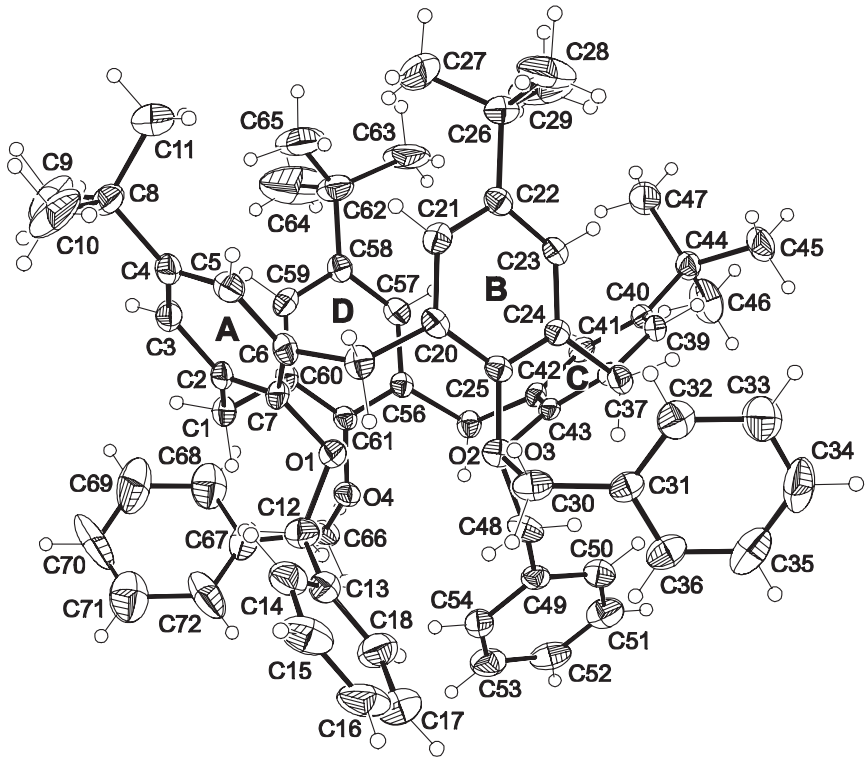
Crystal structure of 25,26,27,28-tetrabenzyloxy-5,11,17,23-*tert*-butylcalix-[4]arene, $C_{72}H_{80}O_4$

Tobias Gruber, Wilhelm Seichter and Edwin Weber*

TU Bergakademie Freiberg, Institut für Organische Chemie, Leipziger Straße 29, 09596 Freiberg, Germany

Received March 5, 2007, accepted and available on-line September 24, 2007; CCDC no. 1267/2012



Abstract

$C_{72}H_{80}O_4$, monoclinic, $P12_1/n1$ (no. 14), a = 10.3709(3) Å, b = 23.2467(6) Å, c = 25.1444(7) Å, β = 92.660(1)°, V = 6055.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.060, $wR_{ref}(F^2)$ = 0.190, T = 273 K.

Source of material

4.0 g (100 mmol) NaOH in 7 ml water and 7.58 g (10.2 mmol) *p-tert*-butylcalix[4]arene [1] were added under stirring to 50 ml DMSO. To this mixture, 7.39 g (43.2 mmol) of benzyl bromide were added at 323 K. Stirring was continued for 3 h at 343 K. After cooling to room temperature, the reaction mixture was quenched with diluted hydrochloric acid. Extraction with chloroform, drying over sodium sulphate, evaporation of the solvent and recrystallization from acetonitrile/acetone (1:3, *v*/*v*) gave the title compound as colorless needles (yield 49 %, m.p. 515-516 K).

Discussion

In the title compound, the calixarene framework adopts a pinched-cone conformation [2], which is an usual behavior of disubstituted calix[4]arenes [3] rather than a tetrasubstituted calix[4]arene such as here. Moreover, the interplanar angles, formed by the opposite phenyl rings, i.e. A/C (86.46(7)°) and B/D (4.8(1)°), indicate an asymmetric overall conformation. By way of contrast, the title compound in the structure of its complex with acetontrile and sodium iodide (1:1:1) was found almost in a perfect cone conformation suggesting environmental effects [4]. Corresponding to the hydrophobic nature of the molecule, intermolecular contacts are restricted to weak van der Waals forces. Thus, the molecular assembly in the crystal structure follows close-packing requirements.

Table 1. Data collection and handling.

Crystal:	colorless needle fragment, size 0.08 × 0.11 × 0.54 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.67 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX 2 CCD, φ/ω
$2\theta_{max}$:	48.92°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	45635, 9971
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5647
$N(param)_{refined}$:	698
Programs:	SHELXS-97 [5], SHELXL-97 [6]

* Correspondence author (e-mail: edwin.weber@chemie.tu-freiberg.de)

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	4*e*	0.4384	0.2532	–0.0373	0.039
H(1B)	4*e*	0.4145	0.1990	–0.0018	0.039
H(3)	4*e*	0.2676	0.3182	–0.0565	0.043
H(5)	4*e*	–0.0574	0.3180	0.0222	0.043
H(9A)	4*e*	0.1544	0.3644	–0.1234	0.137
H(9B)	4*e*	0.2193	0.4068	–0.0817	0.137
H(9C)	4*e*	0.1040	0.4278	–0.1193	0.137
H(10A)	4*e*	–0.0607	0.3275	–0.1113	0.165
H(10B)	4*e*	–0.1119	0.3908	–0.1085	0.165
H(10C)	4*e*	–0.1414	0.3469	–0.0633	0.165
H(11A)	4*e*	–0.0054	0.4601	–0.0439	0.147
H(11B)	4*e*	0.1017	0.4371	–0.0032	0.147
H(11C)	4*e*	–0.0426	0.4188	0.0023	0.147
H(12A)	4*e*	0.3408	0.1208	0.0564	0.049
H(12B)	4*e*	0.2551	0.1409	0.0069	0.049
H(14)	4*e*	0.0069	0.1269	0.0159	0.055
H(15)	4*e*	–0.1420	0.0557	0.0317	0.073
H(16)	4*e*	–0.0843	–0.0226	0.0832	0.082
H(17)	4*e*	0.1236	–0.0308	0.1196	0.082
H(18)	4*e*	0.2742	0.0387	0.1018	0.066
H(19A)	4*e*	–0.0006	0.1954	0.0980	0.041
H(19B)	4*e*	–0.0948	0.2481	0.0909	0.041
H(21)	4*e*	0.0020	0.3449	0.1290	0.039
H(23)	4*e*	0.2227	0.3334	0.2621	0.037
H(27A)	4*e*	0.0738	0.4888	0.1632	0.143
H(27B)	4*e*	0.0026	0.4364	0.1358	0.143
H(27C)	4*e*	0.1531	0.4416	0.1346	0.143
H(28A)	4*e*	–0.0384	0.4643	0.2451	0.141
H(28B)	4*e*	–0.0184	0.4034	0.2711	0.141
H(28C)	4*e*	–0.1014	0.4099	0.2177	0.141
H(29A)	4*e*	0.2837	0.4334	0.2227	0.150
H(29B)	4*e*	0.2081	0.4226	0.2743	0.150
H(29C)	4*e*	0.1918	0.4810	0.2435	0.150
H(30A)	4*e*	0.0065	0.1026	0.1805	0.046
H(30B)	4*e*	–0.0664	0.1611	0.1869	0.046
H(32)	4*e*	–0.0896	0.2014	0.2754	0.058
H(33)	4*e*	–0.0625	0.1928	0.3667	0.078
H(34)	4*e*	0.0576	0.1182	0.4038	0.089
H(35)	4*e*	0.1494	0.0514	0.3492	0.081
H(36)	4*e*	0.1247	0.0599	0.2582	0.059

Table 2. Continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(37A)	4*e*	0.2347	0.2304	0.3055	0.036
H(37B)	4*e*	0.2521	0.1813	0.2636	0.036
H(39)	4*e*	0.4172	0.2827	0.3361	0.036
H(41)	4*e*	0.7417	0.2885	0.2567	0.037
H(45A)	4*e*	0.4886	0.3523	0.3861	0.076
H(45B)	4*e*	0.6161	0.3633	0.4206	0.076
H(45C)	4*e*	0.5656	0.3004	0.4115	0.076
H(46A)	4*e*	0.7836	0.2744	0.3772	0.096
H(46B)	4*e*	0.8227	0.3381	0.3906	0.096
H(46C)	4*e*	0.8422	0.3134	0.3335	0.096
H(47A)	4*e*	0.7051	0.3905	0.2882	0.103
H(47B)	4*e*	0.6990	0.4191	0.3445	0.103
H(47C)	4*e*	0.5712	0.4059	0.3110	0.103
H(48A)	4*e*	0.3508	0.1085	0.1704	0.048
H(48B)	4*e*	0.3605	0.1235	0.2312	0.048
H(50)	4*e*	0.5698	0.1122	0.2810	0.054
H(51)	4*e*	0.7673	0.0651	0.2886	0.064
H(52)	4*e*	0.8429	0.0170	0.2168	0.065
H(53)	4*e*	0.7251	0.0157	0.1372	0.062
H(54)	4*e*	0.5294	0.0631	0.1289	0.051
H(55A)	4*e*	0.6683	0.1850	0.1630	0.038
H(55B)	4*e*	0.7664	0.2348	0.1768	0.038
H(57)	4*e*	0.6687	0.3373	0.1547	0.040
H(59)	4*e*	0.4539	0.3488	0.0201	0.041
H(63A)	4*e*	0.5956	0.4837	0.1447	0.205
H(63B)	4*e*	0.6792	0.4291	0.1587	0.205
H(63C)	4*e*	0.5303	0.4285	0.1671	0.205
H(64A)	4*e*	0.6697	0.4218	0.0196	0.270
H(64B)	4*e*	0.7638	0.4256	0.0701	0.270
H(64C)	4*e*	0.6842	0.4798	0.0511	0.270
H(65A)	4*e*	0.3803	0.4363	0.0848	0.155
H(65B)	4*e*	0.4427	0.4385	0.0292	0.155
H(65C)	4*e*	0.4625	0.4898	0.0693	0.155
H(66A)	4*e*	0.6822	0.1111	0.0669	0.048
H(66B)	4*e*	0.7461	0.1723	0.0695	0.048
H(68)	4*e*	0.7635	0.2302	–0.0067	0.074
H(69)	4*e*	0.7397	0.2434	–0.0973	0.095
H(70)	4*e*	0.6397	0.1726	–0.1497	0.101
H(71)	4*e*	0.5680	0.0895	–0.1126	0.088
H(72)	4*e*	0.5799	0.0799	–0.0187	0.080

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.4074(3)	0.2406(1)	–0.0034(1)	0.034(2)	0.040(2)	0.024(2)	0.002(1)	0.002(1)	0.001(1)
C(2)	4*e*	0.2673(3)	0.2580(1)	0.0005(1)	0.034(2)	0.035(2)	0.023(2)	0.000(1)	–0.006(1)	–0.003(1)
C(3)	4*e*	0.2173(3)	0.3030(1)	–0.0303(1)	0.041(2)	0.040(2)	0.026(2)	–0.002(2)	–0.002(1)	–0.000(2)
C(4)	4*e*	0.0957(3)	0.3266(1)	–0.0238(1)	0.041(2)	0.039(2)	0.029(2)	0.002(2)	–0.007(2)	–0.002(2)
C(5)	4*e*	0.0239(3)	0.3030(1)	0.0165(1)	0.034(2)	0.041(2)	0.033(2)	0.006(2)	–0.006(1)	–0.005(2)
C(6)	4*e*	0.0691(3)	0.2575(1)	0.0486(1)	0.031(2)	0.040(2)	0.028(2)	–0.001(1)	–0.005(1)	–0.007(2)
C(7)	4*e*	0.1893(3)	0.2339(1)	0.0386(1)	0.032(2)	0.033(2)	0.022(2)	0.002(1)	–0.007(1)	–0.001(1)
C(8)	4*e*	0.0429(3)	0.3764(1)	–0.0579(1)	0.057(2)	0.042(2)	0.039(2)	0.014(2)	–0.005(2)	0.001(2)
C(9)	4*e*	0.1393(5)	0.3957(2)	–0.0995(2)	0.104(4)	0.095(4)	0.076(3)	0.034(3)	0.018(3)	0.045(3)
C(10)	4*e*	–0.0787(5)	0.3588(2)	–0.0879(2)	0.111(4)	0.076(3)	0.134(5)	–0.004(3)	–0.077(4)	0.040(3)
C(11)	4*e*	0.0223(6)	0.4278(2)	–0.0225(2)	0.158(5)	0.061(3)	0.073(3)	0.041(3)	0.001(3)	0.002(3)
C(12)	4*e*	0.2560(3)	0.1350(1)	0.0451(1)	0.041(2)	0.035(2)	0.045(2)	0.006(2)	0.002(2)	–0.001(2)
C(13)	4*e*	0.1570(3)	0.0906(1)	0.0573(1)	0.042(2)	0.036(2)	0.037(2)	0.000(2)	0.003(2)	–0.004(2)
C(14)	4*e*	0.0313(3)	0.0951(2)	0.0365(1)	0.045(2)	0.045(2)	0.047(2)	0.002(2)	0.005(2)	–0.009(2)
C(15)	4*e*	–0.0581(4)	0.0525(2)	0.0461(2)	0.047(2)	0.053(3)	0.085(3)	–0.005(2)	0.015(2)	–0.027(2)
C(16)	4*e*	–0.0237(4)	0.0058(2)	0.0769(2)	0.075(3)	0.042(2)	0.092(3)	–0.018(2)	0.036(3)	–0.015(2)
C(17)	4*e*	0.1004(5)	0.0006(2)	0.0984(2)	0.097(3)	0.041(2)	0.068(3)	–0.011(2)	0.008(3)	0.008(2)
C(18)	4*e*	0.1899(4)	0.0426(2)	0.0880(2)	0.065(2)	0.039(2)	0.059(3)	–0.002(2)	–0.007(2)	0.003(2)
C(19)	4*e*	–0.0048(3)	0.2370(1)	0.0957(1)	0.028(2)	0.040(2)	0.034(2)	–0.001(1)	–0.002(1)	–0.002(2)
C(20)	4*e*	0.0526(3)	0.2633(1)	0.1470(1)	0.024(2)	0.036(2)	0.030(2)	–0.001(1)	0.003(1)	–0.002(1)
C(21)	4*e*	0.0476(3)	0.3228(1)	0.1543(1)	0.031(2)	0.036(2)	0.032(2)	0.003(1)	0.002(1)	0.006(1)
C(22)	4*e*	0.1078(3)	0.3503(1)	0.1977(1)	0.029(2)	0.034(2)	0.033(2)	0.002(1)	0.004(1)	–0.001(2)
C(23)	4*e*	0.1776(3)	0.3158(1)	0.2336(1)	0.033(2)	0.034(2)	0.026(2)	–0.002(1)	0.004(1)	–0.004(1)

Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(24)	4*e*	0.1833(3)	0.2562(1)	0.2292(1)	0.024(1)	0.032(2)	0.026(2)	0.000(1)	0.004(1)	–0.002(1)
C(25)	4*e*	0.1179(3)	0.2301(1)	0.1860(1)	0.024(2)	0.028(2)	0.031(2)	–0.000(1)	0.007(1)	–0.003(1)
C(26)	4*e*	0.0936(3)	0.4152(1)	0.2065(1)	0.043(2)	0.031(2)	0.047(2)	0.002(1)	0.003(2)	–0.000(2)
C(27)	4*e*	0.0795(6)	0.4485(2)	0.1554(2)	0.176(5)	0.041(2)	0.068(3)	0.002(3)	–0.004(3)	0.010(2)
C(28)	4*e*	–0.0274(5)	0.4240(2)	0.2381(2)	0.101(4)	0.049(3)	0.136(5)	0.014(2)	0.046(3)	–0.018(3)
C(29)	4*e*	0.2044(5)	0.4403(2)	0.2398(2)	0.101(4)	0.036(2)	0.157(5)	–0.005(2)	–0.049(4)	–0.012(3)
C(30)	4*e*	0.0111(3)	0.1400(1)	0.1975(1)	0.030(2)	0.034(2)	0.052(2)	–0.007(1)	–0.001(2)	–0.001(2)
C(31)	4*e*	0.0171(3)	0.1322(1)	0.2568(1)	0.029(2)	0.033(2)	0.050(2)	–0.008(1)	0.004(2)	0.004(2)
C(32)	4*e*	–0.0403(3)	0.1715(2)	0.2900(2)	0.043(2)	0.048(2)	0.055(2)	0.001(2)	0.011(2)	0.002(2)
C(33)	4*e*	–0.0246(4)	0.1661(2)	0.3448(2)	0.069(3)	0.073(3)	0.055(3)	–0.007(2)	0.025(2)	–0.003(2)
C(34)	4*e*	0.0468(4)	0.1215(2)	0.3670(2)	0.079(3)	0.099(4)	0.045(3)	–0.022(3)	0.009(2)	0.020(3)
C(35)	4*e*	0.1020(4)	0.0819(2)	0.3344(2)	0.066(3)	0.067(3)	0.068(3)	–0.009(2)	–0.001(2)	0.032(2)
C(36)	4*e*	0.0872(3)	0.0870(2)	0.2799(2)	0.042(2)	0.039(2)	0.066(3)	–0.004(2)	0.004(2)	0.010(2)
C(37)	4*e*	0.2641(3)	0.2221(1)	0.2703(1)	0.031(2)	0.033(2)	0.027(2)	–0.001(1)	0.003(1)	–0.001(1)
C(38)	4*e*	0.4060(3)	0.2366(1)	0.2685(1)	0.030(2)	0.025(2)	0.024(2)	0.002(1)	0.001(1)	0.002(1)
C(39)	4*e*	0.4645(3)	0.2718(1)	0.3072(1)	0.037(2)	0.031(2)	0.022(2)	0.003(1)	0.001(1)	0.001(1)
C(40)	4*e*	0.5912(3)	0.2916(1)	0.3045(1)	0.038(2)	0.027(2)	0.023(2)	0.000(1)	–0.004(1)	0.001(1)
C(41)	4*e*	0.6580(3)	0.2750(1)	0.2601(1)	0.028(2)	0.031(2)	0.033(2)	–0.002(1)	–0.003(1)	0.004(1)
C(42)	4*e*	0.6046(3)	0.2391(1)	0.2207(1)	0.029(2)	0.030(2)	0.025(2)	0.005(1)	–0.002(1)	0.003(1)
C(43)	4*e*	0.4782(3)	0.2191(1)	0.2260(1)	0.027(2)	0.025(2)	0.023(2)	0.002(1)	–0.006(1)	0.001(1)
C(44)	4*e*	0.6515(3)	0.3330(1)	0.3455(1)	0.050(2)	0.039(2)	0.029(2)	–0.013(2)	–0.003(2)	–0.003(2)
C(45)	4*e*	0.5731(4)	0.3377(2)	0.3956(1)	0.067(2)	0.053(2)	0.031(2)	–0.014(2)	–0.002(2)	–0.011(2)
C(46)	4*e*	0.7878(3)	0.3128(2)	0.3634(2)	0.047(2)	0.094(3)	0.050(2)	–0.015(2)	–0.013(2)	–0.016(2)
C(47)	4*e*	0.6572(5)	0.3927(2)	0.3199(2)	0.117(4)	0.038(2)	0.050(3)	–0.025(2)	0.011(2)	–0.008(2)
C(48)	4*e*	0.4052(3)	0.1262(1)	0.1982(1)	0.036(2)	0.033(2)	0.050(2)	–0.001(1)	0.002(2)	–0.013(2)
C(49)	4*e*	0.5290(3)	0.0934(1)	0.2042(1)	0.036(2)	0.029(2)	0.037(2)	–0.002(1)	0.004(2)	–0.001(2)
C(50)	4*e*	0.6008(3)	0.0931(1)	0.2517(1)	0.053(2)	0.036(2)	0.046(2)	–0.006(2)	0.001(2)	–0.004(2)
C(51)	4*e*	0.7193(3)	0.0646(2)	0.2565(2)	0.050(2)	0.041(2)	0.066(3)	–0.008(2)	–0.018(2)	0.007(2)
C(52)	4*e*	0.7641(3)	0.0361(1)	0.2137(2)	0.036(2)	0.032(2)	0.094(3)	0.003(2)	0.003(2)	0.006(2)
C(53)	4*e*	0.6939(3)	0.0353(1)	0.1662(2)	0.054(2)	0.040(2)	0.062(3)	0.012(2)	0.018(2)	0.002(2)
C(54)	4*e*	0.5767(3)	0.0638(1)	0.1613(1)	0.053(2)	0.035(2)	0.040(2)	0.007(2)	0.004(2)	0.000(2)
C(55)	4*e*	0.6756(3)	0.2257(1)	0.1709(1)	0.026(2)	0.037(2)	0.032(2)	0.002(1)	0.000(1)	0.000(1)
C(56)	4*e*	0.6198(3)	0.2604(1)	0.1240(1)	0.024(2)	0.035(2)	0.027(2)	0.003(1)	0.006(1)	0.001(1)
C(57)	4*e*	0.6238(3)	0.3199(1)	0.1261(1)	0.030(2)	0.038(2)	0.033(2)	–0.003(1)	0.001(1)	–0.004(2)
C(58)	4*e*	0.5639(3)	0.3549(1)	0.0875(1)	0.034(2)	0.037(2)	0.033(2)	–0.001(1)	0.002(1)	0.001(2)
C(59)	4*e*	0.4968(3)	0.3267(1)	0.0462(1)	0.033(2)	0.038(2)	0.033(2)	0.003(1)	0.000(1)	0.008(2)
C(60)	4*e*	0.4903(3)	0.2671(1)	0.0417(1)	0.027(2)	0.038(2)	0.026(2)	0.002(1)	0.004(1)	–0.001(1)
C(61)	4*e*	0.5561(3)	0.2342(1)	0.0803(1)	0.028(2)	0.029(2)	0.026(2)	0.000(1)	0.004(1)	–0.001(1)
C(62)	4*e*	0.5726(3)	0.4206(1)	0.0896(2)	0.061(2)	0.032(2)	0.062(3)	–0.002(2)	–0.008(2)	0.001(2)
C(63)	4*e*	0.5966(7)	0.4424(2)	0.1449(2)	0.251(8)	0.040(3)	0.110(5)	0.039(4)	–0.096(5)	–0.027(3)
C(64)	4*e*	0.6829(7)	0.4386(2)	0.0543(4)	0.184(7)	0.057(3)	0.31(1)	–0.043(4)	0.131(7)	0.004(5)
C(65)	4*e*	0.4539(5)	0.4488(2)	0.0661(2)	0.134(4)	0.046(3)	0.123(5)	0.031(3)	–0.063(4)	–0.016(3)
C(66)	4*e*	0.6722(3)	0.1507(1)	0.0553(1)	0.036(2)	0.043(2)	0.042(2)	0.013(2)	0.002(2)	–0.008(2)
C(67)	4*e*	0.6692(3)	0.1530(2)	–0.0037(1)	0.035(2)	0.067(3)	0.040(2)	0.017(2)	0.002(2)	–0.002(2)
C(68)	4*e*	0.7209(4)	0.2027(2)	–0.0277(2)	0.053(2)	0.083(3)	0.051(3)	0.000(2)	0.012(2)	0.006(2)
C(69)	4*e*	0.7086(4)	0.2102(2)	–0.0817(2)	0.075(3)	0.110(4)	0.055(3)	–0.002(3)	0.022(2)	0.008(3)
C(70)	4*e*	0.6489(4)	0.1674(3)	–0.1131(2)	0.072(3)	0.141(5)	0.042(3)	0.001(3)	0.015(2)	–0.014(3)
C(71)	4*e*	0.6040(4)	0.1186(2)	–0.0913(2)	0.069(3)	0.104(4)	0.046(3)	0.016(3)	0.000(2)	–0.012(3)
C(72)	4*e*	0.6134(4)	0.1126(2)	–0.0344(2)	0.059(3)	0.076(3)	0.066(3)	0.015(2)	0.001(2)	–0.017(2)
O(1)	4*e*	0.2337(2)	0.18922(8)	0.07090(8)	0.041(1)	0.033(1)	0.030(1)	0.0036(9)	0.0004(9)	0.001(1)
O(2)	4*e*	0.1228(2)	0.17062(8)	0.18013(8)	0.030(1)	0.030(1)	0.038(1)	–0.0007(9)	0.0037(9)	–0.003(1)
O(3)	4*e*	0.4232(2)	0.18595(8)	0.18548(8)	0.032(1)	0.033(1)	0.031(1)	0.0009(9)	–0.0035(9)	–0.007(1)
O(4)	4*e*	0.5551(2)	0.17434(8)	0.07623(8)	0.034(1)	0.031(1)	0.032(1)	0.0042(9)	0.0037(9)	–0.0034(9)

Acknowledgment. Financial support from the German Federal Ministry of Economics and Technology (BMWi) under grant no. 16IN0218 ′ChemoChips′ is gratefully acknowledged.

References

1. Gutsche, C. D.; Iqbal, M.; Stewart, D.: Synthesis Procedures for *p-tert*-Butylcalix[4]arene. J. Org. Chem. **51** (1986) 742-745.
2. Scheerder, J.; Vreekamp, R. H.; Engbersen, J. F. J.; Verboom, W.; van Duynhoven, J. P. M.; Reinhoudt, D. N.: The Pinched Cone Conformation of Calix[4]arenes: Noncovalent Rigidification of the Calix[4]arene Skeleton. J. Org. Chem. **61** (1996) 3476-3481.
3. Gruber, T.; Weber, E.; Seichter, W.; Bombicz, P.: Versatile Inclusion Behaviour of a Dinitrocalix[4]arene Having Two Ester Pendants – Preparation and X-ray Crystal Structures of Complexes. Supramol. Chem. **18** (2006) 537-547.
4. Ferdani, R.; Barbour, L. J.; Gokel, G. W.: Cation-π Interactions in the Crystal Structures of Alkali Metal Calixarene Complexes. J. Supramol. Chem. **2** (2002) 343-348.
5. Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
6. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.