Table 1S Scaling factors for the force fields of the molecules **6 - 9**.

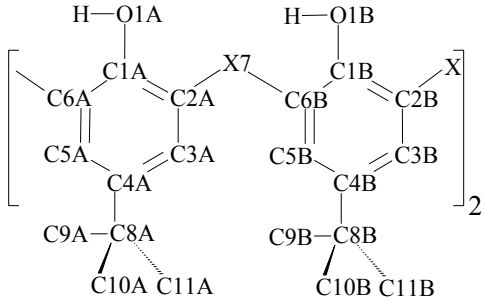
scaling factor		value
stretch	C-C	0.9207 [a]
stretch	C-H (arom.)	0.915 [b]
stretch	C-H (aliph.)	0.889 [b]
stretch	C-O	0.9207 [a]
stretch	O-H	0.9527 [a]
stretch	C-S	1.040 [c]
bend	C-S-C	1.070 [c]
bend	C-C-C	1.0144 [a]
bend	C-C-H	0.9431 [a]
bend	C-O-H	0.9431 [a]
bend	H-C-H	0.9016 [a]
torsion	all	0.9523 [a]
out of plane	Ring-H	0.976 [a]

[a] Ref. **9**

[b] Ref. **5**

[c] Ref. **17**

Table 2S Comparison of the results obtained from the B3LYP/6-31G* geometry optimisation for the *cone* conformer of the calixarenes **6 – 9** with the corresponding X-ray data.



	6		**7**		**8**		**9**	
	x-ray[a]	calc.	x-ray[b]	calc.	x-ray[b]	calc.	x-ray[b]	calc.
Bond, Å								
C1-C2	1.395	1.405	1.398	1.411	1.384	1.402	1.408	1.407
C2-C3	1.383	1.397	1.377	1.399	1.390	1.401	1.375	1.401
C3-C4	1.383	1.394	1.373	1.393	1.397	1.398	1.384	1.397
C4-C5	1.383	1.393	1.373	1.394	1.385	1.403	1.383	1.403
C5-C6	1.383	1.399	1.377	1.398	1.388	1.394	1.382	1.394
C6-C1	1.395	1.406	1.398	1.410	1.398	1.404	1.396	1.409
C1-O1	1.388	1.382	1.368	1.357	1.385	1.382	1.349	1.358
C4-C8					1.535	1.540	1.584	1.540
C8-C9					1.560	1.547	1.595	1.547
C8-C9					1.536	1.547	1.587	1.547
C8-C10					1.523	1.541	1.548	1.547
C2-X7	1.513	1.525	1.778	1.802	1.519	1.527	1.789	1.803
Angle, ^{0}								
C1-C2-C3	117.40	118.08	119.18	119.18	118.05	118.09	120.27	119.83
C2-C3-C4	121.47	121.18	120.35	120.35	122.68	122.81	122.84	122.43
C3-C4-C5	119.77	119.51	120.78	120.78	116.37	116.84	116.46	116.65
C4-C5-C6	121.29	121.45	120.61	120.61	123.89	122.76	122.45	122.55
C5-C6-C1	117.39	117.73	119.18	119.18	116.91	118.25	120.61	119.79
C6-C1-C2	122.76	122.05	120.14	120.14	122.10	121.24	117.29	118.76
O1-C1-C2	118.76	116.94	119.93	119.93	119.02	121.46	121.19	122.79
O1-C1-C6	118.61	120.98	119.93	119.93	118.87	117.28	121.5	118.45
C1-C2-X7	122.36	121.30	120.63	120.63	122.18	122.23	118.93	120.76

C3-C2-X7	120.23	120.58	120.1	120.1	119.68	119.65	121.8	119.18
C3-C4-C8					123.61	123.11	121.68	120.18
C5-C4-C8					120.02	120.05	121.82	123.18
C4-C8-C9					112.55	112.34	109.28	112.12
C4-C8-C10					109.08	109.28	106.2	109.52
C4-C8-C11					109.65	109.52	105.9	109.4
CA-X7-C6B	113.07	113.77	102.66	102.66	112.48	113.69	100.74	104.09
C1A-C2A-X7-C6B	88.00	86.88	89.69	89.69	88.17	87.19	94.16	88.84
C1B-C6B-X7-C2A	-88.31	-88.32	-89.68	-89.68	-88.48	-88.68	-93.89	-87.24

[a]Reference **18**; [b]Reference **11**

Table 3S. IR spectra of *p-tert*-Bu-calix[4]arene **8**

Experiment		**Computations**		
IR, solid (CCl_4) $\nu(cm^{-1})$, I[a]	Raman, solid $\nu(cm^{-1})$, I[a]	$\nu(cm^{-1})$[b]	I_{IR} km/mole	Assignment[c]
		3242	0	ν_1 OH (B)[d]
3229 sh (3216 sh)				
3166 vs (3129 s)		3198, 3198	3768	ν_2 OH (E)[d]
		3104	16	ν_3 OH (A)[d]
3056 m (3056 w)		3071, 3071, 3071, 3071	42	ν CH
3027 m (3025 w)		3044, 3044, 3044, 3044	68	ν CH
(2965 vs)	2954 w	2944, 2944, 2944, 2944	141	ν_{as} CH_3
2959 vs		2942, 2942, 2942, 2942	94	ν_{as} CH_3
(2953 vs)		2937, 2937, 2937, 2937	407	ν_{as} CH_3
		2935, 2935, 2935, 2935	97	ν_{as} CH_3
2934 m (2931 vs)		2930, 2930, 2930, 2930	10	ν_{as} CH_3
		2929, 2929, 2929, 2929	14	ν_{as} CH_3
2906 m (2906 m)		2927, 2927, 2927, 2927	31	ν_{as} CH_2
		2891, 2890, 2890, 2890	105	ν_s CH_2
(2871 m)		2876, 2876, 2876, 2876	118	ν_s CH_3
2869 m		2868, 2868, 2868, 2868	96	ν_s CH_3
(2858 m)		2868, 2868, 2868, 2868	100	ν_s CH_3
2804 w sh				
2743 m	2742 vw			
2716 sh				
1739 w				
		1609, 1606, 1606, 1604	7	Ring 5
1606 m	1611 m	1598, 1594, 1594, 1592	38	Ring 4
		1496, 1490, 1490, 1488	53	δ_{as} CH_3
1482 vs		1485, 1484, 1484, 1483	205	δ_{as} CH_3
1462 sh	1460 m	1476, 1468, 1466, 1466	163	δ CH_2
		1471, 1471, 1471, 1471	13	δ_{as} CH_3
		1470, 1470, 1469, 1467	22	δ_{as} CH_3
		1455, 1455, 1455, 1455	70	δ_{as} CH_3
	1447 m	1451, 1451, 1451, 1451	2	δ_{as} CH_3
		1447, 1447, 1447, 1447	20	ν CO, ν CC
1430 m		1445, 1431, 1431, 1429	50	Ring 6

1408 w sh		1417	7	δ OH
1392 m		1406, 1406, 1406, 1406	12	δ_s CH_3
		1378, 1378, 1376, 1376	98	δ_s CH_3
		1376, 1376, 1376, 1375	14	δ_s CH_3
1362 s-m		1368, 1368	8	δ OH
		1352	0	δ OH
1307 m	1302 w	1315, 1314, 1314, 1311	9	ω CH_2
		1315, 1303, 1303, 1289	7	Ring 8
1285 m		1283, 1279, 1279, 1274	164	Ring 9
1257 w	1252 w	1273, 1264, 1264, 1262	47	Ring 10
1242 m	1237 w	1260, 1241, 1241, 1225	46	ν CC
		1207, 1206, 1206, 1206	10	ρ CH_3, ν CC(t-Bu)
		1206, 1206, 1206, 1205	15	ρ CH_3, ν CC(t-Bu)
1202 s	1202 m	1202, 1200, 1200, 1199	176	ρ CH_3
1158 w		1174, 1165, 1165, 1152	6	τ CH_2
1124 w	1124 m	1129	7	Ring 13
1103 w		1107, 1107, 1092	12	Ring 13
1039 vw		1035, 1035, 1035, 1035	0	ρ CH_3
1026 sh	1026 w	1030, 1029, 1029, 1029	1	ρ CH_3
978 vw	977 w	969, 969, 967	24	ρ CH_2, νAr-C
		966	0	ρ CH_2
		948, 947, 947, 947	0	ρ CH_3
947 m	949 vw	938	102	ν CC(t-Bu), ρ CH_2
		929	0	ν CC(t-Bu), νAr-C
		928, 928, 927, 919	225	Ring 15
917 vw	925 m	919, 915, 913	17	ν CC(t-Bu)
	910 m	911, 908, 906	2	ν CC(t-Bu)
		911, 911, 905, 905	9	ν CC(t-Bu)
890 sh		896, 896, 894, 889	70	Ring 16
871 m	885 vw	885, 882, 882, 880	39	Ring 14
857 m		875	0	tors OH
818 m	820 m	807, 802, 802, 800	95	ν CC, ν CO
	797 w	789	6	Breathing

783 s-m	782 w	780,	76	Ring 17
		780, 738	119	Breathing
742 m	745 w	734, 734	43	Breathing
		727	0	Ring 17
710 m	699 m	705, 705, 703, 701	75	δ Ar–C-Ar, ν CC, ν CO
676 m	673 w	673, 673, 671	2	Ring 17
619 w		639, 619, 619	1	Ring 18
605 w		607	1	tors OH
593 m	592 vw	606, 596, 596	35	Ring 22
		577	0	tors OH
570 vw	567 s	561	4	Breathing of macrocycle
		560	0	δ Ar-C-Ar
554 w		552, 552, 551	12	Ring 20
523 w	520 w	518, 518	12	δ CCC
513 w	497 w	512, 512	9	Ring 23
		510	0	Ring 23
		498	0	Ring 24
474 vw	472 w	473, 473	8	Ring 23
443 w	445 w	447, 443, 443, 440	12	macrocycle
430 w	439 w	435	0	macrocycle
		428, 428, 425	14	macrocycle
	410 vw	413	0	macrocycle
		393, 393, 373	25	macrocycle
		369, 369, 368, 366	0	macrocycle
	340 vw	340, 340, 332, 331	14	macrocycle
	320 vw	318, 318, 315	4	macrocycle
		307, 301	3	macrocycle
	297 w	297, 297, 295, 288	5	macrocycle
		284, 284,	2	macrocycle
		272, 267	1	macrocycle
	262 w	260, 260, 260	4	macrocycle
		247, 247, 247, 246	14	macrocycle
	227 vw	224, 224	0	macrocycle
		217, 211	0	macrocycle
	199 m	209, 207, 207	1	macrocycle

[a]w, weak; m, medium; s, strong; v, very; sh, shoulder; br, broad.

[b] SQM scaled wavenumbers.

[c] ν, stretch; δ, bend; ω, wagging; τ, twisting; ρ, rocking; s, symmetrical; as, antisymmetrical. "Ring" is used for the vibrations of the phenyl rings (Fig. 1S).

[d] See Fig. 3. In parenthesis – symmetry type of the vibrations.

Table 4S. IR spectra of *p-tert*-Bu-thiacalix[4]arene **9**

Experiment		Computations		
IR, solid (CS_2) $\nu(cm^{-1})$, I[a]	Raman, solid $\nu(cm^{-1})$, I[a]	$\nu(cm^{-1})$[c]	**I_{IR}** km/mole	**Assignment[b]**
3392 w sh				
		3332	0	ν_1 OH (B)[d]
3251 vs (3338 s)		3307	2288	ν_2 OH (E)[d]
		3260	25	ν_3 OH (A)[d]
3123 w sh (3086 w)		3093, 3093, 3093, 3093	7	ν CH
3073 w sh (3031 w)		3069, 3069, 3069, 3069	21	ν CH
2964 vs (2960 s)	2955 vw	2944, 2944, 2944, 2944	150	ν_{as} CH_3
2950 s sh		2942, 2942, 2942, 2942	103	ν_{as} CH_3
		2940, 2940, 2940, 2940	399	ν_{as} CH_3
2934 sh (2922 m)		2937, 2937, 2937, 2937	80	ν_{as} CH_3
		2933, 2933, 2933, 2933	27	ν_{as} CH_3
		2931, 2931, 2931, 2931	17	ν_{as} CH_3
2909 m	2890 w	2877, 2877, 2877, 2877	98	ν_s CH_3
		2870, 2870, 2870, 2870	100	ν_s CH_3
2869 m (2861 m)		2870, 2870, 2870, 2870	91	ν_s CH_3
		1587, 1583, 1583, 1580	4	Ring 5
1563 w (1562 m)	1565 w	1555, 1550, 1550, 1546	54	Ring 4
1477 m (1482 s)		1486, 1486, 1486, 1486	53	δ_{as} CH_3
		1474, 1474, 1474, 1474	19	δ_{as} CH_3
		1471, 1471, 1470, 1470	41	δ_{as} CH_3
	1463 w	1464, 1451, 1451, 1444	16	δ_{as} CH_3
		1459, 1458, 1457, 1455	0	δ_{as} CH_3
		1452, 1452, 1452, 1452	0	δ_{as} CH_3
1458 vs (1455 m)	1440 w	1448, 1448, 1448, 1448	399	ν CO, ν CC
1406 s		1409	142	Ring 6 + δ OH
		1409, 1409, 1409, 1405	9	δ_s CH_3
1394 s (1397 m)		1402, 1401, 1401	64	Ring 6
		1379, 1378, 1378, 1378	33	δ_s CH_3
1366 m (1364 m)		1378, 1376, 1376, 1375	52	δ_s CH_3
		1359	19	δ OH, Ring 8
1348 m (1343 m)		1335, 1335, 1328	52	δ OH

1282 sh	1280 m	1279	23	Ring 9
1271 s (1273 m)		1268, 1268, 1264	100	ν CO, Ring 10
		1261	4	Ring 10
1259 m		1259, 1259, 1257	122	ν CC
1245 s (1247 m)		1253, 1247, 1247, 1242	146	ν CC
1212 w	1200 w	1223, 1215, 1215, 1211	12	ρ CH_3
1203 w		1206, 1206, 1206, 1206	14	ν CC, ρ CH_3
1189 m (1185 m)		1199, 1190, 1190, 1178	48	ρ CH_3
1130 vw (1124 m)	1136 w	1137, 1133, 1133, 1130	3	Ring 13
1087 w (1085 w)	1085 w	1094, 1088, 1088, 1080	2	ν CS
		1035, 1035, 1035, 1035	0	ρ CH_3
1026 vw (1034 w)	1022 w	1030, 1030, 1030, 1030	2	ρ CH_3
	952 w	949, 949, 949, 949	0	ρ CH_3
923 vw (925 vw)		923, 920, 920, 918	5	ν CC (Bu)
		918, 918, 918, 917	11	ν CC (Bu)
911 vw		910, 910, 910, 910	7	ν CC (Bu)
	900 m	896, 894, 894, 893	25	Ring 16
889 m (885 m)	892 sh, w	891, 890, 890, 888	4	Ring 14
824 m (822 m-w)	825 s	811, 809, 809, 806	38	ν CO, ν CC (Bu)
792 w (784 m)		796, 796, 796, 795	46	ν CS
753 m		754, 742	66	Ring 17
743 s (745 m)		742, 729	11	Ring 17
721 w		709, 706, 706, 705	313	Breathing
642 m (645m)		647, 642, 642, 634	4	torsion OH
		631	2	Ring 18
616 m		611, 600, 600	164	δ CSC
587 m		590, 584	510	Ring 22
555 m-w (555 m)		561, 561	124	Ring 22
540 m		547, 546, 531	12	δ CSC
520 m (508 m)	520 m	516	8	Breathing of macrocycle
		516, 516, 516	2	δ CCC
		490	0	Ring 23
		489, 485, 485, 476	9	Ring 23
	455 m-w	457	8	δ CSC
449 w (452 w)		439, 439, 435	2	macrocycle
416 vw	415 w	413	6	macrocycle
		402, 399, 399, 397	13	macrocycle
	394 m	390, 390	2	macrocycle

		381	0	macrocycle
	360 m	366, 361, 361, 355	0	macrocycle
		349, 348	5	macrocycle
		333, 322, 322, 321	7	macrocycle
	315 vs	317	1	macrocycle
		306, 305, 305, 305	1	macrocycle
		290, 290, 286, 278	5	macrocycle
	273 m	267, 267, 266, 265	2	macrocycle

[a,b,c,d] See the corresponding footnotes to Table 3S.

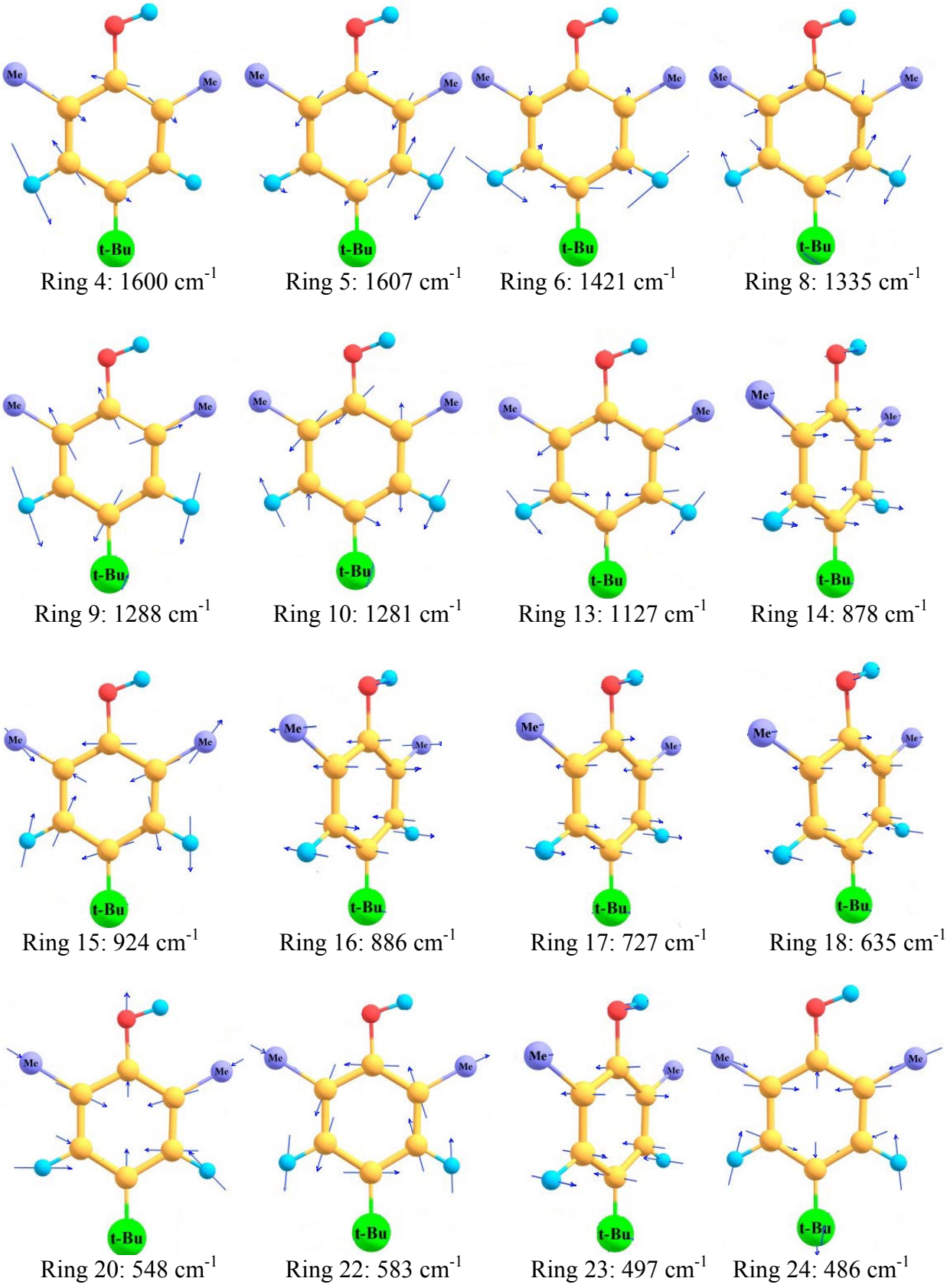


Figure 1S Katsyuba et al.

Legend for figure

Fig. 1S: SQM calculated frequencies (in cm^{-1}) and the diagrams of atomic displacements during vibrations of aromatic ring of 2,6-dimethyl-4-*tert*-Bu-phenol taken as a model of phenolic units of *p-tert*-Bu-calixarenes **8** and **9**. The vibrations are numbered according to the numbers of the most closely resembling "Ring" diagrams of 2,6-dimethylanysole[8]. "Missing" numbers correspond to the strongly mixed vibrations of the aromatic ring and *tert*-Bu residue of 2,6-dimethyl-4-*tert*-Bu-phenol.