

## Structure of 5-Chloro-2-{3-[(diethylamino)methyl]-5-methyl-4*H*-1,2,4-triazol-4-yl}benzophenone (I) and of its Methylamino Analogue (II)\*

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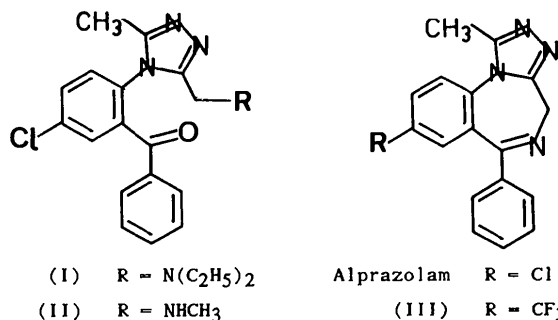
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**Abstract.** (I)  $C_{21}H_{23}ClN_4O$ ,  $M_r = 382.9$ , monoclinic,  $C2/c$ ,  $a = 8.914(4)$ ,  $b = 15.553(4)$ ,  $c = 28.808(7)$  Å,  $\beta = 92.88(3)^\circ$ ,  $V = 3988.9$  Å<sup>3</sup>,  $Z = 8$ ,  $D_x = 1.275$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 2.03$  cm<sup>-1</sup>,  $F(000) = 1616$ ,  $T = 294$  K,  $R = 0.0547$  for 795 observed reflections. (II)  $C_{18}H_{17}ClN_4O$ ,  $M_r = 340.8$ , triclinic,  $P\bar{1}$ ,  $a = 7.381(6)$ ,  $b = 8.345(3)$ ,  $c = 14.955(4)$  Å,  $\alpha = 89.72(2)$ ,  $\beta = 78.89(4)$ ,  $\gamma = 68.97(4)^\circ$ ,  $V = 841.6$  Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 1.345$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 2.32$  cm<sup>-1</sup>,  $F(000) = 356$ ,  $T = 293$  K,  $R = 0.0412$  for 2447 observed reflections. Both benzophenones can be formally derived from the triazolobenzodiazepine alprazolam by splitting of the C=N double bond of the seven-membered heterocyclic ring. In (I) the N(5)⋯C(6) distance is 4.94(1) Å and the seven-atom chain bears little resemblance to its seven-membered ring precursor. In (II), however, the corresponding N⋯C distance is only 3.494(3) Å and the seven-atom chain is more nearly ring shaped. Corresponding bond lengths and angles in the two structures are generally similar and agree well with accepted values.

**Introduction.** Certain *N*-alkylaminobenzophenones, which may be considered as open-ring analogues of benzodiazepines, have been found to possess anxiolytic activity. In general this activity, as measured by the pentylenetetrazole and other tests, is comparable to that of the analogous benzodiazepine (Gall, Hester, Rudzik & Lahti, 1976). However, the benzophenones show a low affinity for the benzodiazepine receptor *in vitro* (Hirai, Ishiba, Sugimoto, Fujishita, Tsukinoki & Hirose, 1981). Lahti & Gall (1976) and Hirai, Fujishita, Ishiba, Sugimoto, Matsutani, Tsukinoki & Hirose (1982) have suggested that benzophenones of this type can act as prodrugs, undergoing *N*-dealkylation and ring closure *in vivo* to form the corresponding benzodiazepine. The observed pharmacological activity of these benzophenones may therefore be due to the formation of active benzodiazepines rather than to any intrinsic activity of their own. We now report the crystal

structures of the title compounds which, in the pentylenetetrazole test, have activity comparable to that of alprazolam (III),† their benzodiazepine analogue.



**Experimental.** Compound (I): crystals were grown from amyl acetate/ethanol. A crystal of size 0.15 × 0.15 × 0.3 mm was mounted on an Enraf–Nonius CAD-4 diffractometer; cell dimensions from setting angles of 24 reflections having  $8 < \theta < 12^\circ$ . Data collection by  $\omega$ - $2\theta$  scans,  $2 < \theta < 25^\circ$ ; two standard reflections measured every 2 h showed no significant variation; 3757 reflections scanned, 3515 unique,  $R_{int} = 0.026$ ; of these 795 having  $I > 2.5\sigma(I)$  were considered observed and used in the analysis, index range  $-10 \leq h \leq 10$ ,  $0 \leq k \leq 16$ ,  $0 \leq l \leq 32$ ; no absorption corrections applied.

Structure determined by direct methods; full-matrix least-squares refinement on  $F$  magnitudes; owing to poor quality of data only Cl, N and O atoms refined with anisotropic temperature factors, C atoms treated isotropically; H atoms placed in calculated positions riding on their respective bonded atoms, overall temperature factor refined to 0.11(2) Å<sup>2</sup> for methyl H atoms and to 0.08(1) Å<sup>2</sup> for remaining H atoms. Final  $R = 0.0547$ ,  $wR = 0.0529$  for the 795 observed reflections,  $w = 1/[\sigma^2(F) + 0.0002F^2]$ , maximum shift/e.s.d. 0.02; residual electron density in final difference map  $\pm 0.3$  e Å<sup>-3</sup>. No correction for secondary extinction.

\* Contribution from the Crystallography Unit, Universities of Aston and Birmingham.

† 8-Chloro-1-methyl-6-phenyl-4*H*-s-triazolo[4,3-*a*][1,4]benzodiazepine. Marketed as Xanax (Upjohn).

Compound (II): diffractometer measurements and structure determination as for compound (I) except: crystal size 0.3 × 0.6 × 0.7 mm,  $\theta$  range for cell refinement 17–24°. 3235 reflections scanned, 2981 unique,  $R_{\text{int}} = 0.014$ , 2447 considered observed [ $I > 2.5\sigma(I)$ ], index range  $-8 \leq h \leq 8$ ,  $-9 \leq k \leq 9$ ,  $0 \leq l \leq 17$ ; all non-H atoms refined anisotropically, H atoms located from difference syntheses and refined with isotropic temperature factors. Final  $R = 0.0412$ ,  $wR = 0.0685$ ,  $w = 1/[\sigma^2(F) + 0.0015F^2]$ , max. shift/e.s.d. = 0.04; residual electron density  $\pm 0.33 \text{ e \AA}^{-3}$ . The atomic coordinates for molecules (I) and (II) are listed in Tables 1 and 2\* respectively.

Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Computations were carried out on the University of Birmingham Honeywell DPS 8/70 computer and on the CDC 7600 at the University of Manchester Regional Computer Centre with the *SHELX76* (Sheldrick, 1978) and *PLUTO78* (Motherwell & Clegg, 1978) programs.

**Discussion.** Bond lengths and angles for molecules (I) and (II) are listed in Tables 3 and 4 and selected torsion angles are compared in Table 5. The structures are illustrated in Figs. 1 and 2.

In view of the possible biotransformation of the title compounds into the triazolobenzodiazepine alprazolam (Lahti & Gall, 1976; Hirai *et al.*, 1982), it is of interest to compare their structures with that of alprazolam, in which N(5) and C(6) are linked by a double bond. It can be seen from Figs. 1 and 2 that in neither structure is there evidence of any attractive interaction between N(5) and C(6). In (I) the N(5) to C(6) distance is 4.936 (12) Å and the conformation about C(3)—C(4) is such as to rotate N(5) away from the C(6)=O carbonyl group. In (II), on the other hand, the N(5)···C(6) distance is 3.494 (3) Å, and the seven-atom chain, C(6)—C(12)—C(11)—N(1)—C(3)—C(4)—N(5), takes up a vaguely cyclic shape. There is, however, no hydrogen bonding between the carbonyl O atom and the H atom linked to N(5) since these atoms point away from one another (see Fig. 2).

The relative spatial positions of N(5) and C(6) are determined largely by the conformations about the bonds C(11)—N(1) and C(3)—C(4), the conformation angles about the cyclic bonds C(12)—C(11) and N(1)—C(3) being geometrically limited to values near to zero. In Table 5 the relevant torsion angles are compared with the corresponding values found in

Table 1. Fractional atomic coordinates ( $\times 10^4$ ) with e.s.d.'s in parentheses and isotropic temperature factors ( $\text{\AA}^2 \times 10^3$ ) for compound (I)

	x	y	z	$U_{\text{iso}}$
Cl(8)	990 (3)	2635 (2)	3352 (1)	51*
O	7543 (9)	2893 (5)	3076 (2)	61*
N(1)	7214 (9)	2790 (6)	4165 (3)	33*
N(2)	9272 (10)	2437 (7)	4560 (3)	51*
N(3)	9450 (9)	3267 (7)	4385 (3)	49*
N(5)	7081 (9)	4874 (5)	4205 (3)	39*
C(1)	7936 (12)	2161 (7)	4430 (4)	35 (3)
C(3)	8200 (13)	3453 (7)	4152 (4)	34 (3)
C(4)	7869 (12)	4279 (7)	3904 (4)	40 (3)
C(6)	6709 (12)	2326 (7)	3185 (3)	34 (3)
C(7)	3976 (11)	2490 (7)	3310 (3)	43 (3)
C(8)	2827 (10)	2675 (7)	3595 (3)	33 (3)
C(9)	3046 (12)	2864 (6)	4059 (4)	38 (3)
C(10)	4530 (11)	2897 (6)	4244 (3)	37 (3)
C(11)	5705 (11)	2728 (7)	3965 (4)	34 (3)
C(12)	5451 (10)	2530 (6)	3502 (3)	31 (3)
C(13)	7288 (13)	1323 (7)	4546 (4)	56 (4)
C(14)	8197 (13)	5342 (7)	4511 (4)	56 (4)
C(15)	7449 (15)	5828 (8)	4896 (4)	75 (4)
C(16)	6198 (13)	5507 (7)	3915 (4)	54 (4)
C(17)	4779 (13)	5095 (8)	3702 (4)	68 (4)
C(1')	6810 (12)	1437 (7)	3008 (4)	35 (3)
C(2')	6008 (13)	762 (7)	3180 (4)	49 (3)
C(3')	6157 (14)	-77 (8)	3019 (4)	67 (4)
C(4')	7161 (13)	-205 (8)	2657 (4)	56 (4)
C(5')	7949 (14)	455 (7)	2499 (5)	69 (4)
C(6')	7848 (12)	1289 (8)	2660 (3)	47 (3)

\* Atoms refined anisotropically;  $U_{\text{eq}}$  shown, where  $U_{\text{eq}} = 1/3 \times$  (trace of the orthogonalized  $U$  tensor).

Table 2. Fractional atomic coordinates ( $\times 10^4$ ) with e.s.d.'s in parentheses and equivalent isotropic temperature factors ( $\text{\AA}^2 \times 10^3$ ) for compound (II)

$U_{\text{eq}}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U_{\text{eq}}$
Cl(8)	6335 (1)	-427 (1)	2875 (1)	55
O	-1090 (2)	6014 (2)	3290 (1)	57
N(1)	554 (2)	5246 (2)	1358 (1)	36
N(2)	-2233 (2)	6538 (2)	918 (1)	44
N(3)	-1005 (3)	7445 (2)	646 (1)	47
N(5)	2975 (3)	7430 (3)	1590 (2)	62
C(1)	-1284 (3)	5227 (3)	1335 (1)	39
C(3)	652 (3)	6651 (3)	914 (1)	41
C(4)	2426 (4)	7154 (4)	751 (2)	56
C(6)	658 (3)	5537 (3)	3306 (1)	43
C(7)	3509 (3)	2723 (3)	2987 (1)	40
C(8)	4787 (3)	1315 (2)	2410 (1)	38
C(9)	4809 (3)	1260 (3)	1490 (2)	41
C(10)	3428 (3)	2586 (3)	1150 (1)	39
C(11)	2066 (3)	3957 (2)	1729 (1)	35
C(12)	2119 (3)	4073 (3)	2649 (1)	38
C(13)	-2027 (4)	3894 (4)	1716 (2)	54
C(14)	1665 (5)	9015 (4)	2115 (3)	78
C(1')	1403 (3)	6301 (3)	3979 (1)	45
C(2')	3349 (4)	6223 (3)	3845 (2)	58
C(3')	3939 (5)	7008 (4)	4484 (2)	72
C(4')	2617 (6)	7828 (5)	5267 (3)	82
C(5')	676 (6)	7930 (4)	5401 (2)	79
C(6')	75 (4)	7176 (3)	4766 (2)	59

\* 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 52355 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

the crystal structure of the 8-trifluoromethyl analogue of alprazolam (Kemmish & Hamor, 1988).

It can be seen that the major difference between structure (II) and the alprazolam analogue (III) is in

Table 3. Bond lengths (Å) and bond angles (°) with *e.s.d.*'s in parentheses for compound (I)

C(8)—C(8)	1.749 (9)	C(7)—C(8)	1.374 (11)
O—C(6)	1.205 (11)	C(7)—C(12)	1.402 (11)
N(1)—C(1)	1.382 (12)	C(8)—C(9)	1.373 (11)
N(1)—C(3)	1.357 (11)	C(9)—C(10)	1.402 (12)
N(1)—C(11)	1.439 (11)	C(10)—C(11)	1.377 (12)
N(2)—N(3)	1.397 (12)	C(11)—C(12)	1.375 (11)
N(2)—C(1)	1.303 (12)	C(14)—C(15)	1.523 (13)
N(3)—C(3)	1.305 (12)	C(16)—C(17)	1.520 (13)
N(5)—C(4)	1.471 (12)	C(1')—C(2')	1.375 (13)
N(5)—C(14)	1.486 (12)	C(1')—C(6')	1.417 (13)
N(5)—C(16)	1.491 (11)	C(2')—C(3')	1.394 (14)
C(1)—C(13)	1.470 (13)	C(3')—C(4')	1.421 (14)
C(3)—C(4)	1.493 (13)	C(4')—C(5')	1.335 (13)
C(6)—C(12)	1.516 (12)	C(5')—C(6')	1.382 (13)
C(6)—C(1')	1.479 (13)		

C(1)—N(1)—C(3)	105.6 (8)	C(8)—C(8)—C(9)	118.8 (8)
C(1)—N(1)—C(11)	125.0 (10)	C(7)—C(8)—C(9)	123.5 (9)
C(3)—N(1)—C(11)	129.4 (10)	C(8)—C(9)—C(10)	117.5 (10)
N(3)—N(2)—C(1)	108.7 (10)	C(9)—C(10)—C(11)	120.2 (10)
N(2)—N(3)—C(3)	106.3 (10)	N(1)—C(11)—C(10)	118.5 (9)
C(4)—N(5)—C(14)	109.4 (8)	N(1)—C(11)—C(12)	120.5 (9)
C(4)—N(5)—C(16)	109.8 (8)	C(10)—C(11)—C(12)	121.0 (9)
C(14)—N(5)—C(16)	109.2 (8)	C(6)—C(12)—C(7)	117.4 (9)
N(1)—C(1)—N(2)	108.6 (10)	C(6)—C(12)—C(11)	122.8 (8)
N(1)—C(1)—C(13)	125.2 (10)	C(7)—C(12)—C(11)	119.9 (10)
N(2)—C(1)—C(13)	126.3 (12)	N(5)—C(14)—C(15)	111.7 (9)
N(1)—C(3)—N(3)	110.8 (10)	N(5)—C(16)—C(17)	110.7 (9)
N(1)—C(3)—C(4)	123.7 (10)	C(6)—C(1')—C(2')	123.3 (11)
N(3)—C(3)—C(4)	125.5 (11)	C(6)—C(1')—C(6')	116.6 (11)
N(5)—C(4)—C(3)	110.3 (9)	C(2')—C(1')—C(6')	120.0 (11)
O—C(6)—C(12)	119.3 (10)	C(1')—C(2')—C(3')	122.4 (12)
O—C(6)—C(1')	123.1 (11)	C(2')—C(3')—C(4')	116.6 (13)
C(12)—C(6)—C(1')	117.6 (10)	C(3')—C(4')—C(5')	120.3 (12)
C(8)—C(7)—C(12)	117.9 (9)	C(4')—C(5')—C(6')	124.2 (13)
C(8)—C(8)—C(7)	117.7 (7)	C(1')—C(6')—C(5')	116.4 (12)

Table 4. Bond lengths (Å) and bond angles (°) with *e.s.d.*'s in parentheses for compound (II)

C(8)—C(8)	1.734 (2)	C(6)—C(1')	1.481 (3)
O—C(6)	1.211 (3)	C(7)—C(8)	1.384 (3)
N(1)—C(1)	1.369 (3)	C(7)—C(12)	1.393 (3)
N(1)—C(3)	1.361 (3)	C(8)—C(9)	1.373 (3)
N(1)—C(11)	1.443 (2)	C(9)—C(10)	1.381 (3)
N(2)—N(3)	1.382 (3)	C(10)—C(11)	1.385 (3)
N(2)—C(1)	1.299 (3)	C(11)—C(12)	1.389 (3)
N(3)—C(3)	1.305 (3)	C(1')—C(2')	1.389 (4)
N(5)—C(4)	1.435 (4)	C(1')—C(6')	1.389 (3)
N(5)—C(14)	1.450 (4)	C(2')—C(3')	1.380 (4)
C(1)—C(13)	1.474 (3)	C(3')—C(4')	1.371 (5)
C(3)—C(4)	1.490 (3)	C(4')—C(5')	1.379 (5)
C(6)—C(12)	1.509 (3)	C(5')—C(6')	1.365 (4)

C(1)—N(1)—C(3)	105.3 (2)	C(8)—C(8)—C(9)	120.0 (1)
C(1)—N(1)—C(11)	125.6 (2)	C(7)—C(8)—C(9)	121.4 (2)
C(3)—N(1)—C(11)	129.0 (2)	C(8)—C(9)—C(10)	118.9 (2)
N(3)—N(2)—C(1)	108.0 (2)	C(9)—C(10)—C(11)	120.2 (2)
N(2)—N(3)—C(3)	107.3 (2)	N(1)—C(11)—C(10)	118.3 (2)
C(4)—N(5)—C(14)	114.1 (3)	N(1)—C(11)—C(12)	120.6 (2)
N(1)—C(1)—N(2)	109.5 (2)	C(10)—C(11)—C(12)	121.1 (2)
N(1)—C(1)—C(13)	124.4 (2)	C(6)—C(12)—C(7)	118.8 (2)
N(2)—C(1)—C(13)	126.1 (2)	C(6)—C(12)—C(11)	122.8 (2)
N(1)—C(3)—N(3)	109.9 (2)	C(7)—C(12)—C(11)	118.2 (2)
N(1)—C(3)—C(4)	124.1 (2)	C(6)—C(1')—C(2')	122.9 (2)
N(3)—C(3)—C(4)	126.0 (2)	C(6)—C(1')—C(6')	118.3 (2)
N(5)—C(4)—C(3)	111.7 (2)	C(2')—C(1')—C(6')	118.8 (2)
O—C(6)—C(12)	119.4 (2)	C(1')—C(2')—C(3')	120.2 (3)
O—C(6)—C(1')	121.8 (2)	C(2')—C(3')—C(4')	120.0 (3)
C(12)—C(6)—C(1')	118.7 (2)	C(3')—C(4')—C(5')	120.1 (3)
C(8)—C(7)—C(12)	120.0 (2)	C(4')—C(5')—C(6')	120.2 (3)
C(8)—C(8)—C(7)	118.6 (2)	C(1')—C(6')—C(5')	120.6 (3)

Table 5. Selected torsion angles (°) for compounds (I) and (II) and for alprazolam analogue (III) (Kemmish &amp; Hamor, 1988)

*E.s.d.*'s are approximately 1.5 (I), 0.4 (II) and 0.8° (III).

	(I)	(II)	(III)
C(6)—C(12)—C(11)—N(1)	3.0	-1.2	0.6
C(12)—C(11)—N(1)—C(3)	81.1	96.8	44.2
C(11)—N(1)—C(3)—C(4)	-1.1	-1.9	-6.7
N(1)—C(3)—C(4)—N(5)	85.5	-58.4	-67.0
O—C(6)—C(12)—C(11)	-70.1	45.0	-44.7*
C(3)—C(4)—N(5)—H(5)	—	168	68.0†
C(12)—C(6)—C(1')—C(2')	-11.9	24.4	-30.1

\* Torsion angle N(5)—C(6)—C(12)—C(11) in (III).

† Torsion angle C(3)—C(4)—N(5)—C(6) in (III).

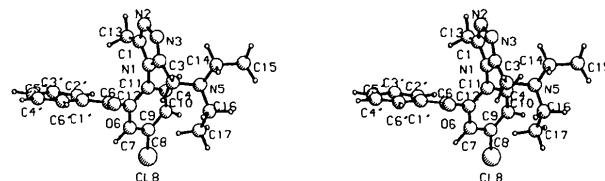


Fig. 1. Stereoscopic view of molecule (I) showing the atom numbering.

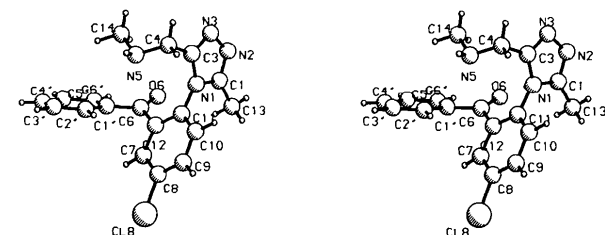


Fig. 2. Stereoscopic view of molecule (II).

the conformation about C(11)—N(1), *i.e.* a difference of 52.6° in the orientation of the triazolo ring relative to the chlorophenyl ring. A rotation of some 53° would, in fact, bring C(6) and N(5) into close proximity.

In the case of structure (I), the differences are greater; the major difference is in the conformation about C(3)—C(4); the torsion angles about this bond differ by 152.5° so that N(5) is directed away from C(6). Furthermore, the orientation of the triazolo ring relative to the chlorophenyl ring differs by 37.6° from that in (III).

The orientation of the C(6)=O carbonyl bond with respect to the N(5)—H bond in (II), of interest in connection with the possibility of hydrogen bond formation, involves also the conformations about C(6)—C(12) and C(4)—N(5). The pertinent torsion angles are listed in Table 5.

Bond lengths and angles are unexceptional. The lengths of the N(2)—C(1) and N(3)—C(3) formal double bonds are 1.303 (12) and 1.305 (12) Å in (I), and 1.299 (3) and 1.305 (3) Å in (II), in good agreement with the value of 1.303 Å in (III). These lengths are slightly greater than the standard N=C

value of 1.28 Å (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987), while the N(1)—C(1) and N(1)—C(3) formal single bonds are shortened from the theoretical N—C(*sp*<sup>2</sup>) single-bond value of *ca* 1.45 Å, indicative of electron delocalization in the triazolo ring. The triazolo ring is planar to within ±0.004 Å in both structures. The angles C(11)—N(1)—C(3) and N(1)—C(3)—C(4) are 129.4 (10) and 123.7 (10)°, respectively, in (I), and 129.0 (2) and 124.1 (2)° in (II), so that the geometry of the N(1)—C(3) bond resembles that of a double bond, as in (III) and in the classical benzodiazepin-2-ones (Hamor & Martin, 1983).

The bond lengths at the C(6) carbonyl group appear to show that there is little if any conjugation between the O atom and the aromatic rings. The C—C bonds are in the range 1.479–1.516 Å and the C=O bonds are 1.205 (11) and 1.211 (3) Å, corresponding, respectively, to C(*sp*<sup>2</sup>)—C(*sp*<sup>2</sup>) single and C=O double bonds. These values are similar to those in 2-*tert*-butylbenzophenone (Wagner, Giri, Scaiano, Ward, Gabe & Lee, 1985) and other benzophenones in which the carbonyl O atom is not involved in hydrogen bonding (Faerman, Nyburg, Punte, Rivero, Vitale & Nudelman, 1985). The angle between the two aromatic rings is 73 (2)° in (I) and 61.1 (5)° in (II). The comparable dihedral angle in the alprazolam analogue (III) is similar, 63.5°.

In both structures intermolecular contacts involve only normal van der Waals interactions.

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## Crystal Studies of Acridinium Dyes. X. 10-Methyl-9-[2-methyl-4-(1,4,7,10-tetraoxa-13-aza-13-cyclopentadecyl)phenyl]acridinium Barium Perchlorate Acetonitrile (1/1)

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**Abstract.** C<sub>31</sub>H<sub>37</sub>N<sub>2</sub>O<sub>4</sub><sup>+</sup>.Ba<sup>2+</sup>.3ClO<sub>4</sub><sup>-</sup>.C<sub>2</sub>H<sub>3</sub>N, *M*<sub>r</sub> = 978.4, monoclinic, *P*2<sub>1</sub>/*a*, *a* = 22.089 (5), *b* = 13.707 (3), *c* = 13.081 (4) Å, β = 93.50 (2)°, *V* = 3953 (2) Å<sup>3</sup>, *Z* = 4, *D*<sub>x</sub> = 1.64 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.71069 Å, μ = 12.8 cm<sup>-1</sup>, *F*(000) = 1976, room temperature. Final *R* = 0.056 for 4074 observed reflections. The angle between the acridinium and phenyl groups is 79°. The mean cavity radius for the crown ether is 1.51 Å. There are nine Ba—O distances in the range 2.77 (1)–3.00 (1) Å. In addition, there are

two larger Ba—O (perchlorate) and Ba—N distances of 3.29 (2) and 3.26 (1) Å respectively.

**Introduction.** The title compound is the tenth structure in a series of acridinium dyes (I: Goubitz, Reiss, Heijdenrijk, Jonker & Verhoeven, 1989; II, IV: Reiss, Goubitz & Heijdenrijk, 1989*a,b*; III, VII: Kronenburg, Goubitz, Reiss & Heijdenrijk, 1989*a,b*; V, VIII: Goubitz, Reiss & Heijdenrijk, 1989*a,b*; VI: Zoutberg, Reiss, Goubitz & Heijdenrijk, 1989; IX: Reiss, Gou-