N1—C17	107.6 (3)	C33—N2—C36	112.7 (4)
C15—N1—C18	109.8 (4)	C34—N2—C35	108.7 (4)
C16—N1—C17	109.0 (4)	C34—N2—C36	108.2 (4)
C16—N1—C18	108.5 (4)	C35—N2—C36	108.7 (4)
C17—N1—C18	108.4 (4)	N1—C15—C1	114.7 (3)
C33—N2—C34	110.9 (4)	N2—C33—C19	116.3 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H43$\cdots$Cl1	0.83 (6)	2.44 (6)	3.190 (5)	150 (8)
O1—H44$\cdots$Cl1^i	1.05 (6)	2.25 (6)	3.185 (5)	148 (4)
O2—H41$\cdots$Cl2^{ii}	1.10 (5)	2.10 (5)	3.159 (4)	163 (4)
O2—H42$\cdots$Cl2	0.89 (5)	2.33 (5)	3.191 (5)	165 (4)

Symmetry codes: (i) $-2 - x, \frac{1}{2} + y, -z$; (ii) $-1 - x, y - \frac{1}{2}, -1 - z$.

The water H atoms were located in a difference Fourier map and their positions were refined. All other H atoms were calculated geometrically and not refined. Assignment of the correct enantio-
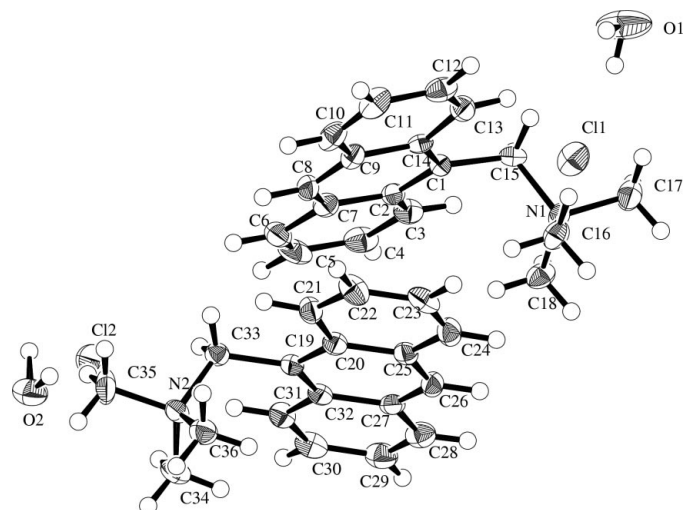

Figure 1
The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

morph was accomplished by comparison of the intensities of Friedel pairs of reflections. The correct enantiomorph is shown in Fig. 1.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN*; molecular graphics: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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