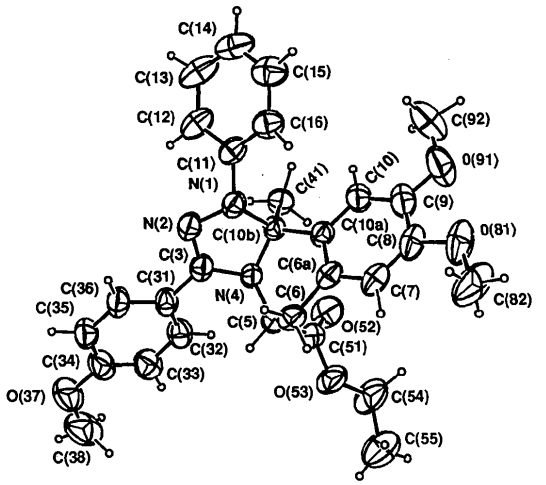

Fig. 1. *ORTEP*II (Johnson, 1976) view of the molecule.

(3), but not the stereochemistry; thus the crystal structure determination of (3) was undertaken.

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Ethanol Complex of 1,3-Diethoxy-*p*-*tert*-butylcalix[4]arene

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Abstract. 26,28-Diethoxy-5,11,17,23-tetrakis(1,1-dimethylethyl)pentacyclo[19.3.1.1^{3,7}.1^{9,13}.1^{15,19}]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-25,27-diol–ethanol (1/1), $C_{48}H_{64}O_4.C_2H_5OH$, $M_r = 751.1$, triclinic, $P\bar{1}$, $a = 12.384$ (1), $b = 17.786$ (1), $c = 21.903$ (2) Å, $\alpha = 97.68$ (1), $\beta = 96.96$ (1), $\gamma = 105.73$ (1)°, $V = 4539$ (1) Å^3, $Z = 4$, $D_x = 1.099$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 5.04$ cm^{-1}, $F(000) = 1640$, $T = 148$ (5) K, final $R = 0.080$ for 8510 observed reflections. The unit cell contains two independent calixarene molecules, with the same cone conformation. In both calixarenes an ethanol molecule could be located, with rather high thermal parameters, indicating disorder.

Experimental. The title compound was obtained as colourless crystals, with dimensions 0.4 × 0.5 × 0.7 mm, by recrystallization of 1,3-diethoxy-*p*-*tert*-butylcalix[4]arene (Ghidini, Ugozolli, Ungaro, Harkema, Abu El-Fadl & Reinhoudt, 1990) from a 1:1 mixture of chloroform and ethanol. The complex loses ethanol at about 395 K and has an ultimate m.p. of 551–554 K. A preliminary structure determination at room temperature indicated disorder. Therefore intensities were measured at 148 (5) K on a Philips PW 1100 diffractometer using graphite-monochromated Cu $K\alpha$ radiation. Lattice parameters were determined from 21 reflections ($6 < \theta < 15$°) by repeated measurement.

A total of 11384 unique reflections up to $\theta = 55$° ($-13 \le h \le 12$, $-18 \le k \le 18$, $0 \le l \le 23$) were measured in the $\omega/2\theta$ scan mode [scan width (ω) = (1.90 + 0.80tanθ)°, scan speed (ω) = 0.2° s^{-1}]; 8510 were considered observed [$F_o^2 > 2\sigma(F_o^2)$]. Three reference reflections were measured every 60 min; a correction for long-term variations (Dam, Harkema & Feil, 1983) was applied (maximum variation 5%). No absorption correction was applied.

The crystal contains two independent calixarene molecules in a cone conformation. In the cavity of both calixarenes an ethanol molecule was found and refined, resulting in rather high thermal parameters

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for non-*H *atoms with e.s.d.'s in parentheses*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$. Atoms indicated with an asterisk were refined with isotropic thermal parameters.

	x	*y*	*z*	B_{eq}
O12	0.1730 (2)	0.4738 (2)	0.0922 (1)	1.97 (7)
O32	0.0792 (3)	0.4102 (2)	−0.0272 (1)	2.59 (8)
O52	0.2937 (3)	0.3976 (2)	−0.0673 (1)	2.16 (7)
O72	0.3872 (3)	0.4513 (2)	0.0543 (1)	2.42 (8)
O101*A*	0.0614 (9)	0.0849 (6)	−0.0117 (4)	7.3 (3)
O101*B*	−0.0219 (9)	0.1355 (6)	0.0773 (5)	8.7 (3)
O412	1.0423 (2)	0.3464 (2)	0.5395 (2)	2.32 (8)
O432	0.9216 (3)	0.4510 (2)	0.5579 (1)	2.45 (8)
O452	0.9149 (2)	0.4271 (2)	0.6890 (1)	2.12 (7)
O472	1.0354 (3)	0.3224 (2)	0.6737 (2)	2.75 (8)
O501	0.4903 (5)	0.2183 (3)	0.5402 (3)	9.3 (2)
C1	0.1402 (4)	0.4181 (3)	0.1308 (2)	1.8 (1)
C2	0.0276 (4)	0.3740 (3)	0.1229 (2)	1.8 (1)
C3	−0.0036 (4)	0.3196 (3)	0.1619 (2)	2.0 (1)
C4	0.0749 (4)	0.3084 (3)	0.2084 (2)	2.0 (1)
C5	0.1882 (4)	0.3517 (3)	0.2126 (2)	1.9 (1)
C6	0.2245 (4)	0.4055 (3)	0.1745 (2)	1.7 (1)
C7	0.0413 (4)	0.2501 (3)	0.2532 (2)	2.2 (1)
C8	0.1015 (5)	0.1851 (3)	0.2438 (3)	3.7 (1)
C9	−0.0864 (4)	0.2105 (3)	0.2435 (3)	3.4 (1)
C10	0.0789 (5)	0.2945 (3)	0.3211 (2)	3.5 (1)
C11	−0.0607 (4)	0.3817 (3)	0.0708 (2)	2.1 (1)
C13	0.1814 (4)	0.5544 (3)	0.1203 (2)	2.4 (1)
C14	0.2579 (4)	0.6094 (3)	0.0870 (3)	3.2 (1)
C21	−0.0022 (4)	0.3387 (3)	−0.0325 (2)	2.0 (1)
C22	−0.0750 (4)	0.3224 (3)	0.0107 (2)	1.9 (1)
C23	−0.1605 (4)	0.2510 (3)	−0.0017 (2)	2.1 (1)
C24	−0.1784 (4)	0.1953 (3)	−0.0555 (2)	2.0 (1)
C25	−0.1013 (4)	0.2137 (3)	−0.0966 (2)	2.1 (1)
C26	−0.0134 (4)	0.2829 (3)	−0.0863 (2)	1.9 (1)
C27	−0.2759 (4)	0.1188 (3)	−0.0713 (2)	2.7 (1)
C28	−0.2298 (5)	0.0471 (3)	−0.0784 (3)	4.2 (2)
C29	−0.3529 (5)	0.1101 (3)	−0.0210 (3)	3.8 (1)
C30	−0.3504 (5)	0.1183 (3)	−0.1327 (3)	3.8 (1)
C31	0.0717 (4)	0.2983 (3)	−0.1315 (2)	2.0 (1)
C41	0.2761 (4)	0.3158 (3)	−0.0824 (2)	1.9 (1)
C42	0.1723 (4)	0.2670 (3)	−0.1143 (2)	1.8 (1)
C43	0.1594 (4)	0.1868 (3)	−0.1300 (2)	2.2 (1)
C44	0.2452 (4)	0.1530 (3)	−0.1129 (2)	2.3 (1)
C45	0.3463 (4)	0.2041 (3)	−0.0781 (2)	2.3 (1)
C46	0.3647 (4)	0.2850 (3)	−0.0618 (2)	1.9 (1)
C47	0.2311 (5)	0.0646 (3)	−0.1334 (3)	4.2 (2)
C48*B*	0.3207 (8)	0.0605 (5)	−0.1843 (5)	2.8 (2)
C48*A*	0.196 (2)	0.037 (1)	−0.1981 (9)	8.9 (5)*
C49*B*	0.1143 (8)	0.0199 (5)	−0.1735 (5)	2.9 (3)
C49*A*	0.312 (1)	0.0329 (7)	−0.0939 (6)	4.7 (3)*
C50*B*	0.263 (1)	0.0278 (6)	−0.0763 (6)	5.2 (3)
C50*A*	0.109 (1)	0.017 (1)	−0.1059 (8)	8.6 (5)*
C51	0.4732 (4)	0.3375 (3)	−0.0194 (2)	2.2 (1)
C53	0.3222 (4)	0.4408 (3)	−0.1178 (2)	2.7 (1)
C54	0.2842 (5)	0.5141 (3)	−0.1077 (3)	3.6 (1)
C61	0.4195 (4)	0.3932 (3)	0.0813 (2)	2.0 (1)
C62	0.4643 (4)	0.3393 (3)	0.0490 (2)	1.8 (1)
C63	0.4998 (4)	0.2853 (3)	0.0806 (2)	2.2 (1)
C64	0.4933 (4)	0.2831 (3)	0.1430 (2)	2.0 (1)
C65	0.4476 (4)	0.3381 (3)	0.1738 (2)	2.0 (1)
C66	0.4087 (4)	0.3917 (3)	0.1443 (2)	1.9 (1)
C67	0.5335 (4)	0.2242 (3)	0.1785 (2)	2.6 (1)
C68	0.5791 (5)	0.1686 (3)	0.1373 (3)	4.5 (1)
C69	0.4326 (5)	0.1732 (3)	0.2029 (3)	3.8 (1)
C70	0.6286 (5)	0.2710 (3)	0.2343 (3)	3.7 (1)
C71	0.3510 (4)	0.4467 (3)	0.1783 (2)	2.1 (1)
C102	0.0766 (8)	0.1344 (8)	0.0478 (4)	17.1 (4)
C103	0.1728 (6)	0.2110 (4)	0.0607 (3)	5.9 (2)
C401	0.9780 (4)	0.2743 (3)	0.5030 (2)	2.1 (1)
C402	0.9010 (4)	0.2746 (3)	0.4501 (2)	2.2 (1)
C403	0.8346 (4)	0.2017 (3)	0.4157 (2)	2.6 (1)
C404	0.8411 (4)	0.1298 (3)	0.4299 (2)	2.8 (1)
C405	0.9191 (4)	0.1331 (3)	0.4830 (2)	2.7 (1)
C406	0.9865 (4)	0.2032 (3)	0.5209 (2)	2.3 (1)
C407	0.7696 (5)	0.0501 (3)	0.3923 (3)	3.6 (1)
C408	0.6839 (5)	0.0580 (4)	0.3395 (3)	4.6 (2)
C409	0.7024 (7)	0.0018 (4)	0.4353 (3)	7.4 (2)
C410	0.8462 (6)	0.0070 (3)	0.3638 (3)	5.3 (2)
C411	0.8865 (4)	0.3518 (3)	0.4343 (2)	2.3 (1)
C413	1.1571 (4)	0.3741 (3)	0.5269 (2)	2.9 (1)
C414	1.2230 (5)	0.4385 (3)	0.5792 (3)	3.6 (1)
C421	0.8140 (4)	0.4202 (3)	0.5240 (2)	1.9 (1)
C422	0.7927 (4)	0.3752 (3)	0.4639 (2)	2.0 (1)
C423	0.6822 (4)	0.3512 (3)	0.4315 (2)	2.3 (1)
C424	0.5915 (4)	0.3690 (3)	0.4555 (2)	2.2 (1)
C425	0.6163 (4)	0.4126 (3)	0.5161 (2)	2.1 (1)
C426	0.7248 (4)	0.4377 (3)	0.5508 (2)	1.8 (1)
C427	0.4730 (4)	0.3451 (3)	0.4154 (2)	2.8 (1)
C428	0.4771 (4)	0.3972 (3)	0.3641 (3)	3.5 (1)
C429	0.4392 (5)	0.2587 (3)	0.3837 (3)	4.0 (2)
C430	0.3827 (4)	0.3584 (3)	0.4526 (3)	3.7 (1)
C431	0.7461 (4)	0.4801 (3)	0.6187 (2)	2.1 (1)
C441	0.8000 (4)	0.3936 (3)	0.6926 (2)	2.0 (1)
C442	0.7170 (4)	0.4211 (3)	0.6622 (2)	1.9 (1)
C443	0.6054 (4)	0.3891 (3)	0.6698 (2)	2.2 (1)
C444	0.5728 (4)	0.3299 (3)	0.7051 (2)	2.3 (1)
C445	0.6586 (4)	0.3009 (3)	0.7317 (2)	2.4 (1)
C446	0.7722 (4)	0.3322 (3)	0.7261 (2)	2.1 (1)
C447	0.4501 (4)	0.2958 (3)	0.7150 (2)	3.1 (1)
C448	0.4056 (6)	0.2103 (5)	0.6851 (5)	9.4 (3)
C449	0.3732 (5)	0.3407 (4)	0.6921 (3)	6.8 (2)
C450	0.4461 (5)	0.3003 (4)	0.7844 (3)	6.3 (2)
C451	0.8626 (4)	0.2988 (3)	0.7553 (2)	2.3 (1)
C453	0.9722 (4)	0.4966 (3)	0.7354 (2)	2.9 (1)
C454	1.0881 (5)	0.5302 (3)	0.7221 (3)	4.4 (2)
C461	0.9658 (4)	0.2473 (3)	0.6726 (2)	2.1 (1)
C462	0.8848 (4)	0.2321 (3)	0.7118 (2)	2.1 (1)
C463	0.8224 (4)	0.1546 (3)	0.7096 (2)	2.8 (1)
C464	0.8366 (4)	0.0905 (3)	0.6711 (2)	2.7 (1)
C465	0.9176 (4)	0.1088 (3)	0.6326 (2)	2.7 (1)
C466	0.9815 (4)	0.1858 (3)	0.6313 (2)	2.2 (1)
C467	0.7673 (4)	0.0055 (3)	0.6721 (3)	3.6 (1)
C468	0.6433 (6)	−0.0036 (4)	0.6553 (5)	9.3 (3)
C469	0.7988 (6)	−0.0556 (3)	0.6271 (3)	5.2 (2)
C470	0.7924 (6)	−0.0136 (3)	0.7373 (3)	5.8 (2)
C471	1.0568 (4)	0.2024 (3)	0.5825 (2)	2.4 (1)
C502	0.5700 (7)	0.1585 (7)	0.5130 (8)	24.4 (5)
C503	0.6862 (5)	0.2022 (4)	0.5682 (4)	6.3 (2)

Table 2. *Bond distances* (Å) *and angles* (°) *for the heavy atoms with e.s.d.'s in parentheses*

The atom labels given are for ring 1. The values on one line are the corresponding distances and angles for the other rings. Distances and angles involving disordered atoms are indicated with an asterisk.

	Ring 1	Ring 2	Ring 3	Ring 4
O12—C1	1.395 (6)	1.372 (5)	1.399 (5)	1.380 (6)
O12—C13	1.454 (6)		1.453 (6)	
C1—C2	1.379 (6)	1.390 (7)	1.382 (5)	1.391 (8)
C1—C6	1.413 (7)	1.403 (6)	1.407 (7)	1.407 (7)
C2—C3	1.383 (7)	1.385 (6)	1.382 (7)	1.389 (7)
C2—C11	1.529 (6)	1.532 (6)	1.526 (7)	1.512 (7)
C3—C4	1.392 (7)	1.388 (6)	1.393 (8)	1.384 (7)
C4—C5	1.391 (6)	1.396 (7)	1.393 (6)	1.396 (7)
C4—C7	1.533 (7)	1.520 (6)	1.533 (7)	1.536 (8)
C5—C6	1.375 (7)	1.375 (6)	1.385 (7)	1.378 (7)
C6—C71	1.526 (7)	1.527 (7)	1.524 (5)	1.527 (7)
C7—C8	1.541 (9)	1.529 (9)	1.41 (2)*	1.517 (8)
			1.67 (1)*	
C7—C9	1.521 (7)	1.539 (9)	1.52 (2)*	1.533 (7)
			1.54 (2)*	
C7—C10	1.540 (6)	1.533 (7)	1.74 (2)*	1.556 (6)
			1.55 (1)*	
C13—C14	1.498 (7)		1.502 (9)	
O101*A*—C102	1.43 (1)*			
O101*B*—C102	1.46 (2)*			
C102—C103	1.51 (1)			
O412—C401	1.391 (5)	1.372 (5)	1.402 (5)	1.375 (6)
O412—C413	1.446 (6)		1.441 (6)	
C401—C402	1.411 (7)	1.402 (7)	1.391 (8)	1.394 (7)
C401—C406	1.400 (7)	1.398 (8)	1.386 (7)	1.396 (7)
C402—C403	1.390 (6)	1.388 (6)	1.385 (6)	1.378 (6)
C402—C411	1.510 (7)	1.522 (7)	1.510 (7)	1.525 (7)
C403—C404	1.376 (8)	1.388 (7)	1.390 (8)	1.389 (7)
C404—C405	1.403 (8)	1.399 (6)	1.402 (8)	1.388 (7)
C404—C407	1.517 (6)	1.535 (6)	1.530 (7)	1.527 (7)
C405—C406	1.390 (6)	1.385 (6)	1.393 (7)	1.390 (6)
C406—C471	1.518 (7)	1.532 (6)	1.517 (7)	1.508 (7)
C407—C408	1.521 (8)	1.546 (9)	1.50 (1)	1.495 (9)
C407—C409	1.53 (1)	1.522 (7)	1.48 (1)	1.529 (9)
C407—C410	1.51 (1)	1.510 (9)	1.518 (9)	1.526 (9)
C413—C414	1.485 (6)		1.479 (8)	
O501—C502	1.73 (1)			
C502—C503	1.69 (1)			

Table 2 (*cont.*)

	Ring 1	Ring 2	Ring 3	Ring 4
C1—O12—C13	113.8 (3)		114.4 (3)	
O12—C1—C2	119.2 (4)	123.0 (4)	120.2 (4)	122.3 (4)
O12—C1—C6	118.9 (4)	116.5 (4)	118.1 (3)	117.3 (4)
C2—C1—C6	121.8 (4)	120.5 (4)	121.6 (4)	120.3 (5)
C1—C2—C3	118.4 (4)	118.4 (5)	118.5 (5)	118.5 (4)
C1—C2—C11	121.4 (4)	120.8 (3)	122.3 (4)	121.6 (4)
C3—C2—C11	120.1 (4)	120.8 (4)	119.2 (3)	119.9 (4)
C2—C3—C4	122.1 (4)	123.4 (4)	122.6 (4)	123.1 (5)
C3—C4—C5	117.4 (4)	115.9 (4)	116.7 (4)	116.8 (5)
C3—C4—C7	122.8 (4)	123.9 (4)	121.7 (4)	123.3 (5)
C5—C4—C7	119.8 (4)	120.2 (4)	121.5 (5)	119.9 (4)
C4—C5—C6	123.0 (4)	123.4 (5)	123.2 (5)	122.6 (4)
C1—C6—C5	117.0 (4)	118.4 (4)	117.2 (4)	118.7 (5)
C1—C6—C71	122.5 (5)	120.5 (3)	121.4 (5)	120.2 (4)
C5—C6—C71	120.4 (4)	121.1 (4)	121.3 (4)	121.1 (4)
C4—C7—C8	109.6 (4)	110.3 (4)	114.3 (9)*	112.4 (4)
			105.6 (5)*	
C4—C7—C9	112.6 (5)	112.4 (4)	113.9 (5)*	109.0 (4)
			112.7 (6)*	
C4—C7—C10	109.5 (4)	109.2 (4)	104.2 (7)*	109.2 (4)
			110.0 (6)*	
C8—C7—C9	108.6 (4)	108.2 (5)	123 (2)*	107.5 (5)
			102.6 (7)*	
C8—C7—C10	108.5 (4)	109.4 (4)	100.2 (9)*	108.9 (4)
			110.3 (8)*	
C9—C7—C10	107.9 (4)	107.3 (4)	96.2 (9)*	109.7 (4)
			115.0 (7)*	
C2—C11—C22	112.8 (5)	111.8 (4)	112.0 (4)	110.9 (3)

Table 2 (*cont.*)

	Ring 1	Ring 2	Ring 3	Ring 4
O12—C13—C14	107.5 (5)		107.7 (4)	
O101*A*—C102—O101*B*	119.3 (8)*			
O101*A*—C102—C103	116.7 (8)*			
O101*B*—C102—C103	116 (1)*			
C401—O412—C413	114.2 (4)		114.5 (4)	
O412—C401—C402	118.9 (4)	122.3 (4)	120.1 (5)	122.0 (4)
O412—C401—C406	119.8 (4)	117.5 (4)	118.3 (4)	117.1 (4)
C402—C401—C406	121.3 (4)	120.3 (4)	121.6 (5)	120.9 (4)
C401—C402—C403	117.7 (5)	118.1 (5)	117.9 (4)	118.2 (4)
C401—C402—C411	120.5 (4)	121.9 (4)	121.2 (5)	121.7 (4)
C403—C402—C411	121.7 (4)	120.0 (4)	120.7 (4)	120.1 (4)
C402—C403—C404	123.9 (4)	123.7 (5)	123.1 (5)	123.7 (5)
C403—C404—C405	116.0 (4)	116.2 (4)	116.8 (4)	115.8 (4)
C403—C404—C407	124.1 (5)	120.9 (5)	123.2 (5)	121.5 (5)
C405—C404—C407	119.9 (5)	122.9 (5)	120.0 (4)	122.8 (5)
C404—C405—C406	124.0 (5)	122.7 (5)	122.1 (5)	123.4 (5)
C401—C406—C405	117.1 (4)	119.1 (4)	118.4 (5)	117.9 (5)
C401—C406—C471	121.5 (4)	120.3 (4)	121.1 (5)	121.3 (4)
C405—C406—C471	121.1 (4)	120.7 (4)	120.5 (4)	120.6 (4)
C404—C407—C408	112.5 (5)	108.3 (4)	110.1 (5)	110.0 (5)
C404—C407—C409	109.0 (5)	110.8 (5)	113.4 (5)	112.6 (5)
C404—C407—C410	109.5 (4)	112.7 (4)	109.7 (4)	109.1 (4)
C408—C407—C409	107.2 (5)	108.3 (4)	110.5 (5)	108.8 (5)
C408—C407—C410	107.8 (5)	107.5 (5)	107.5 (6)	110.0 (6)
C409—C407—C410	110.8 (6)	109.4 (4)	105.6 (5)	106.5 (5)
C402—C411—C422	112.4 (4)	110.9 (3)	114.1 (4)	110.3 (4)
O412—C413—C414	107.8 (4)		108.6 (4)	
O501—C502—C503	95.3 (8)			

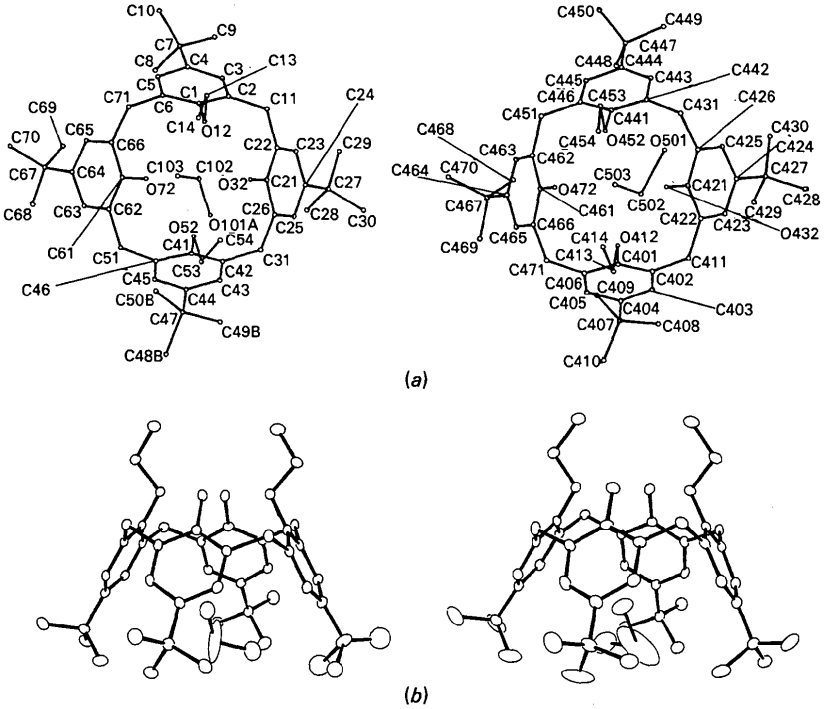

Fig. 1. Views of the two independent calixarene molecules, showing (*a*) atomic numbering (where disorder exists, only one of the disordered atoms is shown) and (*b*) the positioning of the ethanol molecule with respect to the calixarene molecule (thermal ellipsoids are scaled to include 25% probability).

for the ethanol atoms. One of the ethanol O atoms (O101) was found to be disordered over two positions with the same occupancy. A difference Fourier synthesis showed the largest peaks near the ethanol molecules in both cavities. We conclude that there is more disorder in the positions of both ethanols. It was, however, not possible to fit a model with reasonable geometry to these peaks. As usual in this type of compound the terminal C atoms of the *tert*-butyl group show large anisotropic thermal motion, owing to libration. In one of the *tert*-butyl groups disorder was found in the terminal C atoms

(C48–C50). This group was refined in two orientations with the same occupancy. H atoms of the calixarene have been included as riding atoms at calculated positions. The phenolic H atoms were found from a difference Fourier synthesis and were refined with isotropic thermal parameters. Ethanol H atoms and H atoms of the disordered *tert*-butyl group were not included.

The number of parameters refined was 1029 {scale factor, isotropic extinction factor [final value 1.1 (9) $\times 10^{-6}$], positional and anisotropic thermal parameters for the non-H atoms, positions and isotropic thermal parameters for the phenolic H atoms}. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971) and refined by full-matrix least squares. Weights for each reflection in the refinement (on F) were $w = 4F_o^2/\sigma(F_o^2)$, $\sigma(F_o^2) = \sigma^2(I) + (pF_o^2)^2$; the value of the instability factor p was determined as 0.03. Refinement converged at $R = 0.080$, $wR = 0.090$, $(\Delta/\sigma)_{max} = 0.3$, $S = 2.9$. Maximum and minimum heights in the final difference map were 0.92 (near one of the ethanol molecules) and -0.70 e Å^{-3}, respectively. All calculations were performed with *SDP* (B. A. Frenz & Associates, Inc., 1983). Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Atomic parameters are given in Table 1.*

* 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 55094 (77 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB0181]

Bond distances and angles are given in Table 2. The atom numbering is shown in Fig. 1, which displays the two independent calixarene molecules present in the crystal. Both calixarene molecules have the cone conformation (Gutsche, 1989). This conformation is stabilized by almost linear hydrogen bonds from the phenolic H atoms to the O atoms of the ethoxy groups.

Related literature. Several crystal structures of different calixarenes have been reported. A recent review has been given by Andreetti & Ugozzoli (1990). To the best of our knowledge the title compound of this paper represents the first solid-state complex of a calix[4]arene with ethanol.

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Structure du 8-Chloro-11-(4-méthylpipérazin-1-yl)dibenzo[*b*,*f*]-1,4-thiazépine

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Abstract. 8-Chloro-11-(4-methylpiperazin-1-yl)dibenzo[*b*,*f*][1,4]thiazepine, $C_{18}H_{18}ClN_3S$, $M_r = 343.9$, monoclinic, $P2_1/n$, $a = 9.521$ (3), $b = 13.007$ (4), $c = 14.116$ (6) Å, $\beta = 100.77$ (1)°, $V = 1717.4$ (1) Å^3, $Z = 4$, $D_x = 1.330$ g cm^{-3}, m.p. = 439–440 K, λ(Cu $K\bar{\alpha}$) = 1.5418 Å, $\mu = 29.82$ cm^{-1}, $F(000) = 720$, $T =$

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