The molecular structure is presented in Fig. 1 and Fig. 2 shows the molecular packing.

Related literature. This study represents the first in a series of acridines containing 9-alkyl or aryl substituents which we are studying. These acridines are being linked to oligonucleotides in hopes of synthesizing new anti-AIDS or anti-cancer agents. The crystal studies provide important information which will form the basis for molecular modeling studies. Of special interest is the fact that the absolute values of the torsion angles in the two molecules are 98·32, 63·20° and 97·22, 62·11° (for C8*a*—C9—C11—C12 and C9—C11—C12—O12) and are virtually identical, showing the similarity in the conformation of the two molecules per asymmetric unit. Few 9-alkyl or 9-aryl acridines have been studied crystallographically. Pett, Rossi, Glusker, Stezowski & Bogucka-Ledochowska (1982) have reported the structure of 9-methyl-1-nitroacridine. Berman & Neidle (1979) have reviewed the structural studies of acridine intercalators.

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Structure of Phenethylamine Hydrochloride

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Abstract. Phenethylammonium chloride, $C_8H_{12}N^+.Cl^-$, $M_r = 157{\cdot}6$, orthorhombic, $P2_12_12_1$, $a = 4{\cdot}603$ (1), $b = 5{\cdot}906$ (1), $c = 32{\cdot}360$ (2) Å, $V = 880$ (1) Å^3, $D_x = 1{\cdot}190$ Mg m^{-3} for $Z = 4$, Mo $K\bar{\alpha}$ radiation, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}318$ mm^{-1}, $F(000) = 336$, $T = 293$ (2) K, $R = 0{\cdot}036$ for 724 observed reflections. The crystal structure determination of the title compound shows that the ethylamine side chain is fully extended and the C(6)—C(1)—C(7)—C(8) torsion angle is −70°. Each of the three ammonium H atoms forms significant intermolecular contacts with symmetry-related chloride anions such that Cl···H are 2·35, 2·27 and 2·20 Å.

Experimental. Phenethylamine was isolated from *Acacia iteaphylla*, a tall spreading shrub endemic to South Australia. Leaf tissue was extracted with methanol/water (70:30 v/v) and after removal of the methanol component (reduced pressure) the extract was subjected to ion-exchange chromatography on a column containing DOWEX 50W (H^+ form) resin. After washing the column with water phenethylamine was eluted with 4*M* HCl. The product was identified from both its ^{1}H [90 MHz, D_2O, pH 1·5; δ 7·56 (5H), 3·24 (2H) and 3·06 (2H), ref. *tert*-BuOH δ 1·245] and ^{13}C (22·5 MHz, D_2O, pH 1·5, ^{1}H decoupled, δ 139·45, 131·86, 131·70, 130·18, 43·39 and 35·54, ref. *tert*-BuOH δ 32·45) NMR spectra. Suitable crystals for X-ray study obtained from the slow evaporation of a methanol/diethyl ether solution of the compound; colourless needles, m.p. 493–494 K. Enraf–Nonius CAD-4F diffractometer controlled by a PDP8/A computer, graphite-monochromated Mo $K\bar{\alpha}$ radia-

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and* B_{eq} *values* (Å^2)

$$B_{eq} = 8\pi^2/3(U_{11} + U_{22} + U_{33}).$$

	x	y	z	B_{eq}
Cl(1)	3722 (3)	5692 (2)	2112 (1)	3·77
C(1)	−1042 (10)	−70 (7)	1048 (1)	4·04
C(2)	−1424 (13)	1555 (9)	747 (2)	5·05
C(3)	−3212 (14)	1169 (11)	407 (2)	6·01
C(4)	−4625 (13)	−851 (14)	369 (2)	6·79
C(5)	−4297 (15)	−2486 (12)	662 (2)	6·12
C(6)	−2471 (11)	−2107 (9)	1001 (2)	5·17
C(7)	897 (11)	369 (10)	1414 (2)	4·44
C(8)	−853 (9)	602 (9)	1802 (1)	3·62
N(1)	1062 (8)	749 (7)	2171 (1)	3·50

Table 2. *Selected interatomic distances* (Å) *and bond angles* (°)

C(1)—C(2)	1·380 (6)	C(1)—C(6)	1·379 (6)
C(1)—C(7)	1·505 (6)	C(2)—C(3)	1·391 (8)
C(3)—C(4)	1·364 (9)	C(4)—C(5)	1·364 (9)
C(5)—C(6)	1·399 (8)	C(7)—C(8)	1·499 (6)
C(8)—N(1)	1·486 (5)		
C(2)—C(1)—C(6)	117·9 (5)	C(2)—C(1)—C(7)	120·8 (5)
C(6)—C(1)—C(7)	121·3 (5)	C(1)—C(7)—C(8)	110·9 (4)
C(7)—C(8)—N(1)	111·1 (3)		

tion; $\omega/2\theta$ scan technique. Cell parameters on crystal $0{\cdot}15 \times 0{\cdot}20 \times 0{\cdot}60$ mm from a least-squares procedure on 25 reflections ($10 \leq \theta \leq 13°$). No absorption correction applied (Sheldrick, 1976). Total of 1047 reflections ($1 \leq \theta \leq 25{\cdot}0°$) measured in the range $0 \leq h \leq 5$, $0 \leq k \leq 7$, $0 \leq l \leq 38$; some Friedel pairs also included. No significant variation in the net intensities of two reference reflections (2,1,13 and 129) measured every 7200 s. 960 unique reflections ($R_{\rm amal}$ 0·019)* and 724 satisfied $I \geq 2{\cdot}5\sigma(I)$. Structure solved by direct methods (Sheldrick, 1986), full-matrix least-squares refinement of 139 parameters based on F (Sheldrick, 1976). Anisotropic thermal parameters for non-H atoms and H atoms refined with isotropic thermal parameters. At convergence $R = 0{\cdot}036$ (preferred chirality), $wR = 0{\cdot}035$, $w = 2{\cdot}71/[\sigma^2(F) + 0{\cdot}0002F^2]$, $S = 2{\cdot}5$, $(\Delta/\sigma)_{\rm max} \leq 0{\cdot}001$, $(\Delta\rho)_{\rm max} = 0{\cdot}18$, $(\Delta\rho)_{\rm min} = -0{\cdot}18$ e Å^{-3}; no extinction correction. Scattering factors for all atoms given in *SHELX76* (Sheldrick, 1976). All calculations on SUN4/280 computer system. Atomic parameters given in Table 1, selected bond distances and angles in Table 2,† the numbering scheme used is shown in Fig. 1, and a unit-cell diagram is shown in Fig. 2.

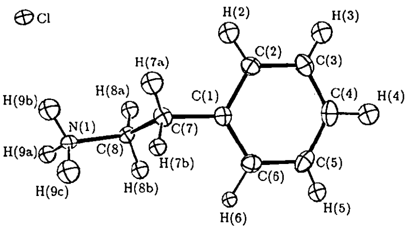

Fig. 1. Molecular structure and numbering scheme for phenethylamine hydrochloride drawn at 25% probability levels (Johnson, 1971).

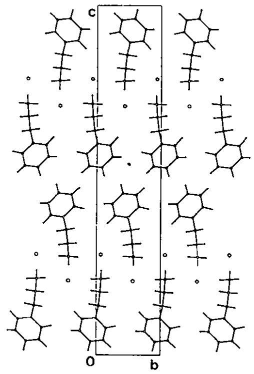

Fig. 2. Unit-cell contents for phenethylamine hydrochloride viewed down the *a* axis (Motherwell, 1976).

Related literature. This report represents a redetermination of the title compound by contemporary methods (Tsoucaris, 1961). Phenethylamine occurs widely in algae, fungi and higher plants (Smith, 1977) and relatively high concentrations of the compound have been reported to occur in Acacias (White, 1944). These high concentrations are associated with a distinct morphological group of *Acacia* (White, 1944) and in *Acacia iteaphylla* phenethylamine concentrations of up to 7% have been observed (Naiola, Jones & Paleg, 1989).

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* $R_{\rm amal} = (\sum\{N\sum[W(F_{\rm mean} - F)^2]\}/\sum[(N-1)\sum(WF^2)])^{1/2}$; the inner summations are over N equivalent reflections and are averaged to give $F_{\rm mean}$, the outer summations are over all unique reflections and the weight W is taken as $[\sigma(F)]^{-2}$.

† Lists of structure factors, H-atom parameters, thermal parameters and all bond distances and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52827 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.