

SUPPLEMENTARY MATERIAL

Deprotonation of Large Calixarenes - Cation Binding and Conformations

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Table S1. Interplanar dihedral angles in the representatives of the 'pleated loop' form of *p*-*t*-butylcalix[8]arene (vertically: the present acetonitrile solvate, that of ref. [4c] (VARHEC), that of ref. [4a] (DOVHIF), and ref. [4b] (SUXFIA) (a chloroform solvate, not isomorphous)).

Plane	1	2	3	4	5	6	7	8
O ₈	40.08(8)	35.02(7)	46.21(7)	42.30(7)	32.78(7)	46.03(7)	44.40(7)	42.96(9)
	39.34(6)	35.59(6)	45.72(6)	41.83(6)	32.68(6)	45.72(6)	44.66(6)	42.70(6)
	33.16(3)	40.35(3)	44.85(3)	36.73(3)	37.64(2)	43.07(3)	43.68(3)	44.64(3)
	36.6(3)	39.3(2)	37.0(2)	37.1(2)	37.6(2)	42.0(3)	38.3(2)	35.6(2)
1		74.83(10)	30.69(10)	36.31(10)	65.55(10)	10.05(10)	73.54(10)	62.27(10)
		74.77(8)	31.88(8)	35.07(8)	65.32(8)	9.24(8)	72.48(8)	63.54(8)
		73.45(3)	48.63(3)	24.94(3)	63.63(3)	15.88(3)	60.35(3)	62.44(3)
		74.8(3)	39.0(2)	41.9(3)	72.8(3)	8.8(3)	57.5(3)	60.9(3)
2			71.24(10)	69.87(10)	22.02(10)	81.02(10)	44.01(1)	40.94(10)
			71.22(8)	69.67(8)	22.39(8)	81.27(8)	40.07(8)	41.02(8)
			64.71(3)	69.37(3)	32.93(3)	81.26(3)	44.46(3)	29.85(3)
			68.3(3)	51.2(3)	24.3(3)	81.1(3)	34.9(3)	45.9(3)
3				65.26(10)	52.69(10)	39.96(10)	89.79(10)	41.09(10)
				65.16(8)	52.06(8)	39.94(8)	89.97(8)	40.62(8)
				70.51(3)	33.63(3)	39.15(3)	88.32(3)	41.18(3)
				79.2(3)	51.3(3)	35.4(3)	75.1(3)	29.5(3)
4					74.90(10)	30.78(10)	46.04(10)	83.81(10)
					74.30(8)	31.01(8)	45.69(8)	83.21(8)
					74.28(3)	40.50(3)	40.01(3)	81.32(3)
					66.1(3)	50.7(3)	19.1(3)	72.2(3)

5	74.20(10)	59.01(10)	19.06(10)
	73.79(8)	59.11(8)	18.83(8)
	63.02(3)	69.59(3)	19.15(3)
	75.9(3)	54.7(3)	23.7(3)

6		73.01(10)	73.16(10)
		73.05(8)	72.27(8)
		75.71(3)	72.17(3)
		66.2(3)	60.8(3)

7			77.39(10)
			77.29(8)
			71.07(3)
			67.9(3)
