Supporting information of

Invariant water inclusion property of 1,3-alternate *p-tert*-butylthiacalix[4]arene tetra-methyleneoxycarboxylic acid

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Table S1. Dihedral angles of aromatic rings and reference molecular plane R (defined as the least squares plane containing the four sulfur atoms of the bridges) of compound **I** in solvate **1**, solvate **2** and complex **3**, and compound **II** in solvate **4**, solvate **5** and complex **6**.

Structure no.	Plane AR	Plane BR	Plane CR	Plane DR
1	103.91	100.26	102.60	102.40
2	104.24	101.25	103.70	105.88
3	104.34	104.69	102.28	100.30
4	104.27	113.66	103.14	109.46
5	102.08	110.31	100.27	107.97
6	80.02	80.02	80.02	80.02

Table S2. Dihedral angles of the apposite aromatic rings of compound **I** in solvate **1**, solvate **2** and complex **3**, and compound **II** in solvate **4**, solvate **5** and complex **6**.

Structure no.	Plane AC	Plane BD
1	26.52	22.66
2	27.94	27.16
3	26.63	25.00
4	27.42	43.14
5	22.36	38.32
6	19.96	19.96

Table S3. Torsion angles in the pendant arms of compound **I** in solvate **1**, solvate **2** and complex **3**.

		1	**2**	**3**
Chain A	C6-O1-C11-C12	-175.6(3)	175.8(8)	178.9(2)
	O1-C11-C12-O2	-1.9(6)	6.0(16)	8.7(4)
	O1-C11-C12-O3	178.2(3)	-174.4(9)	-171.3(2)
Chain B	C14-O4-C23-C24	-175.1(4)	-167.6(11)	166.4(2)
	O4-C23-C24-O5	-4.6(8)	-8(2)	6.8(4)
	O4-C23-C24-06	176.8(5)	175.2(16)	-174.8(3)
Chain C	C30-O7-C35-C36	-173.8(4)	-179.4(11)	-170.6(2)
	O7-C35-C36-09	-7.4(6)	-5(2)	0.6(4)
	O7-C35-C36-08	174.2(4)	169.1(15)	179.3(3)
Chain D	C38-O10-C47-C48	-175.8(4)	-170.6(8)	-175.7(3)
	O10-C47-C48-011	-1.6(7)	-2.6(18)	-4.9(5)
	O10-C47-C48-O12	178.4(5)	179.0(10)	175.0(3)

Table S4. Torsion angles in the pendant arms of compound **II** in solvate **4**, solvate **5** and complex **6**.

		4	**5**	**6**
Chain A	C6-O1-C7-C8	-138.1(2)	139.35(19)	-136.1(6)
	O1-C7-C8-O2	-6.3(4)	9.2(3)	9.4(8)
	O1-C7-C8-O3	176.0(2)	-172.52(18)	-169.6(5)
Chain B	C10-O4-C15-C16	172.1(2)	177.71(19)	
	O4-C15-C16-O5	6.8(4)	176.4(2)	
	O4-C15-C16-06	-173.1(3)	-3.7(4)	
Chain C	C22-O7-C23-C24	-168.7(3)	174.2(2)	
	O7-C23-C24-09	20.8(4)	-22.0(3)	
	O7-C23-C24-08	-162.6(3)	160.8(2)	
Chain D	C26-O10-C31-C32	-75.8(4)	-179.8(2)	
	O10-C31-C32-011	-94.6(5)	-178.3(3)	
	O10-C31-C32-O12	83.0(4)	2.4(4)	

Table S5. Hydrogen bonds of solvent **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(18)#1	0.84	1.73	2.547(5)	162.2
O(15)-H(15)...O(8)#2	0.84	1.90	2.743(6)	176.1
O(16)-H(16A)...O(12)#3	0.84	2.13	2.772(10)	133.3
O(16)-H(16A)...O(16)#3	0.84	1.94	2.531(19)	126.1
O(6)-H(6)...O(17)	0.84	1.78	2.565(6)	153.6
O(11)-H(11)...O(14)	0.84	1.87	2.643(5)	152.2
O(14)-H(14A)...O(5)	0.82	1.84	2.641(5)	166.7
O(14)-H(14B)...O(4)	0.82	2.36	2.908(5)	124.7
O(18)-H(18A)...O(15)	0.84	1.91	2.738(6)	166.2

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z #2 x-1,y-1,z #3 –x+2, -y+1, -z+1

Table S6. Hydrogen bonds of solvent **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(14)#1	0.82(19)	1.8(2)	2.450(17)	139(19)
O(9)-H(9)...O(13)#1	0.82	1.91	2.569(12)	136.4
O(12)-H(12A)...O(15)#1	0.82	2.20	2.710(14)	120.1
O(3)-H(3)...O(16)	0.82	1.79	2.606(14)	175.9
O(13)-H(13B)...O(2)#2	0.82(16)	2.3(3)	2.779(10)	119(26)
O(14)-H(14A)...O(10)#2	0.84(10)	2.3(2)	2.996(11)	137(27)
O(14)-H(14A)...O(11)#2	0.84(10)	2.1(2)	2.783(13)	135(1)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z+1 #2 x,y,z-1

Table S7. Hydrogen bonds of complex **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(14)-H(14D)...O(4)	0.85	2.13	2.978(2)	179.8
O(14)-H(14C)...O(11)	0.85	2.55	2.961(3)	110.8
O(14)-H(14C)...O(10)	0.85	2.14	2.986(3)	179.5
O(13)-H(13D)...O(7)	0.85	1.91	2.761(2)	179.4
O(13)-H(13C)...O(1)	0.85	2.17	3.017(2)	179.5
O(12)-H(12)...N(1)	0.82	1.85	2.655(3)	165.8
O(9)-H(9)...O(13)	0.85	1.72	2.568(3)	179.8
O(5)-H(5A)...O(14)	0.85	1.77	2.620(3)	179.8

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

Table S8. Hydrogen bonds of solvent **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(2)#1	0.82	1.84	2.658(3)	176.3
O(12)-H(12)...O(14)#2	0.82	1.90	2.711(4)	169.9
O(9)-H(9)...O(13)#3	0.82	1.72	2.536(3)	170.9
O(5)-H(5A)...O(4)	0.82	2.04	2.565(3)	121.6
O(13)-H(13B)...O(7)	0.818(10)	2.239(13)	3.047(3)	170(4)
O(13)-H(13B)...O(9)	0.818(10)	2.39(3)	2.881(3)	119(3)
O(13)-H(13A)...O(1)	0.815(10)	2.13(2)	2.883(3)	154(4)
O(13)-H(13A)...O(2)	0.815(10)	2.65(4)	3.129(3)	119(3)
O(14)-H(14)...O(8)#4	0.82	1.90	2.706(3)	167.1

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z #2 x-1,y-1,z #3 -x+1,-y+1,-z

#4 -x+2,-y+1,-z

Table S9. Hydrogen bonds of solvent **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(9)-H(9A)...O(13)#1	0.82	1.75	2.554(3)	165.3
O(5)-H(5)...O(6)#2	0.82	1.86	2.680(2)	175.6
O(3)-H(3)...O(2)#3	0.82	1.83	2.651(2)	173.9
O(12)-H(12)...O(10)	0.82	2.09	2.605(2)	120.5
O(13)-H(13B)...O(2)	0.72(3)	2.63(3)	3.035(3)	118(3)
O(13)-H(13B)...O(1)	0.72(3)	2.21(3)	2.891(3)	157(3)
O(13)-H(13A)...O(9)	0.82(4)	2.34(4)	2.874(3)	124(3)
O(13)-H(13A)...O(7)	0.82(4)	2.24(4)	3.036(3)	166(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,-y+1,-z #3 -x+1,-y+2,-z+1

Table S10. Hydrogen bonds of complex **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4B)...O(2)	0.82(2)	2.45(6)	2.89(5)	114.(4)