Discussion. Final positional parameters for the non-H atoms are listed in Table 1, bond lengths and bond angles in Table 2. A *PLUTO* (Motherwell & Clegg, 1978) drawing of the molecule is given in Fig. 1 and the Newman projection along the C(9)—C(1′) bond in Fig. 2. A least-squares plane through the acridinium atoms shows that the maximum distance from the plane is 0·095 Å [C(2)]. N(10) lies 0·085, C(6) 0·085 and C(9) 0·078 Å from the plane, all other distances are less than 0·061 Å. The phenyl ring is planar {max. distance from the best plane is 0·014 Å [C(3′)]}. The angle between the two planes is 72°.

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Crystal Studies of Acridinium Dyes. III. 10-Methyl-9-(2-methylphenyl)acridinium Perchlorate

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Abstract. $C_{21}H_{18}N^+.ClO_4^-$, $M_r = 383·8$, monoclinic, $P2_1/a$, $a = 14·738\,(2)$, $b = 11·866\,(2)$, $c = 11·041\,(2)$ Å, $\beta = 105·75\,(2)°$, $V = 1858·4\,(6)$ Å^3, $Z = 4$, $D_x = 1·37$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0·71069$ Å, $\mu = 2·28$ cm^{-1}, $F(000) = 800$, room temperature. Final $R = 0·066$ for 1830 observed reflections. The acridinium group and phenyl ring are each nearly planar. The angle between the acridinium plane and the phenyl ring is 76°. There are no unusual bond lengths or angles.

Introduction. The title compound is the third structure in a series of acridinium dyes [I: Goubitz, Reiss, Heijdenrijk, Jonker & Verhoeven (1989); II: Reiss, Goubitz & Heijdenrijk (1989)]. In the structure here presented the phenyl ring is substituted with a methyl group.

Experimental. A bright-yellow cubic-shaped crystal (dimensions 0·30 × 0·30 × 0·30 mm approximately) was used for data collection on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Mo $K\alpha$ radiation and θ–2θ scan. A total of 3862 reflections was measured within the range $-18 \le h \le 18$, $0 \le k \le 14$, $0 \le l \le 13$. Of these, 1830 were above the significance level of $2·5\sigma(I)$. The maximum value of $(\sin\theta)/\lambda$ was 0·61 Å^{-1}. Two standard reflections (021, 201) were measured hourly, the intensity decrease was 4·6% during 43 h collection time. Unit-cell parameters were refined by a least-

Table 1. *Fractional coordinates of the non*-H *atoms and equivalent isotropic thermal parameters*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	y	U_{eq} (Å^2)
Cl	0·3611 (1)	0·7971 (1)	0·3894 (1)	0·0694 (9)
C(1)	0·3063 (4)	1·2380 (5)	0·2828 (5)	0·058 (3)
C(2)	0·3859 (4)	1·2725 (5)	0·3670 (5)	0·067 (4)
C(3)	0·3850 (4)	1·3793 (6)	0·4258 (5)	0·075 (4)
C(4)	0·3084 (4)	1·4443 (5)	0·4021 (5)	0·066 (4)
C(5)	−0·0238 (4)	1·5021 (5)	0·1840 (6)	0·069 (4)
C(6)	−0·1019 (4)	1·4693 (5)	0·0957 (6)	0·076 (4)
C(7)	−0·1028 (4)	1·3710 (6)	0·0247 (6)	0·070 (4)
C(8)	−0·0242 (4)	1·3064 (5)	0·0464 (5)	0·056 (3)
C(9)	−0·1404 (3)	1·2693 (4)	0·1629 (4)	0·045 (3)
C(11)	0·1404 (5)	1·5751 (6)	0·3677 (7)	0·086 (5)
N(10)	0·1421 (3)	1·4700 (3)	0·2954 (4)	0·054 (3)
O(1)	0·2812 (5)	0·7775 (7)	0·2859 (6)	0·156 (6)
O(2)	0·4387 (4)	0·7579 (5)	0·3481 (5)	0·113 (4)
O(3)	0·3764 (8)	0·9076 (6)	0·4172 (10)	0·214 (9)
O(4)	0·3512 (6)	0·7408 (6)	0·4935 (6)	0·146 (6)
C(4a)	0·2235 (4)	1·4080 (4)	0·3175 (4)	0·051 (3)
C(8a)	0·0594 (3)	1·3358 (4)	0·1389 (4)	0·047 (3)
C(9a)	0·2225 (3)	1·3025 (4)	0·2535 (4)	0·048 (3)
C(10a)	0·0605 (4)	1·4382 (4)	0·2086 (5)	0·050 (3)
C(1′)	0·1395 (3)	1·1614 (4)	0·0911 (4)	0·045 (3)
C(2′)	0·1335 (4)	1·0567 (4)	0·1447 (5)	0·052 (3)
C(3′)	0·1358 (4)	0·9610 (5)	0·0716 (5)	0·063 (3)
C(4′)	0·1390 (4)	0·9692 (5)	−0·0508 (5)	0·065 (4)
C(5′)	0·1422 (4)	1·0713 (5)	−0·1052 (5)	0·065 (4)
C(6′)	0·1429 (4)	1·1696 (5)	−0·0349 (5)	0·055 (3)
C(7′)	0·1245 (5)	1·0448 (6)	0·2755 (6)	0·079 (4)

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Table 2. *Bond lengths* (Å) *and bond angles* (°)

Cl—O(1)	1·418 (6)	C(9)—C(9a)	1·399 (5)
Cl—O(2)	1·417 (6)	C(9)—C(1′)	1·501 (6)
Cl—O(3)	1·349 (6)	C(11)—N(10)	1·482 (8)
Cl—O(4)	1·368 (6)	N(10)—C(4a)	1·369 (7)
C(1)—C(2)	1·345 (7)	N(10)—C(10a)	1.369 (6)
C(1)—C(9a)	1·411 (7)	C(4a)—C(9a)	1·433 (7)
C(2)—C(3)	1·423 (8)	C(8a)—C(10a)	1·433 (7)
C(3)—C(4)	1·331 (8)	C(1′)—C(2′)	1·386 (6)
C(4)—C(4a)	1·408 (7)	C(1′)—C(6′)	1·406 (5)
C(5)—C(6)	1·346 (7)	C(2′)—C(3′)	1·396 (6)
C(5)—C(10a)	1·415 (7)	C(2′)—C(7′)	1·489 (6)
C(6)—C(7)	1·401 (8)	C(3′)—C(4′)	1·366 (6)
C(7)—C(8)	1·353 (7)	C(4′)—C(5′)	1·356 (7)
C(8)—C(8a)	1·412 (5)	C(5′)—C(6′)	1·397 (7)
C(9)—C(8a)	1·392 (6)		

O(1)—Cl—O(2)	104·6 (5)	N(10)—C(4a)—C(9a)	119·2 (5)
O(1)—Cl—O(3)	113·1 (6)	C(8)—C(8a)—C(9)	122·1 (4)
O(1)—Cl—O(4)	110·0 (5)	C(8)—C(8a)—C(10a)	118·5 (5)
O(2)—Cl—O(3)	106·9 (6)	C(9)—C(8a)—C(10a)	119·5 (5)
O(2)—Cl—O(4)	112·8 (5)	C(1)—C(9a)—C(9)	122·9 (5)
O(3)—Cl—O(4)	109·4 (6)	C(1)—C(9a)—C(4a)	117·9 (5)
C(2)—C(1)—C(9a)	122·4 (5)	C(9)—C(9a)—C(4a)	119·2 (5)
C(1)—C(2)—C(3)	118·1 (6)	C(5)—C(10a)—N(10)	122·9 (5)
C(2)—C(3)—C(4)	122·5 (6)	C(5)—C(10a)—C(8a)	117·9 (5)
C(3)—C(4)—C(4a)	120·3 (6)	N(10)—C(10a)—C(8a)	119·2 (5)
C(6)—C(5)—C(10a)	121·1 (6)	C(9)—C(1′)—C(2′)	122·0 (5)
C(5)—C(6)—C(7)	121·4 (6)	C(9)—C(1′)—C(6′)	117·6 (4)
C(6)—C(7)—C(8)	119·5 (6)	C(2′)—C(1′)—C(6′)	120·4 (4)
C(7)—C(8)—C(8a)	121·6 (5)	C(1′)—C(2′)—C(3′)	117·8 (5)
C(8a)—C(9)—C(9a)	120·4 (5)	C(1′)—C(2′)—C(7′)	122·0 (4)
C(8a)—C(9)—C(1′)	119·8 (5)	C(3′)—C(2′)—C(7′)	120·3 (5)
C(9a)—C(9)—C(1′)	119·9 (4)	C(2′)—C(3′)—C(4′)	121·6 (5)
C(11)—N(10)—C(4a)	119·8 (5)	C(3′)—C(4′)—C(5′)	121·0 (5)
C(11)—N(10)—C(10a)	117·9 (5)	C(4′)—C(5′)—C(6′)	119·6 (6)
C(4a)—N(10)—C(10a)	122·4 (5)	C(1′)—C(6′)—C(5′)	119·5 (4)
C(4)—C(4a)—N(10)	122·0 (5)		
C(4)—C(4a)—C(9a)	118·8 (5)		

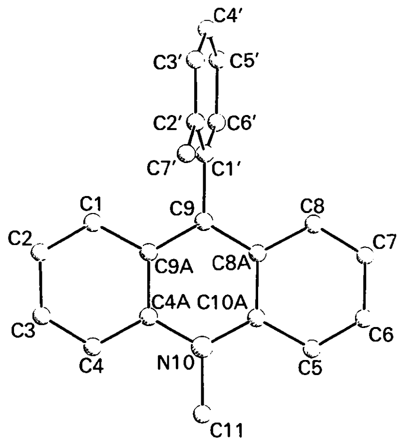

Fig. 1. Structure of $[C_{21}H_{18}N]^+$ showing the numbering scheme.

squares-fitting procedure using 23 reflections with $32 < 2\theta < 39°$. Corrections for Lorentz and polarization effects were applied. The structure was determined by direct methods using the program *SIMPEL* (Schenk & Kiers, 1985). H atoms found on ΔF map. Block-diagonal least-squares refinement on F, anisotropic for the non-H atoms and isotropic for the H atoms, converged to $R = 0{\cdot}066$, $wR = 0{\cdot}094$, $(\Delta/\sigma)_{\max} = 0{\cdot}73$. A weighting scheme $w = (5{\cdot}14 + F_{\rm obs} + 0{\cdot}013F_{\rm obs}{}^2)^{-1}$ was used. An empirical absorption correction was applied with corrections in the range 0·81–1·37 (*DIFABS*; Walker & Stuart, 1983). A final difference Fourier map revealed a residual electron density between −0·3 and 0·4 e Å^{-3}. Scattering factors were taken from Cromer & Mann (1968); *International Tables for X-ray Crystallography* (1974). Anomalous dispersion for Cl was corrected for. All calculations were performed with *XRAY76* (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976), unless stated otherwise.*

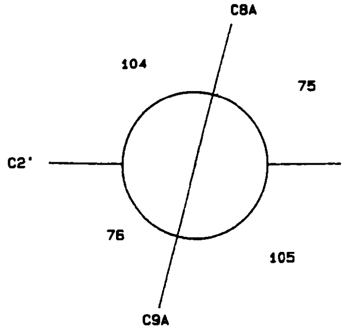

Fig. 2. The Newman projection along the C(9)—C(1′) bond.

Discussion. Final positonal parameters for the non-H atoms are listed in Table 1, bond lengths and bond angles in Table 2. A *PLUTO* (Motherwell & Clegg, 1978) drawing of the molecule is given in Fig. 1 and the Newman projection along the C(9)—C(1′) bond in Fig. 2. The phenyl ring is planar within 0·018 Å and the maximum deviation from the acridinium plane is 0·076 Å. The angle between the two planes is 76°.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51847 (33 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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