1148 reflections were below the $2{\cdot}5\sigma$ level and were treated as unobserved. Two standard reflections (141 and $\bar{1}13$) were measured hourly and showed no systematic change. Corrections for Lorentz and polarization effects were applied. Lattice parameters from least-squares adjustment to $\sin\theta$ values of 23 reflections in the range $60 < 2\theta < 70°$.

The structure was solved from the Patterson synthesis. The asymmetric unit was found to comprise two independent half molecules straddling the crystallographic diad axes at $x = \frac{3}{4}$, $z = 0$ and $x = \frac{1}{4}$, $z = \frac{1}{2}$.

Refinement on F proceeded by means of block-diagonal least-squares calculations, anisotropic for the non-H and isotropic for H atoms. The H atoms were very well indicated in a ΔF synthesis, except those at C(11) which have been omitted. An empirical absorption correction (*DIFABS*; Walker & Stuart, 1983) was applied, with correction in the range 0·50–1·51. A weighting scheme $w = 1/(5{\cdot}2 + F_o + 0{\cdot}0043F_o^2)$ was employed and the anomalous dispersion of Cl was taken into account. The final R value was 0·063 ($wR = 0{\cdot}085$), $(\Delta/\sigma)_{\max} = 0{\cdot}47$. The residual density in a final difference synthesis was between $-0{\cdot}2$ and $0{\cdot}3$ e Å^{-3}. Scattering factors were taken from Cromer & Mann (1968). All calculations were carried out with *XRAY76* (Stewart *et al.*, 1976).

Discussion. Final parameters for the non-H atoms are listed in Table 1.* Bond lengths and angles are given in Table 2. The atomic numbering is indicated in the *PLUTO* drawing of Fig. 1. The two independent molecules are very similar. There is a slight difference in the angle between the planes of the acridinium moiety and the phenyl group (*A* 65·1, *B* 63·8°). The Cl ion is surrounded by six C atoms at distances of 3·4–3·8 Å. The packing is indicated in Fig. 2.

References

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* **A24**, 321–324.

Goubitz, K., Reiss, C. A. & Heijdenrijk, D. (1989*a*). *Acta Cryst.* **C45**, 1356–1358.

Goubitz, K., Reiss, C. A. & Heijdenrijk, D. (1989*b*). *Acta Cryst.* **C45**, 1364–1366.

Goubitz, K., Reiss, C. A., Heijdenrijk, D., Jonker, S. A. & Verhoeven, J. W. (1989). *Acta Cryst.* **C45**, 1348–1350.

Häming, L. P., Reiss, C. A., Goubitz, K. & Heijdenrijk, D. (1990). *Acta Cryst.* **C46**, 462–465.

Jonker, S. A., Ariese, F. & Verhoeven, J. W. (1989). *Recl Trav. Chim. Pays-Bas*, **108**, 109–115.

Kronenburg, M. J., Goubitz, K., Reiss, C. A. & Heijdenrijk, D. (1989*a*). *Acta Cryst.* **C45**, 1352–1353.

Kronenburg, M. J., Goubitz, K., Reiss, C. A. & Heijdenrijk, D. (1989*b*). *Acta Cryst.* **C45**, 1361–1363.

Reiss, C. A., Goubitz, K. & Heijdenrijk, D. (1989*a*). *Acta Cryst.* **C45**, 1350–1352.

Reiss, C. A., Goubitz, K. & Heijdenrijk, D. (1989*b*). *Acta Cryst.* **C45**, 1354–1356.

Reiss, C. A., Goubitz, K., Zoutberg, M. C. & Heijdenrijk, D. (1989). *Acta Cryst.* **C45**, 1366–1369.

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.

Zoutberg, M. C., Reiss, C. A., Goubitz, K. & Heijdenrijk, D. (1989). *Acta Cryst.* **C45**, 1359–1361.

---

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52625 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1990). **C46**, 1081–1084

Crystal Studies of Acridinium Dyes. XIII.* The Structures of 10-Methyl-9-(4-methylphenyl)acridinium Perchlorate (*A*) and 10-Methyl-9-(4-methoxyphenyl)-acridinium Perchlorate (*B*)

By Kees Goubitz, Celeste A. Reiss and Dick Heijdenrijk

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

(*Received* 3 *July* 1989; *accepted* 6 *September* 1989)

Abstract. (*A*): $C_{21}H_{18}N^+.ClO_4^-$, $M_r = 383{\cdot}8$, monoclinic, $P2_1/n$, $a = 8{\cdot}3480\ (8)$, $b = 16{\cdot}9618\ (14)$, $c = 13{\cdot}2145\ (8)$ Å, $\beta = 96{\cdot}106\ (6)°$, $V = 1860{\cdot}5\ (3)$ Å^3, $Z = 4$, $D_x = 1{\cdot}37$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 23{\cdot}7$ cm^{-1}, $F(000) = 800$, room temperature. Final $R = 0{\cdot}067$ for 2242 observed reflections. (*B*):

---

* Part XII, preceding paper.

0108-2701/90/061081-04$03.00

Table 1. *Fractional coordinates and equivalent isotropic thermal parameters*

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

	x	*y*	*z*	U_{eq} (Å^2)
Molecule (*A*)				
Cl	0·5436 (1)	0·29661 (7)	0·26217 (8)	0·0618 (6)
C(1)	0·6180 (5)	0·0206 (3)	0·3407 (3)	0·053 (2)
C(2)	0·7605 (6)	0·0091 (3)	0·3981 (4)	0·069 (3)
C(3)	0·7941 (5)	0·0505 (3)	0·4888 (4)	0·069 (3)
C(4)	0·6891 (5)	0·1027 (3)	0·5220 (3)	0·057 (3)
C(5)	0·1591 (6)	0·2232 (3)	0·4852 (4)	0·065 (3)
C(6)	0·0127 (6)	0·2315 (3)	0·4325 (4)	0·076 (3)
C(7)	−0·0278 (6)	0·1939 (3)	0·3391 (4)	0·074 (3)
C(8)	−0·0811 (5)	0·1468 (3)	0·3007 (4)	0·061 (3)
C(9)	0·3528 (5)	0·0870 (2)	0·3138 (3)	0·043 (2)
C(11)	0·4664 (7)	0·2099 (4)	0·5949 (4)	0·079 (4)
N(10)	0·4256 (4)	0·1645 (2)	0·5003 (2)	0·046 (2)
O(1)	0·6058 (4)	0·2270 (2)	0·2207 (3)	0·077 (2)
O(2)	0·5565 (5)	0·2922 (3)	0·3682 (3)	0·094 (3)
O(3)	0·621 (1)	0·3613 (3)	0·2332 (5)	0·211 (7)
O(4)	0·3725 (6)	0·2984 (3)	0·2290 (4)	0·133 (4)
C(1′)	0·3175 (5)	0·0517 (2)	0·2108 (3)	0·045 (2)
C(2′)	0·3225 (7)	0·0962 (3)	0·1250 (4)	0·075 (3)
C(3′)	0·2878 (7)	0·0648 (3)	0·0289 (4)	0·079 (4)
C(4′)	0·2427 (5)	−0·0130 (3)	0·0161 (3)	0·058 (3)
C(5′)	0·2324 (8)	−0·0561 (3)	0·1009 (4)	0·082 (4)
C(6′)	0·2697 (8)	−0·0262 (3)	0·1975 (4)	0·078 (3)
C(7′)	0·2002 (8)	−0·0473 (4)	−0·0894 (4)	0·091 (4)
C(4*a*)	0·5369 (5)	0·1138 (2)	0·4665 (3)	0·043 (2)
C(8*a*)	0·2393 (5)	0·1361 (2)	0·3524 (3)	0·046 (2)
C(9*a*)	0·5011 (5)	0·0740 (2)	0·3726 (3)	0·042 (2)
C(10*a*)	0·2769 (5)	0·1746 (2)	0·4478 (3)	0·046 (2)
Molecule (*B*)				
Cl	0·5694 (2)	0·2933 (1)	0·2525 (1)	0·084 (1)
C(1)	0·6118 (6)	0·0176 (4)	0·3573 (4)	0·064 (3)
C(2)	0·7537 (7)	0·0087 (4)	0·4143 (5)	0·080 (4)
C(3)	0·7942 (7)	0·0581 (4)	0·4977 (5)	0·078 (4)
C(4)	0·6952 (6)	0·1154 (4)	0·5252 (4)	0·066 (3)
C(5)	0·1756 (8)	0·2351 (5)	0·4858 (5)	0·088 (5)
C(6)	0·0292 (9)	0·2386 (5)	0·4352 (6)	0·100 (5)
C(7)	−0·0138 (7)	0·1972 (5)	0·3466 (5)	0·089 (5)
C(8)	0·0914 (7)	0·1483 (4)	0·3107 (5)	0·073 (4)
C(9)	0·3561 (6)	0·0871 (3)	0·3255 (4)	0·054 (3)
C(11)	0·485 (1)	0·2342 (6)	0·5848 (6)	0·122 (6)
N(10)	0·4387 (5)	0·1793 (3)	0·4990 (3)	0·068 (3)
O(1)	0·6267 (5)	0·2190 (3)	0·2168 (4)	0·093 (3)
O(2)	0·5966 (7)	0·2981 (4)	0·3551 (4)	0·110 (4)
O(3)	0·618 (2)	0·3599 (5)	0·2111 (6)	0·28 (1)
O(4)	0·3993 (9)	0·2883 (5)	0·2253 (7)	0·182 (7)
C(1′)	0·3155 (6)	0·0468 (3)	0·2266 (4)	0·058 (3)
C(2′)	0·337 (1)	0·0853 (5)	0·1451 (5)	0·140 (7)
C(3′)	0·301 (1)	0·0494 (5)	0·0512 (5)	0·144 (8)
C(4′)	0·2391 (6)	−0·0247 (3)	0·0402 (4)	0·061 (3)
C(5′)	0·212 (2)	−0·0644 (6)	0·1210 (6)	0·167 (9)
C(6′)	0·252 (2)	−0·0293 (6)	0·2144 (6)	0·167 (9)
C(7′)	0·229 (1)	−0·0266 (5)	−0·1343 (5)	0·117 (6)
O(1′)	0·2009 (5)	−0·0648 (3)	−0·0485 (3)	0·081 (3)
C(4*a*)	0·5452 (6)	0·1247 (3)	0·4709 (4)	0·056 (3)
C(8*a*)	0·2470 (6)	0·1405 (3)	0·3611 (4)	0·059 (3)
C(9*a*)	0·5011 (6)	0·0761 (3)	0·3831 (4)	0·055 (3)
C(10*a*)	0·2884 (7)	0·1841 (4)	0·4501 (4)	0·066 (3)

$C_{21}H_{18}NO^+.ClO_4^-$, M_r = 399·8, monoclinic, $P2_1/n$, a = 8·6761 (5), b = 16·0533 (8), c = 13·6787 (7) Å, β = 98·733 (8)°, V = 1883·1 (2) Å^3, Z = 4, D_x = 1·41 g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ = 20·9 cm^{-1}, F(000) = 832, room temperature. Final R = 0·084 for 2070 observed reflections. The angle between the acridinium and the phenyl groups is 78° in (*A*) and 88° in (*B*). There are no unusual bond lengths or angles in either structure.

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

	Molecule (*A*)	Molecule (*B*)
Cl—O(1)	1·423 (4)	1·407 (5)
Cl—O(2)	1·396 (4)	1·389 (5)
Cl—O(3)	1·348 (7)	1·31 (1)
Cl—O(4)	1·450 (5)	1·468 (7)
C(1)—C(2)	1·355 (6)	1·361 (8)
C(1)—C(9*a*)	1·428 (6)	1·426 (8)
C(2)—C(3)	1·391 (7)	1·390 (9)
C(3)—C(4)	1·352 (7)	1·350 (9)
C(4)—C(4*a*)	1·411 (5)	1·405 (7)
C(5)—C(6)	1·348 (7)	1·35 (1)
C(5)—C(10*a*)	1·412 (7)	1·42 (1)
C(6)—C(7)	1·397 (8)	1·38 (1)
C(7)—C(8)	1·349 (7)	1·35 (1)
C(8)—C(8*a*)	1·432 (6)	1·425 (7)
C(9)—C(1′)	1·488 (5)	1·492 (7)
C(9)—C(8*a*)	1·398 (6)	1·418 (8)
C(9)—C(9*a*)	1·407 (5)	1·390 (7)
C(11)—N(10)	1·478 (6)	1·47 (1)
N(10)—C(4*a*)	1·374 (5)	1·371 (7)
N(10)—C(10*a*)	1·367 (5)	1·375 (7)
C(1′)—C(2′)	1·366 (6)	1·31 (1)
C(1′)—C(6′)	1·386 (7)	1·34 (1)
C(2′)—C(3′)	1·380 (7)	1·40 (1)
C(3′)—C(4′)	1·377 (8)	1·31 (1)
C(4′)—C(5′)	1·349 (7)	1·33 (1)
C(4′)—C(7′)	1·518 (7)	—
C(4′)—O(1′)	—	1·369 (7)
C(5′)—C(6′)	1·378 (7)	1·39 (1)
C(7′)—O(1′)	—	1·377 (9)
C(4*a*)—C(9*a*)	1·416 (5)	1·433 (7)
C(8*a*)—(10*a*)	1·425 (5)	1·401 (7)
O(1)—Cl—O(2)	110·5 (3)	112·5 (3)
O(1)—Cl—O(3)	111·2 (4)	112·8 (6)
O(1)—Cl—O(4)	106·8 (3)	105·1 (4)
O(2)—Cl—O(3)	110·0 (4)	112·0 (5)
O(2)—Cl—O(4)	105·9 (3)	105·6 (4)
O(3)—Cl—O(4)	112·4 (4)	108·3 (7)
C(2)—C(1)—C(9*a*)	120·9 (4)	120·8 (5)
C(1)—C(2)—C(3)	119·6 (5)	120·3 (6)
C(2)—C(3)—C(4)	122·1 (4)	121·6 (5)
C(3)—C(4)—C(4*a*)	119·8 (4)	120·2 (5)
C(6)—C(5)—C(10*a*)	120·5 (5)	119·4 (6)
C(5)—C(6)—C(7)	122·0 (5)	122·4 (7)
C(6)—C(7)—C(8)	119·5 (5)	119·3 (6)
C(7)—C(8)—C(8*a*)	121·3 (4)	121·2 (6)
C(1′)—C(9)—C(8*a*)	119·8 (3)	119·7 (4)
C(1′)—C(9)—C(9*a*)	121·3 (3)	121·9 (5)
C(8*a*)—C(9)—C(9*a*)	118·9 (3)	118·4 (4)
C(11)—N(10)—C(4*a*)	119·9 (3)	119·4 (5)
C(11)—N(10)—C(10*a*)	118·6 (4)	118·7 (6)
C(4*a*)—N(10)—C(10*a*)	121·5 (3)	121·9 (5)
C(9)—C(1′)—C(2′)	121·1 (4)	121·5 (6)
C(9)—C(1′)—C(6′)	121·7 (4)	123·0 (6)
C(2′)—C(1′)—C(6′)	117·1 (4)	115·5 (6)
C(1′)—C(2′)—C(3′)	121·9 (5)	123·1 (8)
C(2′)—C(3′)—C(4′)	120·8 (5)	120·7 (8)
C(3′)—C(4′)—C(5′)	117·3 (4)	117·7 (7)
C(3′)—C(4′)—C(7′)	121·0 (4)	—
C(3′)—C(4′)—O(1′)	—	124·8 (6)
C(5′)—C(4′)—C(7′)	121·7 (5)	—
C(5′)—C(4′)—O(1′)	—	117·6 (6)
C(4′)—C(5′)—C(6′)	122·8 (5)	121·1 (9)
C(1′)—C(6′)—C(5′)	120·1 (4)	121·7 (8)
C(4′)—O(1′)—C(7′)	—	119·8 (5)
C(4)—C(4*a*)—N(10)	121·1 (3)	121·9 (5)
C(4)—C(4*a*)—C(9*a*)	119·1 (4)	119·6 (5)
N(10)—C(4*a*)—C(9*a*)	119·7 (3)	118·5 (4)
C(8)—C(8*a*)—C(9)	121·9 (4)	121·3 (5)
C(8)—C(8*a*)—C(10*a*)	117·9 (4)	118·4 (5)
C(9)—C(8*a*)—C(10*a*)	120·1 (3)	120·3 (5)
C(1)—C(9*a*)—C(9)	121·7 (3)	121·9 (5)
C(1)—C(9*a*)—C(4*a*)	118·3 (3)	117·5 (4)
C(9)—C(9*a*)—C(4*a*)	120·0 (4)	120·7 (5)
C(5)—C(10*a*)—N(10)	121·7 (4)	121·1 (5)
C(5)—C(10*a*)—C(8*a*)	118·8 (4)	119·2 (5)
N(10)—C(10*a*)—C(8*a*)	119·6 (4)	119·6 (5)

Introduction. This paper contains the structure determinations of two acridinium derivatives, one where the phenyl group is substituted with a methyl group (*A*), the other where it is substituted with a methoxy group (*B*).

Experimental. Structure (*A*): A yellow brick-shaped crystal (dimensions 0·15 × 0·15 × 0·25 mm approximately) was used for data collection on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Cu $K\alpha$ radiation and ω–2θ scans. A total of 3407 unique reflections was measured within the range $0 \le h \le 9$, $0 \le k \le 20$, $-16 \le l \le 15$. Of these, 2242 were above the significance level of $2{\cdot}5\sigma(I)$. The maximum value of $(\sin\theta)/\lambda$ was 0·61 Å^{-1}. Two standard reflections (022, $01\bar{1}$) were measured hourly, the intensity showed no significant decrease during the 38 h collection time. Unit-cell parameters were refined by a least-squares fitting procedure using 23 reflections with $61 < 2\theta < 80°$. Corrections for Lorentz and polarization effects were applied. The structure was determined by direct methods using the program *SIMPEL* (Schenk & Kiers, 1983). The H atoms were derived from a ΔF synthesis. Block-diagonal least-squares refinement on F, anisotropic for the non-H and isotropic for the H atoms, converged to $R = 0{\cdot}067$, $wR = 0{\cdot}092$, $(\Delta/\sigma)_{\max} = 0{\cdot}73$. A weighting scheme $w = (5{\cdot}54 + F_o + 0{\cdot}010F_o^2)^{-1}$ was used. The isotropic secondary-extinction coefficient refined to $1{\cdot}4\,(1) \times 10^{-3}$ (Zachariasen, 1968). An empirical absorption correction was applied, with corrections in the range 0·67–1·52 (*DIFABS*; Walker & Stuart, 1983). A final difference synthesis revealed residual electron density between $-0{\cdot}3$ and 0·5 e Å^{-3}. One O atom of the perchlorate ion (O3) is markedly anisotropic.

Structure (*B*): A brown-yellow pillar-shaped crystal (dimensions 0·10 × 0·10 × 0·38 mm approximately) was used for data collection on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Cu $K\alpha$ radiation and ω–2θ scans. A total of 2866 unique reflections was measured within the range $-8 \le h \le 9$, $0 \le k \le 18$, $0 \le l \le 15$. Of these, 2070 were above the significance level of $2{\cdot}5\,\sigma(I)$. The maximum value of $(\sin\theta)/\lambda$ was 0·56 Å^{-1}. Two standard reflections (213, $\bar{2}01$) were measured hourly, the intensity showed no significant decrease during the 25 h collection time. Unit-cell parameters were refined by a least-squares fitting procedure using 23 reflections with $70 < 2\theta < 80°$. Structure solution and refinement as for (*A*). $R = 0{\cdot}084$, $wR = 0{\cdot}123$, $(\Delta/\sigma)_{\max} = 0{\cdot}77$. A weighting scheme $w = (2{\cdot}88 + F_o + 0{\cdot}011F_o^2)^{-1}$ was used. The isotropic secondary-extinction coefficient refined to $8\,(2) \times 10^{-4}$ (Zachariasen, 1968). An empirical absorption correction was applied, with corrections in the range 0·69–1·27 (*DIFABS*; Walker & Stuart, 1983). A final difference Fourier map revealed residual electron density between $-0{\cdot}4$ and 0·5 e Å^{-3}.

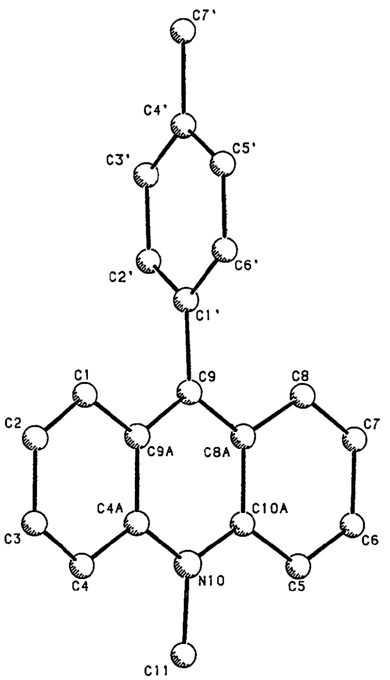

Fig. 1. Structure of $[C_{21}H_{18}N]^+$ showing the numbering scheme.

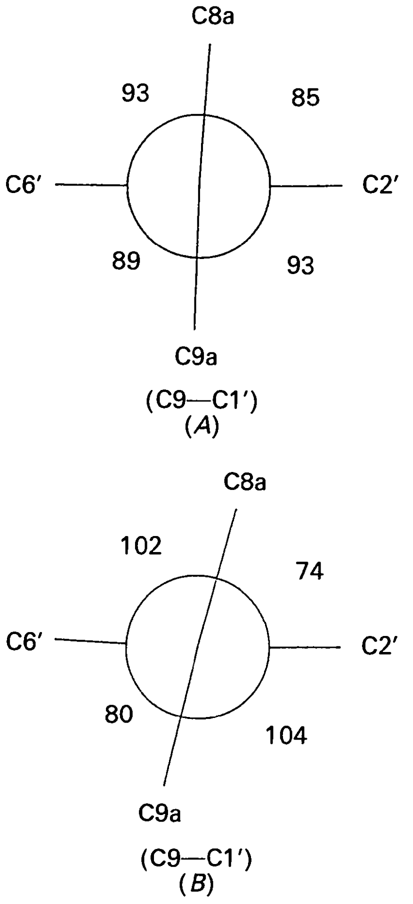

Fig. 2. The Newman projection along the C(9)—C(1') bond.

Here also one O atom of the perchlorate ion (O3) is markedly anisotropic.

For both structures: 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 *et al.*, 1976), unless stated otherwise.

Discussion. Final positional parameters for the non-H atoms for both structures are listed in Table 1.* Bond lengths and bond angles are listed in Table 2. A *PLUTO* (Motherwell & Clegg, 1978) drawing of molecule (*A*), showing the numbering scheme, is given in Fig. 1 [the numbering of (*B*) is similar] and the Newman projections along the C9—C1′ bond for (*A*) and (*B*) are depicted in Fig. 2.

A least-squares plane through the acridinium atoms of (*A*) shows that the maximum distance of one of its constituent atoms from the plane is 0·082 Å. The phenyl ring of (*A*) is planar to within 0·011 Å. The angle between the two planes of (*A*) is 78°. For structure (*B*) the corresponding values are 0·124, 0·011 Å and 88° respectively. The angle between the two least-squares planes through the atoms C(1), C(2), C(3), C(4), C(4*a*), C(9*a*), C(9) and N(10) and the atoms C(5), C(6), C(7), C(8), C(8*a*), C(10*a*), C(9) and N(10) in (*B*) is 7°. The only significant difference between the two structures is in the twist angle. Matching of the two molecules [leaving out the perchlorates, all H atoms and C(7′) in structure (*B*)] resulted in an r.m.s. value of 0·11 Å. The largest distances between the corresponding atoms occur at C2′, C3′, C5′ and C6′ (about 0·2 Å).

References

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* **A24**, 321–324.

International Tables for X-ray Crystallography (1974). Vol. IV, p.55. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

Schenk, H. & Kiers, C. T. (1983). *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.

---

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond distances and angles involving H atoms and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52628 (47 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1990). **C46**, 1084–1086

Crystal Studies of Acridinium Dyes. XIV.* 10-Methyl-9-[2-methyl-4-(1,4,7,10-tetraoxa-13-aza-13-cyclopentadecyl)phenyl]acridinium Potassium Dithiocyanate Acetonitrile Solvate

By Celeste A. Reiss, Kees Goubitz and Dick Heijdenrijk

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

(*Received* 10 *July* 1989; *accepted* 6 *September* 1989)

Abstract. $C_{31}H_{37}N_2O_4^+.K^+.2SCN^-.CH_3CN$, M_r = 698·0, triclinic, $P\bar{1}$, a = 13·460 (2), b = 15·760 (2), c = 8·646 (1) Å, α = 101·88 (2), β = 95·23 (2), γ = 81·52 (2)°, V = 1771·7 (8) Å^3, Z = 2, D_x = 1·31 g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ = 27·6 cm^{-1}, F(000) = 736, room temperature. Final R = 0·048 for 4101 observed reflections. The angle between the planes of the acridinium and the phenyl groups is 85°. The mean cavity radius of the crown ether is 1·47 Å. The K atom is six coordinated by the four O atoms of the crown ether and by two N atoms, one of a thiocyanate ion the other of the acetonitrile solvent.

Introduction. This is the fourteenth paper in a series of acridinium dyes. In this case the phenyl ring is

---

* Part XIII, preceding paper.

0108-2701/90/061084-03$03.00