

Fig. 1. Molecular structure and numbering scheme for the title compound.

eters. 2983 unique reflections, $R_{\text{int}} = 0.025$, 2515 with $F > 4\sigma(F)$. At convergence $R = 0.040$, $wR = 0.049$ (on all data $R = 0.049$, $wR = 0.050$), $S = 1.73$ for 217 parameters, $w = [\sigma^2(F) + 0.0004F^2]^{-1}$, $\Delta/\sigma < 0.001$, data/parameter ratio 11.6:1, $(\Delta\rho)_{\text{max}} = 0.26$, $(\Delta\rho)_{\text{min}} = -0.58 \text{ e } \text{\AA}^{-3}$. Scattering factors for all atoms from *SHELXTL-Plus* (Sheldrick, 1988).

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9-Acridineethanol

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Abstract. $\text{C}_{15}\text{H}_{13}\text{NO}$, $M_r = 223.28$, triclinic, $P\bar{1}$, $a = 7.537$ (4), $b = 9.283$ (5), $c = 16.408$ (4) \AA , $\alpha = 87.50$ (3), $\beta = 83.44$ (3), $\gamma = 79.04$ (3) $^\circ$, $V = 1119$ (1) \AA^3 , $Z = 4$, $D_x = 1.325 \text{ g cm}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.71069 \text{ \AA}$, $\mu = 0.78 \text{ cm}^{-1}$, $F(000) = 472$, $T = 293 \text{ K}$, $R = 0.039$ for 1697 observed reflections. The two molecules per asymmetric unit are in virtually the same conformation. The acridine ring has the expected structure, but the side chain is in the *gauche* conformation. The acridine rings are stacked in pairs held together by hydrogen bonds involving the alcohol functionality and the nitrogen of the acridine ring.

Experimental. Crystals of the synthetic compound were prepared by reacting 9-methylacridine with formaldehyde following published procedures

Atomic parameters are given in Table 1,* bond distances and angles in Table 2, and Fig. 1 shows the molecule together with the atomic numbering scheme used.

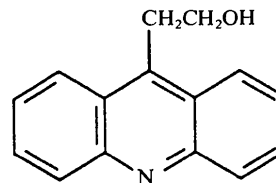
Related literature. The cycloaddition reaction of chromone and diphenylnitrilimine resulted in the formation of the corresponding oxadiazole (Shawali, Eltawil & Albar, 1984).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52648 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(Eisleb, 1936). Crystal: $0.59 \times 0.15 \times 0.14 \text{ mm}$, amber needle from ethyl acetate. Data collected using ω - 2θ scan techniques; scan rate varied from 2 to $20^\circ \text{ min}^{-1}$ (in ω); 2915 intensities recorded on an



Enraf-Nonius CAD-4 diffractometer with graphite-monochromated $\text{Mo } K\alpha$ radiation, $2\theta_{\text{max}} = 45^\circ$, $-7 \geq h \geq 8$, $-9 \geq k \geq 9$, $0 \geq l \geq 17$. Three check reflections measured every 97 reflections, 2% intensity

Table 1. Atom coordinates and isotropic temperature factors

	x	y	z	B* (Å ²)
O(12)	0-0179 (3)	0-2752 (2)	0-8330 (1)	5-36 (6)
O(12')	0-4236 (3)	0-7831 (2)	0-3374 (1)	5-60 (6)
N(10)	0-1888 (3)	-0-0806 (3)	1-0670 (1)	4-09 (6)
N(10')	0-3189 (3)	0-4151 (3)	0-5662 (1)	4-06 (6)
C(1)	0-4379 (4)	-0-1252 (4)	0-8588 (2)	4-52 (8)
C(2)	0-4742 (4)	-0-2740 (4)	0-8567 (2)	5-09 (8)
C(3)	0-4137 (4)	-0-3598 (4)	0-9236 (2)	5-36 (9)
C(4)	0-3195 (4)	-0-2931 (4)	0-9914 (2)	4-68 (8)
C(5)	0-0646 (4)	0-1257 (4)	1-1480 (2)	4-45 (8)
C(6)	0-0263 (4)	0-2722 (4)	1-1596 (2)	5-01 (8)
C(7)	0-0753 (4)	0-3685 (4)	1-0955 (2)	4-97 (8)
C(8)	0-1588 (4)	0-3168 (3)	1-0223 (2)	4-43 (8)
C(9)	0-2950 (3)	0-1019 (3)	0-9344 (2)	3-78 (7)
C(11)	0-2018 (4)	0-3714 (4)	0-3568 (2)	4-81 (8)
C(11')	0-3375 (4)	0-1985 (4)	0-8609 (2)	4-54 (8)
C(12)	0-1960 (4)	0-2082 (4)	0-7995 (2)	5-09 (8)
C(2')	0-2430 (4)	0-2232 (4)	0-3530 (2)	5-28 (8)
C(3')	0-3112 (4)	0-1372 (4)	0-4194 (2)	5-37 (9)
C(4')	0-3338 (4)	0-2029 (4)	0-4885 (2)	4-82 (8)
C(4a)	0-2806 (3)	-0-1383 (3)	0-9970 (2)	3-81 (7)
C(5')	0-3056 (4)	0-6210 (4)	0-6480 (2)	4-55 (8)
C(6')	0-2694 (4)	0-7676 (4)	0-6593 (2)	5-14 (8)
C(7')	0-2016 (4)	0-8651 (4)	0-5970 (2)	5-18 (9)
C(8')	0-1737 (4)	0-8117 (4)	0-5244 (2)	4-66 (8)
C(8a)	0-2044 (3)	0-1632 (3)	1-0080 (2)	3-60 (7)
C(9')	0-1875 (3)	0-5986 (3)	0-4348 (2)	3-84 (7)
C(9a)	0-3383 (3)	-0-0508 (3)	0-9291 (2)	3-71 (7)
C(10a)	0-1553 (3)	0-0665 (3)	1-0729 (2)	3-67 (7)
C(11')	0-1322 (4)	0-6968 (4)	0-3626 (2)	4-81 (8)
C(12')	0-2976 (4)	0-7151 (4)	0-3021 (2)	5-18 (8)
C(4a')	0-2906 (3)	0-3575 (3)	0-4955 (2)	3-88 (7)
C(8a')	0-2110 (3)	0-6586 (3)	0-5092 (2)	3-84 (7)
C(9a')	0-2244 (3)	0-4462 (3)	0-4282 (2)	3-81 (7)
C(10a')	0-2774 (4)	0-5616 (3)	0-5731 (2)	3-89 (7)

* Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as: $B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. Bond lengths (Å) between non-H atoms with e.s.d.'s in parentheses

O(12)—C(12)	1-426 (4)	C(1')—C(2')	1-354 (5)
O(12')—C(12')	1-421 (4)	C(1')—C(9a')	1-430 (4)
N(10)—C(4a)	1-347 (4)	C(11)—C(12)	1-537 (4)
N(10)—C(10a)	1-346 (4)	C(2')—C(3')	1-409 (5)
N(10')—C(4a')	1-353 (4)	C(3')—C(4')	1-353 (5)
N(10')—C(10a')	1-343 (4)	C(4')—C(4a')	1-417 (5)
C(1)—C(2)	1-357 (5)	C(4a)—C(9a)	1-426 (4)
C(1)—C(9a)	1-431 (4)	C(5')—C(6')	1-353 (5)
C(2)—C(3)	1-413 (5)	C(5')—C(10a')	1-422 (4)
C(3)—C(4)	1-355 (5)	C(6')—C(7')	1-409 (5)
C(4)—C(4a)	1-416 (5)	C(7')—C(8')	1-363 (5)
C(5)—C(6)	1-352 (5)	C(8')—C(8a')	1-422 (5)
C(5)—C(10a)	1-417 (4)	C(8a)—C(10a)	1-425 (4)
C(6)—C(7)	1-413 (5)	C(9')—C(11')	1-511 (4)
C(7)—C(8)	1-353 (5)	C(9')—C(8a')	1-407 (4)
C(8)—C(8a)	1-425 (4)	C(9')—C(9a')	1-395 (4)
C(9)—C(11)	1-512 (4)	C(11')—C(12')	1-534 (4)
C(9)—C(8a)	1-404 (4)	C(4a')—C(9a')	1-427 (4)
C(9)—C(9a)	1-398 (4)	C(8a')—C(10a')	1-424 (4)

change. All of the 2915 reflections collected were unique, 1697 with $I > 3.0\sigma(I)$ used for all calculations [program systems *SHELX86* (Sheldrick, 1986) and Enraf-Nonius *SDP* (Enraf-Nonius, 1979)]. Cell constants refined from 25 reflections in the range $17 < \theta < 19^\circ$. No correction for absorption or extinction.

Structure solution by random-start multiresolution direct methods. The final cycle of refinement on $|F|$ included 307 variable parameters and converged (largest parameter shift was 0.00 times its e.s.d.) with

$R = 0.039$, $wR = 0.046$ and $S = 1.042$ (all non-H atoms anisotropic; H atoms were not refined, placed in calculated positions). Weighting scheme defined as in the Killean & Lawrence (1969) method with terms of 0.02 and 1.0. Maximum $\Delta/\sigma = 0.00$. Maximum height on the Fourier ΔF map $\rho = 0.20 \text{ e \AA}^{-3}$. Atomic scattering factors from Cromer & Waber (1974).

Table 1 lists atomic coordinates and isotropic temperature factors and Table 2 gives bond lengths.*

* Lists of structure factors, anisotropic thermal parameters, bond angles and torsion angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52756 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

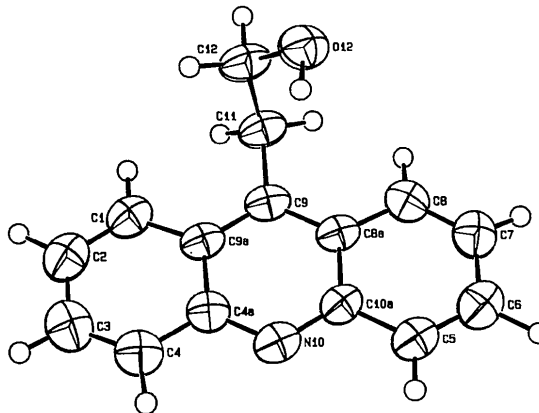


Fig. 1. View of the molecule showing the atomic labeling scheme (the second molecule in the asymmetric unit is labeled with primes). Thermal ellipsoids are scaled to the 50% probability level.

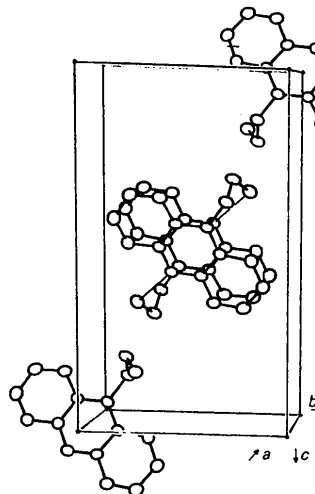


Fig. 2. View of the molecular packing. The axes are shown on the drawing.

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 C8a—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, $C_8H_{12}N^+.Cl^-$, $M_r = 157.6$, orthorhombic, $P2_12_12_1$, $a = 4.603$ (1), $b = 5.906$ (1), $c = 32.360$ (2) Å, $V = 880$ (1) Å³, $D_x = 1.190$ Mg m⁻³ for $Z = 4$, Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å, $\mu = 0.318$ mm⁻¹, $F(000) = 336$, $T = 293$ (2) K, $R = 0.036$ 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 $Cl \cdots H$ 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 4M HCl. The product was identified from both its ¹H [90 MHz, D₂O, pH 1.5; δ 7.56 (5H), 3.24 (2H) and 3.06 (2H), ref. *tert*-BuOH δ 1.245] and ¹³C (22.5 MHz, D₂O, pH 1.5, ¹H 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 $K\alpha$ radi-