Acta Cryst. (1989). C**45**, 1359–1361

Crystal Studies of Acridinium Dyes. VI. 10-Methyl-9-[4-(1,4,7,10-tetraoxa-13-aza-13-cyclopentadecyl)phenyl]acridinium Barium Triperchlorate Acetonitrile Solvate

By Martin C. Zoutberg, Celeste A. Reiss, Kees Goubitz and Dick Heijdenrijk

Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, *Amsterdam, The Netherlands*

(*Received* 11 *November* 1988; *accepted* 28 *April* 1989)

Abstract. $C_{30}H_{35}N_2O_4^+.Ba^{2+}.3ClO_4^-.C_2H_3N$, M_r = 964·4, monoclinic, $P2_1/a$, a = 22·511 (4), b = 13·740 (3), c = 12·443 (2) Å, β = 95·66 (2)°, V = 3830 (1) Å^3, Z = 4, D_x = 1·67 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 13·2 cm^{-1}, F(000) = 1944, room temperature. Final R = 0·042 for 3972 observed reflections. The angle between the acridinium and the phenyl groups is 73°. The mean cavity radius of the crown ether is 1·54 Å. The distance from the Ba atom to nine O atoms is about 3·0 Å, a longer distance of ~3·3 Å exists to another O atom and the N atom of the crown ether.

Introduction. The title compound is the sixth structure in a series of acridinium dyes [I: Goubitz, Reiss, Heijdenrijk, Jonker & Verhoeven (1989); II and IV: Reiss, Goubitz & Heijdenrijk (1989*a*,*b*); III: Kronenburg, Goubitz, Reiss & Heijdenrijk (1989); V: Goubitz, Reiss & Heijdenrijk (1989)]. In this case the phenyl ring is substituted with an aza-15-crown-5 group, which has formed a complex with barium perchlorate.

Experimental. An orange brick-shaped crystal (dimensions 0·15 × 0·15 × 0·38 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 5959 unique reflections was measured within the range $-25 \le h \le 25$, $0 \le k \le 15$, $0 \le l \le 14$. Of these, 3972 were above the significance level of $2{\cdot}5\sigma(I)$. The maximum value of $(\sin\theta)/\lambda$ was 0·57 Å^{-1} ($\theta \le 24°$). Two standard reflections ($\bar{4}02$, 020) were measured hourly, no significant decrease was measured during the 66 h collecting time. Unit-cell parameters were refined by a least-squares-fitting procedure using 23 reflections with $32 < 2\theta < 34°$. Corrections for Lorentz and polarization effects were applied. The Ba- and Cl-atom positions were determined by direct methods using the program *SIMPEL* (Schenk & Kiers, 1985). From a ΔF synthesis the positions of the remaining non-H atoms were derived. After isotropic refinement, a subsequent ΔF synthesis revealed three peaks, which were interpreted as acetonitrile, one of the solvents used in the crystallization of the compound. The positions of the H atoms were calculated. Block-

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	z	U_{eq}(Å^2)
Ba	0·16244 (2)	0·27731 (3)	0·12171 (3)	0·0391 (2)
Cl(1)	0·00105 (8)	0·2958 (1)	0·1463 (1)	0·047 (1)
Cl(2)	0·2076 (1)	0·0687 (2)	0·3072 (2)	0·062 (1)
Cl(3)	0·12719 (9)	0·0834 (1)	−0·0640 (2)	0·048 (1)
C(1)	0·0899 (4)	0·0468 (7)	0·5409 (7)	0·060 (5)
C(2)	0·0820 (4)	−0·0525 (6)	0·5400 (9)	0·070 (6)
C(3)	0·0473 (5)	−0·0953 (7)	0·6137 (9)	0·085 (7)
C(4)	0·0187 (4)	−0·0424 (7)	0·6836 (8)	0·071 (6)
C(5)	−0·0381 (4)	0·2694 (9)	0·8200 (8)	0·074 (7)
C(6)	−0·0343 (5)	0·3669 (9)	0·8188 (8)	0·083 (7)
C(7)	−0·0005 (5)	0·4178 (8)	0·7486 (9)	0·081 (7)
C(8)	0·0331 (4)	0·3652 (6)	0·6834 (7)	0·058 (5)
C(9)	0·0634 (3)	0·2072 (5)	0·6126 (5)	0·039 (4)
C(11)	−0·0430 (5)	0·066 (1)	0·8326 (10)	0·099 (9)
N(10)	−0·0075 (3)	0·1158 (6)	0·7532 (6)	0·059 (4)
O(1)	0·0422 (4)	0·2159 (5)	0·1754 (7)	0·089 (5)
O(2)	−0·0257 (3)	0·3256 (6)	0·2398 (5)	0·072 (4)
O(3)	−0·0426 (3)	0·2672 (9)	0·0661 (6)	0·119 (7)
O(4)	0·0388 (3)	0·3712 (5)	0·1107 (6)	0·082 (5)
O(5)	0·1905 (4)	−0·0267 (5)	0·2796 (8)	0·102 (6)
O(6)	0·2303 (4)	0·0759 (6)	0·4193 (6)	0·100 (6)
O(7)	0·2505 (4)	0·1015 (7)	0·2374 (6)	0·102 (6)
O(8)	0·1592 (4)	0·1335 (6)	0·2897 (6)	0·105 (6)
O(9)	0·1762 (3)	0·0865 (5)	0·0176 (6)	0·078 (4)
O(10)	0·1480 (3)	0·0758 (6)	−0·1670 (5)	0·081 (5)
O(11)	0·0955 (3)	0·1741 (5)	−0·0574 (6)	0·081 (5)
O(12)	0·0893 (3)	0·0042 (5)	−0·0492 (6)	0·085 (5)
C(4a)	0·0221 (4)	0·0597 (7)	0·6854 (7)	0·055 (5)
C(8a)	0·0305 (3)	0·2620 (6)	0·6805 (6)	0·046 (4)
C(9a)	0·0587 (3)	0·1058 (6)	0·6123 (6)	0·043 (4)
C(10a)	−0·0054 (4)	0·2150 (7)	0·7517 (6)	0·057 (5)
C(1*s*)	0·3794 (6)	0·1672 (9)	0·500 (1)	0·103 (9)
C(2*s*)	0·3862 (7)	0·089 (1)	0·427 (1)	0·13 (1)
N(*s*)	0·3723 (8)	0·2297 (8)	0·558 (1)	0·14 (1)
C(2″)	0·1851 (4)	0·5169 (6)	0·3105 (7)	0·053 (5)
C(3″)	0·1971 (4)	0·5524 (6)	0·2006 (8)	0·060 (5)
C(5″)	0·1590 (4)	0·5403 (6)	0·0162 (8)	0·062 (6)
C(6″)	0·1235 (5)	0·4797 (7)	−0·0641 (8)	0·068 (6)
C(8″)	0·1987 (5)	0·3840 (8)	−0·1451 (8)	0·075 (7)
C(9″)	0·2314 (5)	0·2939 (8)	−0·1336 (8)	0·077 (7)
C(11″)	0·3085 (4)	0·3209 (8)	0·0136 (9)	0·071 (6)
C(12″)	0·3261 (4)	0·2939 (8)	0·1276 (8)	0·070 (6)
C(14″)	0·2972 (3)	0·3248 (7)	0·3050 (7)	0·054 (5)
C(15″)	0·2717 (3)	0·4131 (6)	0·3524 (7)	0·050 (5)
N(1″)	0·2059 (3)	0·4168 (4)	0·3317 (5)	0·043 (4)
O(4″)	0·1620 (3)	0·4945 (4)	0·1198 (4)	0·055 (3)
O(7″)	0·1511 (3)	0·3855 (4)	−0·0744 (5)	0·065 (4)
O(10″)	0·2536 (3)	0·2743 (4)	−0·0238 (4)	0·058 (4)
O(13″)	0·2799 (2)	0·3273 (5)	0·1900 (4)	0·052 (3)
C(1′)	0·1020 (3)	0·2592 (5)	0·5388 (6)	0·038 (4)
C(2′)	0·0757 (3)	0·3100 (6)	0·4499 (6)	0·044 (4)
C(3′)	0·1112 (3)	0·3606 (6)	0·3846 (6)	0·045 (4)
C(4′)	0·1726 (3)	0·3641 (5)	0·4030 (6)	0·038 (4)
C(5′)	0·1983 (3)	0·3108 (6)	0·4918 (6)	0·047 (4)
C(6′)	0·1627 (4)	0·2585 (6)	0·5572 (6)	0·051 (5)

0108-2701/89/091359-03$03.00

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

Ba—O(1)	2·973 (8)	C(9)—C(8a)	1·40 (1)
Ba—O(4)	3·058 (7)	C(9)—C(9a)	1·40 (1)
Ba—O(7)	3·358 (9)	C(9)—C(1′)	1·51 (1)
Ba—O(8)	2·882 (8)	C(11)—N(10)	1·50 (1)
Ba—O(9)	2·954 (7)	N(10)—C(4a)	1·36 (1)
Ba—O(11)	2·930 (7)	N(10)—C(10a)	1·36 (1)
Ba—N(1″)	3·310 (6)	C(4a)—C(9a)	1·43 (1)
Ba—O(4″)	2·984 (5)	C(8a)—C(10a)	1·41 (1)
Ba—O(7″)	2·847 (6)	C(1*s*)—C(2*s*)	1·42 (2)
Ba—O(10″)	2·868 (6)	C(1*s*)—N(*s*)	1·14 (2)
Ba—O(13″)	2·782 (5)	C(2″)—C(3″)	1·50 (1)
Cl(1)—O(1)	1·459 (8)	C(2″)—N(1″)	1·468 (10)
Cl(1)—O(2)	1·422 (7)	C(3″)—O(4″)	1·45 (1)
Cl(1)—O(3)	1·387 (8)	C(5″)—C(6″)	1·47 (1)
Cl(1)—O(4)	1·437 (8)	C(5″)—O(4″)	1·43 (1)
Cl(2)—O(5)	1·399 (8)	C(6″)—O(7″)	1·45 (1)
Cl(2)—O(6)	1·441 (8)	C(8″)—C(9″)	1·44 (2)
Cl(2)—O(7)	1·434 (9)	C(8″)—O(7″)	1·45 (1)
Cl(2)—O(8)	1·407 (9)	C(9″)—O(10″)	1·43 (1)
Cl(3)—O(9)	1·424 (7)	C(11″)—C(12″)	1·48 (1)
Cl(3)—O(10)	1·411 (7)	C(11″)—O(10″)	1·43 (1)
Cl(3)—O(11)	1·442 (7)	C(12″)—O(13″)	1·43 (1)
Cl(3)—O(12)	1·406 (8)	C(14″)—C(15″)	1·49 (1)
C(1)—C(2)	1·38 (1)	C(14″)—O(13″)	1·45 (1)
C(1)—C(9a)	1·44 (1)	C(15″)—N(1″)	1·479 (10)
C(2)—C(3)	1·39 (2)	N(11″)—C(4′)	1·416 (10)
C(3)—C(4)	1·35 (2)	C(1′)—C(2′)	1·39 (1)
C(4)—C(4a)	1·40 (1)	C(1′)—C(6′)	1·36 (1)
C(5)—C(6)	1·34 (2)	C(2′)—C(3′)	1·38 (1)
C(5)—C(10a)	1·40 (1)	C(3′)—C(4′)	1·38 (1)
C(6)—C(7)	1·40 (2)	C(4′)—C(5′)	1·40 (1)
C(7)—C(8)	1·37 (1)	C(5′)—C(6′)	1·40 (1)
C(8)—C(8a)	1·42 (1)		

O(1)—Ba—O(4)	44·4 (2)	O(11)—Cl(3)—O(12)	110·6 (4)
O(1)—Ba—O(7)	102·2 (2)	C(2)—C(1)—C(9a)	119·6 (9)
O(1)—Ba—O(8)	63·5 (2)	C(1)—C(2)—C(3)	119·6 (9)
O(1)—Ba—O(9)	89·1 (2)	C(2)—C(3)—C(4)	122·2 (9)
O(1)—Ba—O(11)	67·8 (2)	C(3)—C(4)—C(4a)	121·4 (9)
O(1)—Ba—N(1″)	101·1 (2)	C(6)—C(5)—C(10a)	119·3 (10)
O(1)—Ba—O(4″)	106·4 (2)	C(5)—C(6)—C(7)	123 (1)
O(1)—Ba—O(7″)	109·5 (2)	C(6)—C(7)—C(8)	118 (1)
O(1)—Ba—O(10″)	149·5 (2)	C(7)—C(8)—C(8a)	121·2 (9)
O(1)—Ba—O(13″)	149·3 (2)	C(8a)—C(9)—C(9a)	119·6 (7)
O(4)—Ba—O(7)	145·0 (2)	C(8a)—C(9)—C(1′)	119·0 (6)
O(4)—Ba—O(8)	103·5 (2)	C(9a)—C(9)—C(1′)	121·3 (6)
O(4)—Ba—O(9)	119·3 (2)	C(11)—N(10)—C(4a)	118·4 (9)
O(4)—Ba—O(11)	76·9 (2)	C(11)—N(10)—C(10a)	119·2 (8)
O(4)—Ba—N(1″)	89·3 (2)	C(4a)—N(10)—C(10a)	122·4 (8)
O(4)—Ba—O(4″)	64·9 (2)	Ba—O(1)—Cl(1)	107·5 (4)
O(4)—Ba—O(7″)	74·8 (2)	Ba—O(4)—Cl(1)	104·2 (4)
O(4)—Ba—O(10″)	133·0 (2)	Ba—O(7)—Cl(2)	94·7 (4)
O(4)—Ba—O(13″)	138·0 (2)	Ba—O(8)—Cl(2)	118·1 (5)
O(7)—Ba—O(8)	41·6 (2)	Ba—O(9)—Cl(3)	103·4 (3)
O(7)—Ba—O(9)	57·8 (2)	Ba—O(11)—Cl(3)	104·0 (3)
O(7)—Ba—O(11)	102·4 (2)	C(4)—C(4a)—N(10)	123·0 (8)
O(7)—Ba—N(1″)	87·8 (2)	C(4)—C(4a)—C(9a)	117·7 (8)
O(7)—Ba—O(4″)	136·4 (2)	N(10)—C(4a)—C(9a)	119·3 (8)
O(7)—Ba—O(7″)	137·9 (2)	C(8)—C(8a)—C(9)	122·0 (7)
O(7)—Ba—O(10″)	80·3 (2)	C(8)—C(8a)—C(10a)	117·7 (8)
O(7)—Ba—O(13″)	62·8 (2)	C(9)—C(8a)—C(10a)	120·2 (8)
O(8)—Ba—O(9)	73·8 (2)	C(1)—C(9a)—C(9)	121·5 (7)
O(8)—Ba—O(11)	99·9 (2)	C(1)—C(9a)—C(4a)	119·3 (7)
O(8)—Ba—N(1″)	81·4 (2)	C(9)—C(9a)—C(4a)	119·1 (7)
O(8)—Ba—O(4″)	133·7 (2)	C(5)—C(10a)—N(10)	120·4 (9)
O(8)—Ba—O(7″)	166·6 (2)	C(5)—C(10a)—C(8a)	120·4 (9)
O(8)—Ba—O(10″)	121·3 (2)	N(10)—C(10a)—C(8a)	119·2 (8)
O(8)—Ba—O(13″)	92·2 (2)	C(2*s*)—C(1*s*)—N(*s*)	178 (2)
O(9)—Ba—O(11)	46·0 (2)	C(3″)—C(2″)—N(1″)	112·7 (7)
O(9)—Ba—N(1″)	145·5 (2)	C(2″)—C(3″)—O(4″)	108·5 (7)
O(9)—Ba—O(4″)	152·2 (2)	C(6″)—C(5″)—O(4″)	109·7 (7)
O(9)—Ba—O(7″)	95·3 (2)	C(5″)—C(6″)—O(7″)	110·9 (8)
O(9)—Ba—O(10″)	66·3 (2)	C(9″)—C(8″)—O(7″)	110·6 (8)
O(9)—Ba—O(13″)	102·4 (2)	C(8″)—C(9″)—O(10″)	112·5 (8)
O(11)—Ba—N(1″)	166·1 (2)	C(12″)—C(11″)—O(10″)	109·9 (8)
O(11)—Ba—O(4″)	118·5 (2)	C(12″)—C(11″)—O(13″)	107·4 (8)
O(11)—Ba—O(7″)	66·7 (2)	C(15″)—C(14″)—O(13″)	107·2 (7)
O(11)—Ba—O(10″)	81·9 (2)	C(14″)—C(15″)—N(1″)	112·2 (6)
O(11)—Ba—O(13″)	138·9 (2)	Ba—N(1″)—C(2″)	109·7 (4)
N(1″)—Ba—O(4″)	55·1 (1)	Ba—N(1″)—C(15″)	109·3 (4)
N(1″)—Ba—O(7″)	111·6 (2)	Ba—N(1″)—C(4′)	93·7 (4)
N(1″)—Ba—O(10″)	109·4 (2)	C(2″)—N(1″)—C(15″)	111·1 (6)
N(1″)—Ba—O(13″)	54·4 (2)	C(2″)—N(1″)—C(4′)	114·4 (6)
O(4″)—Ba—O(7″)	58·1 (2)	C(15″)—N(1″)—C(4′)	117·1 (6)
O(4″)—Ba—O(10″)	90·7 (2)	Ba—O(4″)—C(3″)	122·7 (4)
O(4″)—Ba—O(13″)	76·0 (2)	Ba—O(4″)—C(5″)	116·6 (5)
O(7″)—Ba—O(10″)	58·4 (2)	C(3″)—O(4″)—C(5″)	110·9 (6)
O(7″)—Ba—O(13″)	97·8 (2)	Ba—O(7″)—C(6″)	113·2 (5)

Table 2 (*cont.*)

O(10″)—Ba—O(13″)	58·6 (2)	Ba—O(7″)—C(8″)	120·2 (5)
O(1)—Cl(1)—O(2)	108·9 (5)	C(6″)—O(7″)—C(8″)	114·5 (7)
O(1)—Cl(1)—O(3)	110·7 (6)	Ba—O(10″)—C(9″)	113·3 (6)
O(1)—Cl(1)—O(4)	103·8 (4)	Ba—O(10″)—C(11″)	116·0 (5)
O(2)—Cl(1)—O(3)	110·1 (4)	C(9″)—O(10″)—C(11″)	115·8 (8)
O(2)—Cl(1)—O(4)	110·8 (4)	Ba—O(13″)—C(12″)	118·3 (5)
O(3)—Cl(1)—O(4)	112·4 (5)	Ba—O(13″)—C(14″)	116·8 (4)
O(5)—Cl(2)—O(6)	111·4 (5)	C(12″)—O(13″)—C(14″)	112·9 (6)
O(5)—Cl(2)—O(7)	109·3 (6)	C(9)—C(1′)—C(2′)	119·8 (6)
O(5)—Cl(2)—O(8)	111·4 (5)	C(9)—C(1′)—C(6′)	121·6 (6)
O(6)—Cl(2)—O(7)	111·7 (5)	C(2′)—C(1′)—C(6′)	118·6 (7)
O(6)—Cl(2)—O(8)	107·6 (5)	C(1′)—C(2′)—C(3′)	119·7 (7)
O(7)—Cl(2)—O(8)	105·4 (5)	C(2′)—C(3′)—C(4′)	123·2 (7)
O(9)—Cl(3)—O(10)	110·3 (4)	N(1″)—C(4′)—C(3′)	119·8 (6)
O(9)—Cl(3)—O(11)	106·6 (4)	N(1″)—C(4′)—C(5′)	123·9 (6)
O(9)—Cl(3)—O(12)	111·5 (4)	C(3′)—C(4′)—C(5′)	116·2 (7)
O(10)—Cl(3)—O(11)	109·0 (5)	C(4′)—C(5′)—C(6′)	120·8 (7)
O(10)—Cl(3)—O(12)	108·8 (5)	C(1′)—C(6′)—C(5′)	121·5 (7)

diagonal least-squares refinement on F, anisotropic for the non-H atoms and isotropic for the H atoms, converged to $R = 0{\cdot}042$, $wR = 0{\cdot}074$, $(\Delta/\sigma)_{\max} = 0{\cdot}83$. A weighting scheme $w = (4{\cdot}62 + F_{\rm obs} + 0{\cdot}025F^2_{\rm obs})^{-1}$ was used. The isotropic secondary-extinction coefficient refined to 1·8 (4) × 10^{-3} (Zachariasen, 1968). An empirical absorption correction was applied, with corrections in the range 0·81–1·12 (*DIFABS*; Walker & Stuart, 1983). A final difference Fourier map revealed a residual electron density between −0·3 and 0·6 e Å^{-3}. Scattering factors were taken from Cromer & Mann (1968); *International Tables for X-ray Crystallography* (1974). Anomalous dispersion for Ba and Cl was corrected for. All calculations were performed with *XRAY76* (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976), unless stated otherwise.*

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 acridinium group is nearly planar, the maximum distance of atoms from the plane is 0·069 Å. The phenyl ring is planar within 0·014 Å. The angle between the two planes is 73°.

The O atoms of the crown ether form a reasonably planar tetragon, alternately about 0·10 Å above and below their mean plane; the N atom lies 1·059 Å below this plane. For the mean cavity radius, as defined by Mathieu, Metz, Moras & Weiss (1978), a value of 1·54 Å was obtained. The distance from the Ba ion to the centre of gravity of the hetero atoms in the crown ether is 1·78 Å, the angle N(1″)—centre of

---

* 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 51850 (50 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

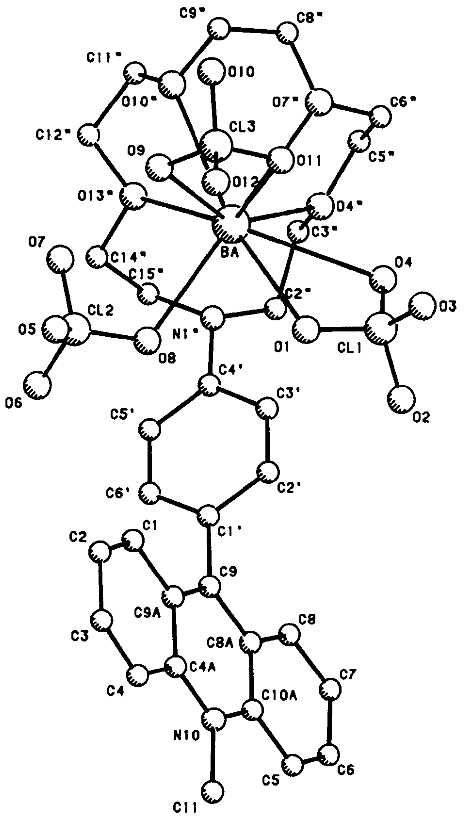

Fig. 1. The molecular structure of the title compound showing the atom numbering.

gravity—Ba is 105°. The Ba ion is coordinated by the four O atoms of the crown ether and by the three perchlorate ions, one unidentate the others bidentate (distances about 3·0 Å). The distance from the Ba ion to the N atom in the crown ether and to the O(7) atom of the unidentate perchlorate is about 3·3 Å. From this it can be argued that the Ba ion is 11 rather than 9 coordinated.

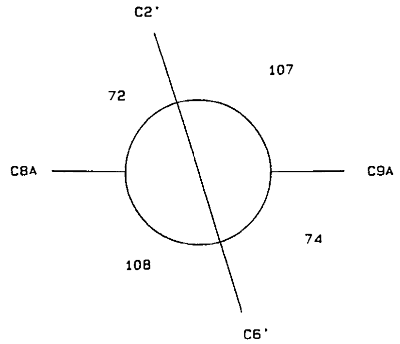

Fig. 2. The Newman projection along the C(9)—C(1') bond.

References

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* **A24**, 321–324.
Goubitz, K., Reiss, C. A. & Heijdenrijk, D. (1989). *Acta Cryst.* **C45**, 1356–1358.
Goubitz, K., Reiss, C. A., Heijdenrijk, D., Jonker, S. A., Verhoeven, J. W. (1989). *Acta Cryst.* **C45**, 1348–1350.
International Tables for X-ray Crystallography (1974). Vol. IV, p. 55. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
Kronenburg, M. J., Goubitz, K., Reiss, C. A. & Heijdenrijk, D. (1989). *Acta Cryst.* **C45**, 1352–1353.
Mathieu, F., Metz, B., Moras, B. & Weiss, R. (1978). *J. Am. Chem. Soc.* **100**, 4412–4416.
Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.
Reiss, C. A., Goubitz, K. & Heidenrijk, D. (1989*a*). *Acta Cryst.* **C45**, 1350–1352.
Reiss, C. A., Goubitz, K. & Heijdenrijk, D. (1989*b*). *Acta Cryst.* **C45**, 1354–1356.
Schenk, H. & Kiers, C. T. (1985). *SIMPEL83, a Program System for Direct Methods*. In *Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 200–205. Oxford: Clarendon Press.
Stewart, J. M., Machin, P. A., Dickinson, C. W., Ammon, H. L., Heck, H. & Flack, H. (1976). The *XRAY76* system. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland, USA.
Walker, N. & Stuart, D. (1983). *Acta Cryst.* **A39**, 158–166.
Zachariasen, W. H. (1968). *Acta Cryst.* **A24**, 212–216.

Acta Cryst. (1989). **C45**, 1361–1363

Crystal Studies of Acridinium Dyes. VII. 10-Methyl-9-[4-(1,4,7,10-tetraoxa-13-aza-13-cyclopentadecyl)phenyl]acridinium Silver Diperchlorate Dichloromethane Solvate

By Maarten J. Kronenburg, Celeste A. Reiss, Kees Goubitz and Dick Heijdenrijk

Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, *Amsterdam, The Netherlands*

(*Received* 11 *November* 1988; *accepted* 28 *April* 1989)

Abstract. $C_{30}H_{35}N_2O_4^+.Ag^+.2ClO_4^-.2CH_2Cl_2$, M_r = 964·3, monoclinic, $P2_1$, a = 14·861 (8), b = 14·810 (8), c = 9·157 (4) Å, β = 101·86 (5)°, V = 1972 (2) Å^3, Z = 2, D_x = 1.624 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 9·75 cm^{-1}, F(000) = 980, room temperature. Final R = 0·055 for 2917 observed reflections. The angle between the acridinium and phenyl groups is 74°. The mean cavity radius of the crown ether is 1·13 Å.

0108-2701/89/091361-03$03.00