

Electronic Supplementary Information (ESI)

Table S1 Torsion angles ($^{\circ}$) of the alkanoyl chains

Table S2 Distances and angles of hydrogen bond type contacts.

Fig. S1 Packing arrangement of the calixarene molecules in the complex of **1**·with (-)-menthone (**1a**) viewed from the crystallographic *a*, *b* and *c* axes, respectively. The two crystallographically independent calixarene molecules are indicated by different colours.

Fig. S2 Packing arrangement of the calixarene molecules in the complex of **1**·with (-)-menthol (**1b**) viewed from the crystallographic *a*, *b* and *c* axes, respectively. The two crystallographically independent calixarene molecules are indicated by different colours.

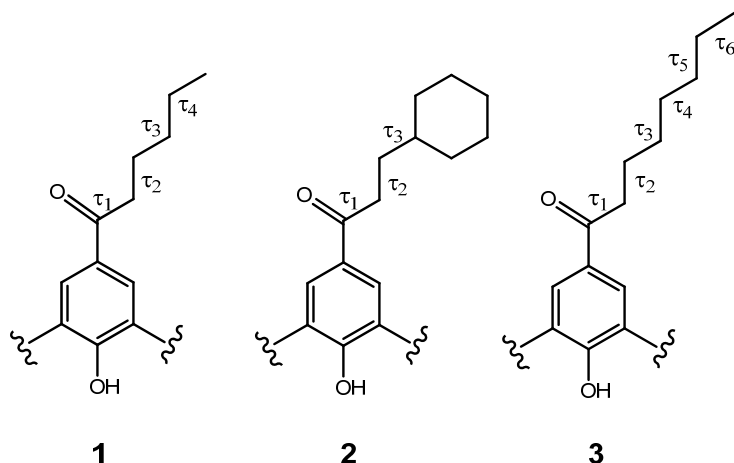
Fig. S3 Packing arrangement of the calixarene molecules in the complex of **2**·with (-)-menthone (**2a**) viewed from the crystallographic *a*, *b* and *c* axes, respectively. The two crystallographically independent calixarene molecules are indicated by different colours.

Fig. S4 Packing arrangement of the calixarene molecules in the complex of **2**·with (+)-carvone (**2b**) viewed from the crystallographic *a*, *b* and *c* axes, respectively. The two crystallographically independent calixarene molecules are indicated by different colours.

Fig. S5 Packing arrangement of the calixarene molecules in the complex of **3**·with (+)-carvone (**3a**) viewed from the crystallographic *a*, *b* and *c* axes, respectively. The two crystallographically independent calixarene molecules are indicated by different colours.

Fig. S6 Packing arrangement of the calixarene molecules in the complex of **3** with *n*-butanol (**3b**) viewed from the crystallographic *a*, *b* and *c* axes, respectively. The space group is the centrosymmetric $P2_1/n$ and there is one complex molecule in the asymmetric unit only.

Table S1.



	τ_1		τ_2		τ_3		τ_4		τ_5		τ_6	
	<i>A</i>	<i>B</i>	<i>A</i>	<i>B</i>	<i>A</i>	<i>B</i>	<i>A</i>	<i>B</i>	<i>A</i>	<i>B</i>	<i>A</i>	<i>B</i>
1a												
branch 1	-173.1	74.2	80.2	63.0	80.4	-176.8	-170.6	-177.4				
branch 2	-178.8	179.3	178.7	-175.3	-165.1	79.5	176.1	168.0				
branch 3	-168.9	-179.2	175.4	-176.9	169.8	-174.8	-174.8	179.2				
branch 4	-75.1	178.5	-165.2	-74.9	-176.1	176.8	-172.4	-176.7				
1b												
branch 1	-170.2	73.3	72.3	65.4	74.4	-176.0	70.7	-177.4				
branch 2	173.1	176.1	171.9	-162.7	-75.7	166.7	-166.1	178.0				
branch 3	-175.3	-174.2	177.4	-176.3	179.9	-170.8	179.9	170.8				
branch 4	-79.9	166.8	-163.8	-170.9	-177.5	77.2	-172.1	163.2				
2a												
branch 1	165.5	-167.1	-72.0	71.5	-59.5	60.0	-167.6	166.7	-170.2	171.0	-60.0	58.5
branch 2	72.5	-72.0	161.5	-163.3	-179.3	179.5	174.9	-174.9	-175.6	175.4	-176.2	174.8
branch 3	177.4	-178.2	-179.9	178.2	-176.6	177.8	171.8	-172.5	-178.1	178.3	179.3	-179.4
branch 4	176.6	-175.4	-167.8	172.7	176.7	-178.3	-178.1	177.2	171.0	-170.9	-171.7	172.0
2b												
branch 1	-114.1	115.4	67.7	-63.6	170.5	-174.1	177.2	-179.3	-131.1	177.4	-87.0	-176.5
branch 2	-174.3	-172.1	75.5	-72.6	177.9	-179.7	73.4	-71.7	176.2	179.9	179.6	-178.1
branch 3	-166.7	171.4	176.6	-178.5	-176.5	174.2	-173.4	174.6	-172.5	173.0	174.7	-172.3
branch 4	152.8	-147.2	179.6	177.8	-73.3	73.3	-176.1	176.8	172.4	-172.8	-176.2	177.1
3a												
branch 1	155.0	-149.6	-70.7	79.1	159.5	-171.1						
branch 2	98.9	-105.4	173.7	-177.0	-162.3	161.9						
branch 3	147.4	-156.8	-82.7	74.0	174.5	-166.5						
branch 4	164.9	-161.6	176.3	-171.5	173.0	-172.4						
3b												
branch 1	-179.9		-69.0		174.1							
branch 2	82.8		165.6		179.2							
branch 3	73.0		-179.0		179.7							
branch 4	150.8		161.5		152.7							

Table S2.

Atoms involved	Symmetry	Distances (Å)		Angles (°)
		D...A	H...A	D-H...A
1a				
O(1)-H(1)···O(4)	x, y, z	2.726(4)	1.90	166.6
O(2)-H(2)···O(1)	x, y, z	2.670(4)	1.86	162.1
O(3)-H(3)···O(2)	x, y, z	2.655(4)	1.85	161.1
O(4)-H(4)···O(3)	x, y, z	2.667(4)	1.83	171.8
C(24A)-H(24)···O(5)	$-x, -0.5+y, 2-z$	3.356(4)	2.47	155.2
C(3A)-H(3A2)···O(6)	$-x, -0.5+y, 1-z$	3.393(4)	2.50	157.0
C(7A)-H(7C)···O(7)	$1-x, -0.5+y, 1-z$	3.364(4)	2.51	144.1
C(10A)-H(10A)···O(7)	$1-x, -0.5+y, 1-z$	3.293(4)	2.43	150.6
C(17A)-H(17A)···O(8)	$1-x, -0.5+y, 2-z$	3.304(4)	2.44	151.7
C(14A)-H(14A)···O(8)	$1-x, -0.5+y, 2-z$	3.402(4)	2.55	144.2
O(1A)-H(1A)···O(4A)	x, y, z	2.739(4)	2.06	137.3
O(2A)-H(2A)···O(1A)	x, y, z	2.709(4)	1.90	160.1
O(3A)-H(3A)···O(2A)	x, y, z	2.670(4)	1.84	172.1
O(4A)-H(4A)···O(3A)	x, y, z	2.672(4)	1.86	161.2
C(24)-H(24)···O(5A)	$1-x, 0.5+y, 1-z$	3.386(4)	2.47	156.7
C(19)-H(19)···O(5A)	$1-x, 0.5+y, 1-z$	3.568(4)	2.68	155.8
C(3)-H(3A1)···O(6A)	$1-x, 0.5+y, 2-z$	3.302(4)	2.38	162.2
C(5)-H(5)···O(7A)	$-x, 0.5+y, 2-z$	3.421(4)	2.55	152.0
C(10)-H(10)···O(7A)	$-x, 0.5+y, 2-z$	3.239(4)	2.36	153.2
C(14)-H(14A)···O(8A)	$-x, 0.5+y, 1-z$	3.386(4)	2.55	144.5
C(17)-H(17A)···O(8A)	$-x, 0.5+y, 1-z$	3.298(4)	2.44	149.8
1b				
O(1)-H(1)···O(4)	x, y, z	2.723(4)	1.89	170.5
O(2)-H(2)···O(1)	x, y, z	2.709(4)	1.99	142.5
O(3)-H(3)···O(2)	x, y, z	2.676(4)	1.85	167.6
O(4)-H(4)···O(3)	x, y, z	2.682(4)	1.83	177.8
O(1A)-H(1A)···O(3)	x, y, z	2.196(4)	2.58	130.8
O(1H)-H(1H)···O(5)	x, y, z	3.187(4)	2.41	154.2
C(36)-H(36B)···O(1H)	x, y, z	3.371(4)	2.43	158.7
C(21A)-H(21C)···O(5)	$-x, -0.5+y, -z$	3.495(5)	2.61	149.4
C(3A)-H(3C)···O(6)	$-x, -0.5+y, 1-z$	3.313(5)	2.41	157.6
C(7A)-H(7C)···O(7)	$1-x, -0.5+y, 1-z$	3.415(5)	2.54	147.8
C(10A)-H(10A)···O(7)	$1-x, -0.5+y, 1-z$	3.354(4)	2.50	149.7
C(17A)-H(17A)···O(8)	$1-x, -0.5+y, -z$	3.306(5)	2.42	154.7
O(1A)-H(1A)···O(4A)	x, y, z	2.744(4)	2.03	142.6
O(2A)-H(2A)···O(1A)	x, y, z	2.691(4)	1.86	168.7
O(3A)-H(3A)···O(2A)	x, y, z	2.675(4)	1.86	162.4
O(4A)-H(4A)···O(3A)	x, y, z	2.680(4)	1.85	171.4
C(21)-H(21B)···O(5A)	$1+x, 0.5+y, 1-z$	3.501(5)	2.65	144.3
C(24)-H(24)···O(5A)	$1-x, 0.5+y, 1-z$	3.337(4)	2.46	152.6
C(3)-H(3B)···O(6A)	$1-x, 0.5+y, -z$	3.314(4)	2.39	163.3
O(1G)-H(1G)···O(7A)	x, y, z	3.138(4)	2.32	161.5
C(17)-H(17)···O(8A)	$-x, 0.5+y, 1-z$	3.339(5)	2.48	149.9
C(14)-H(14B)···O(8A)	$-x, 0.5+y, 1-z$	3.473(5)	2.60	146.8
2a				
O(1)-H(1)···O(2)	x, y, z	2.722(5)	1.95	152.1
O(2)-H(2)···O(3)	x, y, z	2.694(5)	1.86	173.5
O(3)-H(3)···O(4)	x, y, z	2.679(5)	1.83	179.5
O(4)-H(4)···O(1)	x, y, z	2.673(5)	1.88	156.3
C(46A)-H(46C)···O(1G)	x, y, z	2.587(5)	2.59	122.0
C(12A)-H(12A)···O(5)	$1-x, -0.5+y, -z$	3.399(6)	2.49	159.9
C(17A)-H(17A)···O(5)	$1-x, -0.5+y, -z$	3.422(6)	2.52	159.0
C(19A)-H(19A)···O(6)	$2-x, -0.5+y, -z$	3.318(6)	2.43	154.9
C(24A)-H(24A)···O(6)	$2-x, -0.5+y, -z$	3.501(6)	2.61	156.1
C(3A)-H(3A2)···O(7)	$2-x, -0.5+y, 1-z$	3.428(6)	2.53	158.0
C(26A)-H(26A)···O(7)	$2-x, -0.5+y, 1-z$	3.399(6)	2.48	161.7
C(5A)-H(5A)···O(8)	$1-x, -0.5+y, 1-z$	3.367(6)	2.44	163.9

O(1A)-H(1A)···O(2A)	x, y, z	2.729(5)	1.89	173.0
O(2A)-H(2A)···O(3A)	x, y, z	2.692(5)	1.84	178.6
O(3A)-H(3A)···O(4A)	x, y, z	2.692(5)	1.85	176.6
O(4A)-H(4A)···O(1A)	x, y, z	2.672(5)	1.84	171.5
C(54)-H(54)···O(1H)	x, y, z	3.087(6)	2.49	118.2
C(12)-H(12)···O(5A)	$2-x, 0.5+y, 1-z$	3.441(6)	2.54	159.1
C(17)-H(17)···O(5A)	$2-x, 0.5+y, 1-z$	3.406(6)	2.50	159.7
C(19)-H(19)···O(6A)	$1-x, 0.5+y, 1-z$	3.298(6)	2.41	155.5
C(24)-H(24)···O(6A)	$1-x, 0.5+y, 1-z$	3.478(6)	2.60	156.2
C(3)-H(3A1)···O(7A)	$1-x, 0.5+y, -z$	3.414(6)	2.51	158.1
C(26)-H(26)···O(7A)	$1-x, 0.5+y, -z$	3.400(6)	2.50	158.5
C(5)-H(5)···O(8A)	$2-x, 0.5+y, -z$	3.338(6)	2.41	166.4
C(3)-H(3B)···O(7A)	$1+x, y, z$	3.428(6)	2.53	158.0
C(7H)-H(7H2)··· <i>centroid</i> (ringA) ^a	x, y, z	3.599(7)	2.76	143.9
C(7G)-H(7G1)··· <i>centroid</i> (ringA') ^a	x, y, z	3.576(7)	2.80	136.5

2b

O(1)-H(1)···O(4)	x, y, z	2.714(6)	1.88	174.5
O(2)-H(2)···O(1)	x, y, z	2.691(6)	1.91	155.4
O(3)-H(3)···O(2)	x, y, z	2.691(6)	1.86	172.5
O(4)-H(4)···O(3)	x, y, z	2.686(6)	1.84	174.4
C(5G)-H(5G)···O(5)	x, y, z	3.432(6)	2.67	137.8
C(17A)-H(17A)···O(5)	$1-x, -0.5+y, -z$	3.401(6)	2.49	161.6
C(26A)-H(26A)···O(5)	$1-x, -0.5+y, -z$	3.412(6)	2.50	159.8
C(5A)-H(5A)···O(6)	$1-x, -0.5+y, 1-z$	3.421(6)	2.51	160.8
C(3A)-H(3C)···O(7)	$-x, -0.5+y, 1-z$	3.461(6)	2.55	161.5
C(12A)-H(12A)···O(7)	$-x, -0.5+y, 1-z$	3.361(6)	2.43	165.0
C(19A)-H(19A)···O(8)	$-x, 0.5+y, 2-z$	3.325(6)	2.42	159.3
O(2)-H(2)···O(1G)	$1-x, 0.5+y, 2-z$	2.883(6)	2.59	101.9
O(1A)-H(1A)···O(4A)	x, y, z	2.716(6)	1.91	161.1
O(2A)-H(2A)···O(1A)	x, y, z	2.693(6)	1.87	167.9
O(3A)-H(3A)···O(2A)	x, y, z	2.688(6)	1.93	149.4
O(4A)-H(4A)···O(3A)	x, y, z	2.701(6)	1.88	166.8
C(5H)-H(5H)···O(5A)	x, y, z	3.361(6)	2.65	132.6
C(19)-H(19)···O(5A)	$-x, 0.5+y, 1-z$	3.408(6)	2.50	160.8
C(3)-H(3B)···O(6A)	$-x, 0.5+y, -z$	3.387(6)	2.47	161.4
C(17)-H(17)···O(8A)	$1-x, 0.5+y, 1-z$	3.333(6)	2.41	163.3
C(5)-H(5)···O(7A)	$1-x, 0.5+y, -z$	3.401(6)	2.49	161.4
C(10)-H(10)···O(7A)	$1-x, 0.5+y, -z$	3.412(6)	2.50	165.1
O(2A)-H(2A)···O(1H)	x, y, z	2.787(6)	2.46	103.8
C(52)-H(52B)··· <i>centroid</i> (ringC) ^a	$1-x, -0.5+y, 1-z$	3.553(7)	2.69	146.9
C(10G)-H(10C)··· <i>centroid</i> (ringD) ^a	x, y, z	3.556(6)	2.84	130.4
C(10H)-H(10H)··· <i>centroid</i> (ringB') ^a	x, y, z	3.742(6)	2.80	160.1
C(52A)-H(52A)··· <i>centroid</i> (ringC') ^a	$-x, 0.5+y, -z$	3.599(6)	2.70	152.3
C(10H)-H(10D)··· <i>centroid</i> (ringD') ^a	x, y, z	3.506(6)	2.86	124.3

3a

O(1)-H(1)···O(2)	x, y, z	2.714(5)	1.91	160.3
O(2)-H(2)···O(3)	x, y, z	2.677(5)	1.86	166.2
O(3)-H(3)···O(4)	x, y, z	2.724(5)	1.89	170.5
O(4)-H(4)···O(1)	x, y, z	2.662(5)	1.81	179.1
C(10A)-H(10A)···O(5)	$-1+x, y, z$	3.452(6)	2.52	165.7
C(19A)-H(19A)···O(7)	$x, y, 1+z$	3.365(7)	2.48	158.1
C(24A)-H(24A)···O(7)	$x, y, 1+z$	3.437(7)	2.56	154.8
C(12A)-H(12A)···O(8)	$-1+x, y, 1+z$	3.553(6)	2.62	169.3
C(17A)-H(17A)···O(8)	$-1+x, y, 1+z$	3.585(4)	2.65	168.1
O(1A)-H(1A)···O(4A)	x, y, z	2.694(5)	1.87	166.7
O(2A)-H(2A)···O(1A)	x, y, z	2.685(5)	1.91	148.4
O(3A)-H(3A)···O(2A)	x, y, z	2.704(5)	1.89	161.3
O(4A)-H(4A)···O(3A)	x, y, z	2.694(5)	1.91	152.3
C(3)-H(3A)···O(5A)	$1+x, y, z$	3.419(6)	2.52	157.6
C(26)-H(26)···O(5A)	$1+x, y, z$	3.536(7)	2.65	153.6
C(19)-H(19)···O(6A)	$1+x, y, -1+z$	3.338(6)	2.41	166.0
C(24)-H(24)···O(6A)	$1+x, y, -1+z$	3.442(6)	2.52	162.9

C(12)-H(12)···O(7A)	$x, y, -1+z$	3.469(6)	2.54	165.5
C(17)-H(17)···O(7A)	$x, y, -1+z$	3.597(6)	2.67	165.5
O(3)-H(3)···O(1G)	$1-x, 0.5+y, 1-z$	2.987(6)	2.64	106.4
O(2A)-H(2A)···O(1H)	$1-x, -0.5+y, 1-z$	3.010(6)	2.66	105.5
C(9H)-H(9H1)··· <i>centroid</i> (ringA) ^a	x, y, z	3.614(6)	2.82	139.0
C(8H)-H(8HA)··· <i>centroid</i> (ringC) ^a	x, y, z	3.882(6)	2.93	175.2
C(8G)-H(8GA)··· <i>centroid</i> (ringA') ^a	x, y, z	3.782(6)	2.92	151.1
C(9G)-H(9G2)··· <i>centroid</i> (ringC') ^a	x, y, z	3.659(6)	2.80	147.0

3b

O(1)-H(1)···O(2)	x, y, z	2.728(3)	1.93	157.1
O(2)-H(2)···O(3)	x, y, z	2.686(3)	1.85	172.4
O(3)-H(3)···O(4)	x, y, z	2.709(3)	1.90	162.4
O(4)-H(4)···O(1)	x, y, z	2.691(3)	1.87	166.2
O(1G)-H(1G)···O(5)	x, y, z	3.065(3)	2.36	141.4
C(12)-H(12)···O(5)	$0.5+x, 0.5-y, -0.5+z$	3.532(3)	2.60	168.7
C(24)-H(24)···O(6)	$-0.5+x, 0.5-y, -0.5+z$	3.371(3)	2.47	159.2
C(19)-H(19)···O(6)	$-0.5+x, 0.5-y, -0.5+z$	3.206(3)	2.29	161.9
C(3)-H(3A)···O(7)	$-0.5+x, 0.5-y, 0.5+z$	3.425(3)	2.51	162.7
C(26)-H(26)···O(7)	$-0.5+x, 0.5-y, 0.5+z$	3.351(3)	2.43	164.6
C(5)-H(5)···O(8)	$0.5+x, 0.5-y, 0.5+z$	3.544(3)	2.60	173.0

^a ring A: C(1)...C(6); ring C: C(15)...C(20); ring D: C(22)...C(27); ring A': C(1A)...C(6A); ring B': C(8A)...C(13A); ring C': C(15A)...C(20A); ring D': C(22A)...C(27A); ring B'': C(8B)...C(13B); ring D'': C(22B)...C(27B).

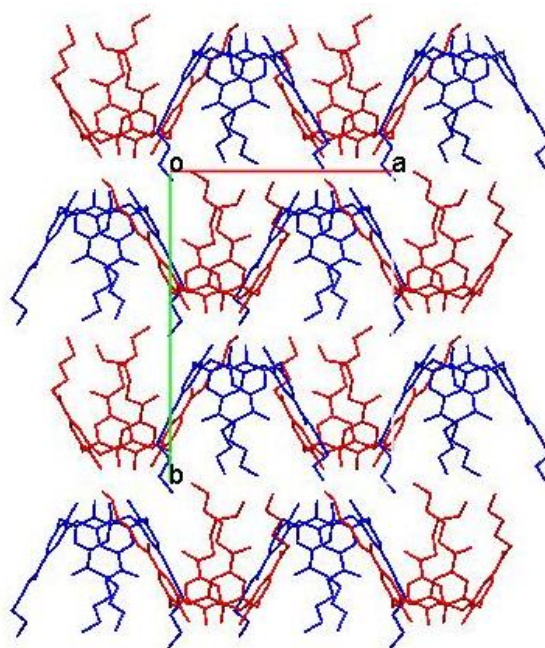
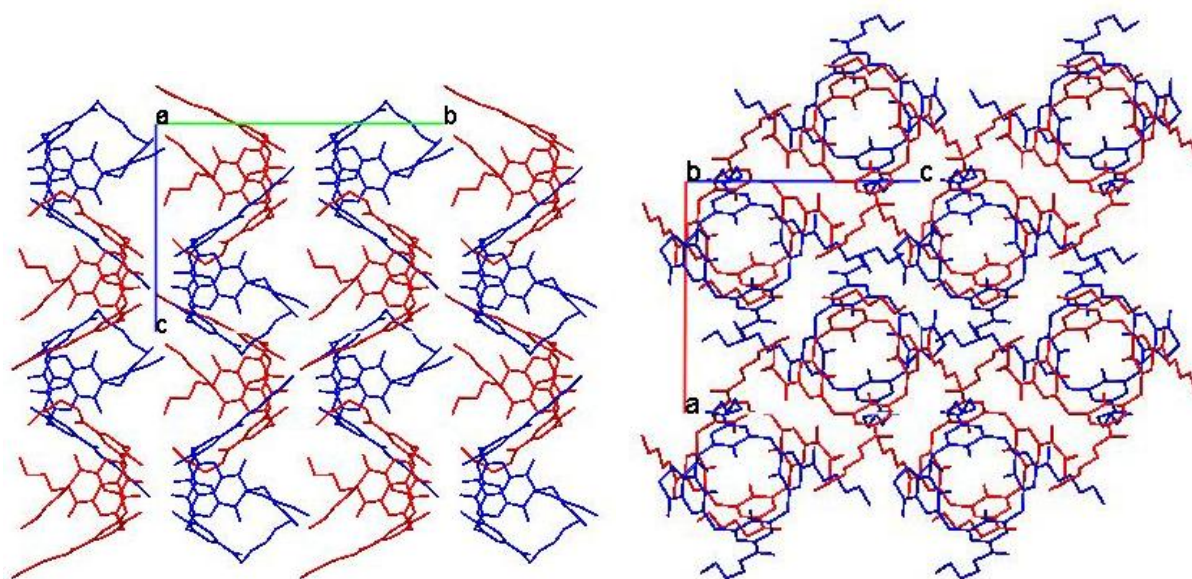


Fig. S1

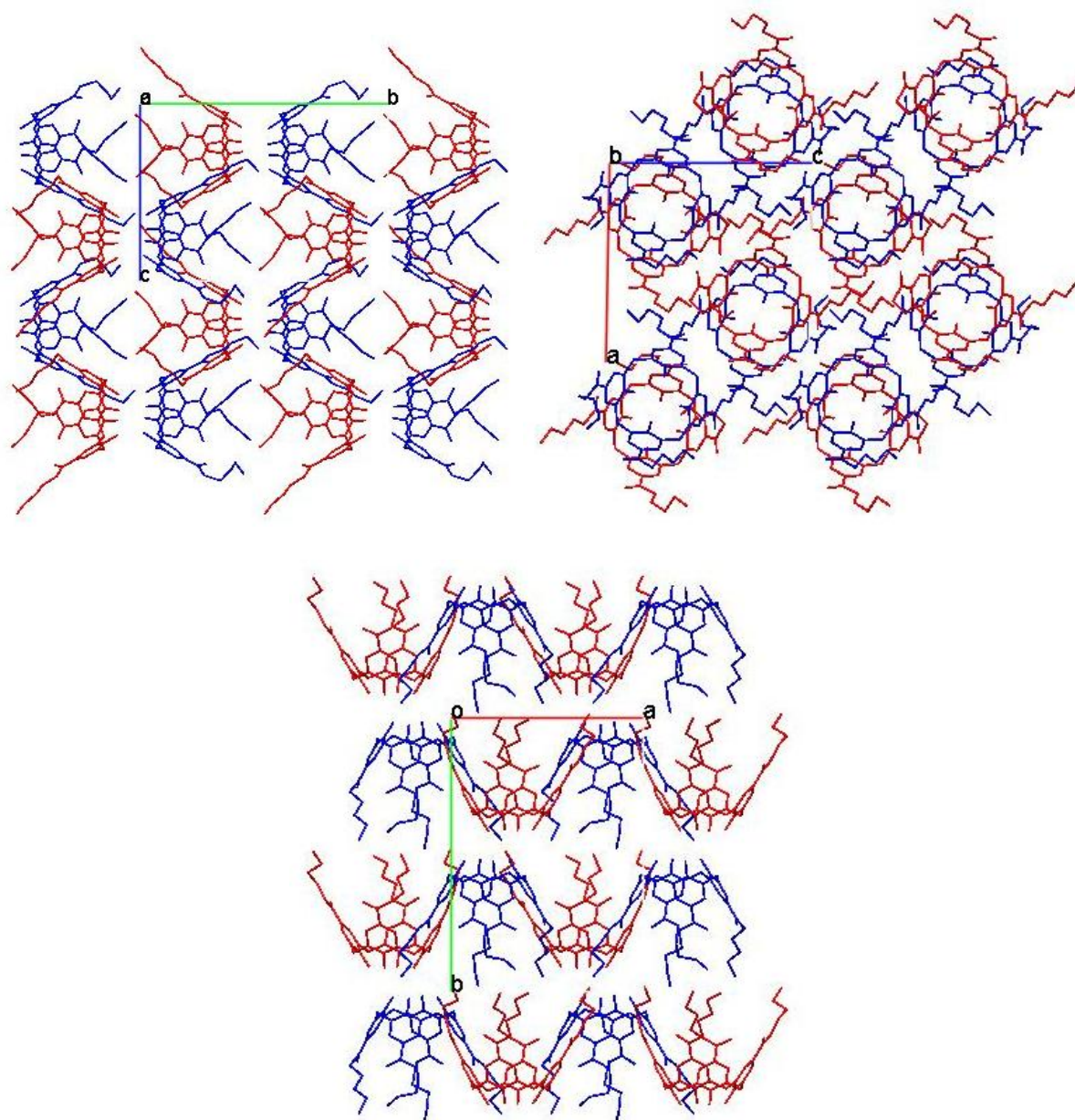


Fig. S2

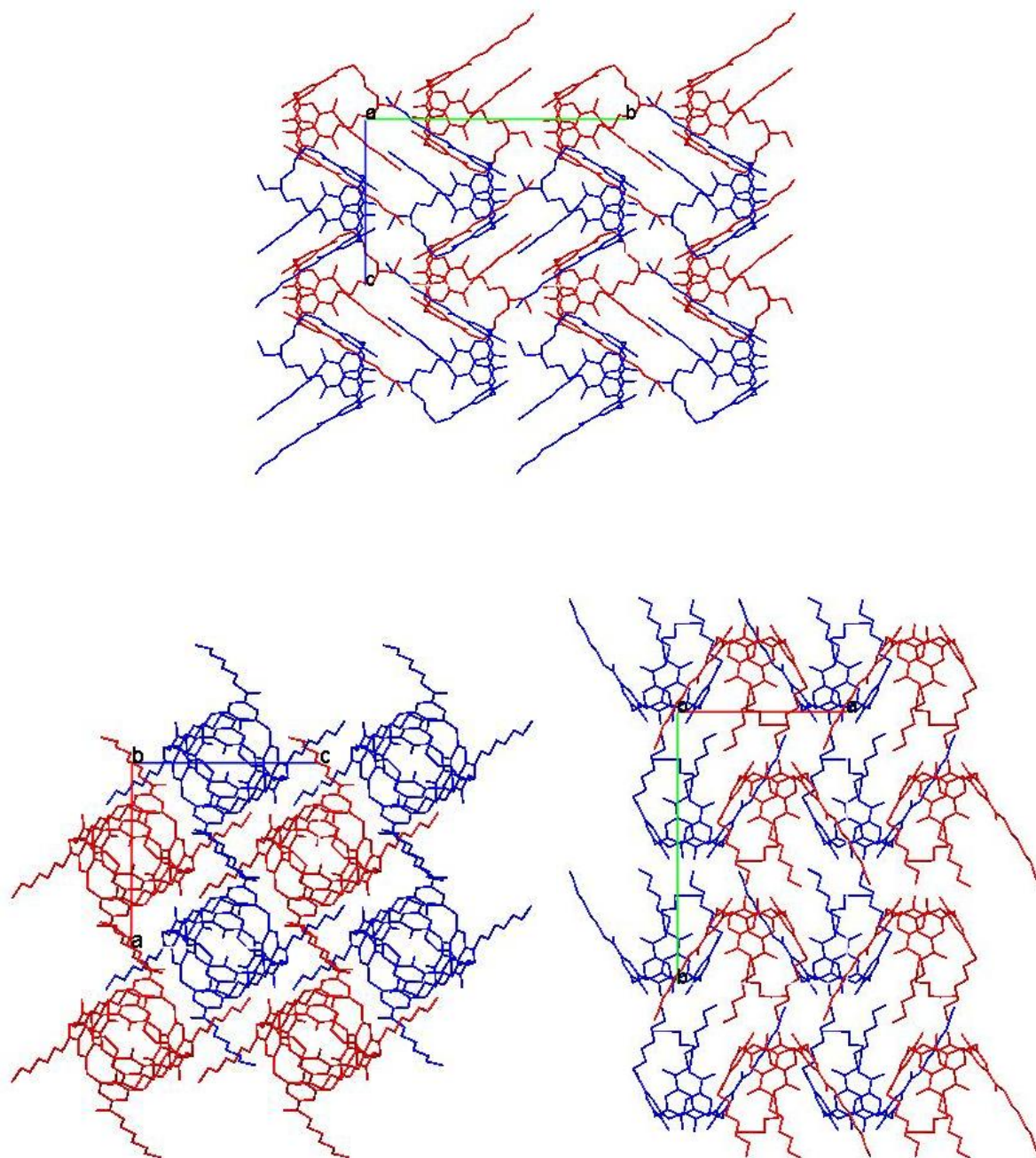


Fig. S3

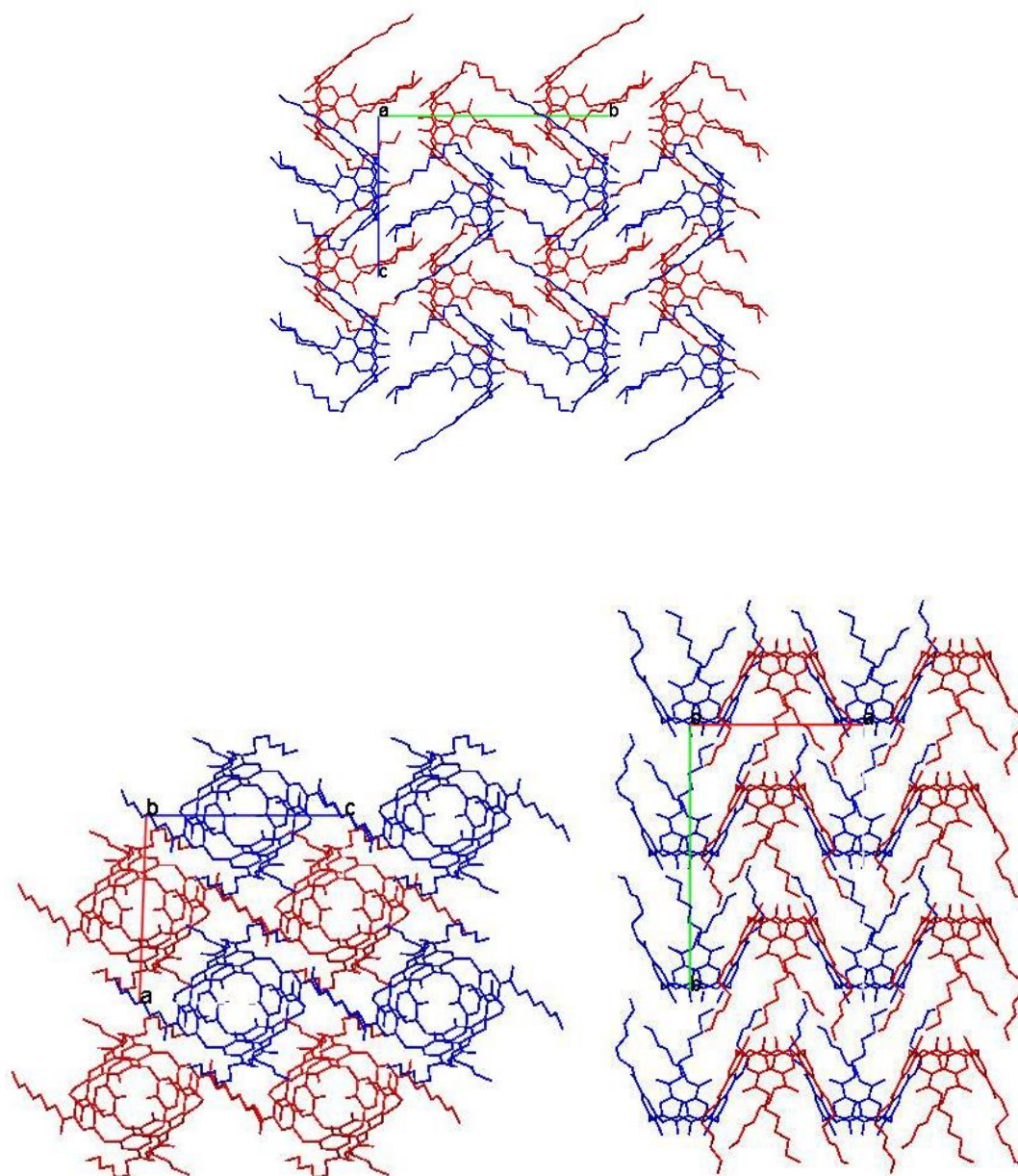


Fig. S4

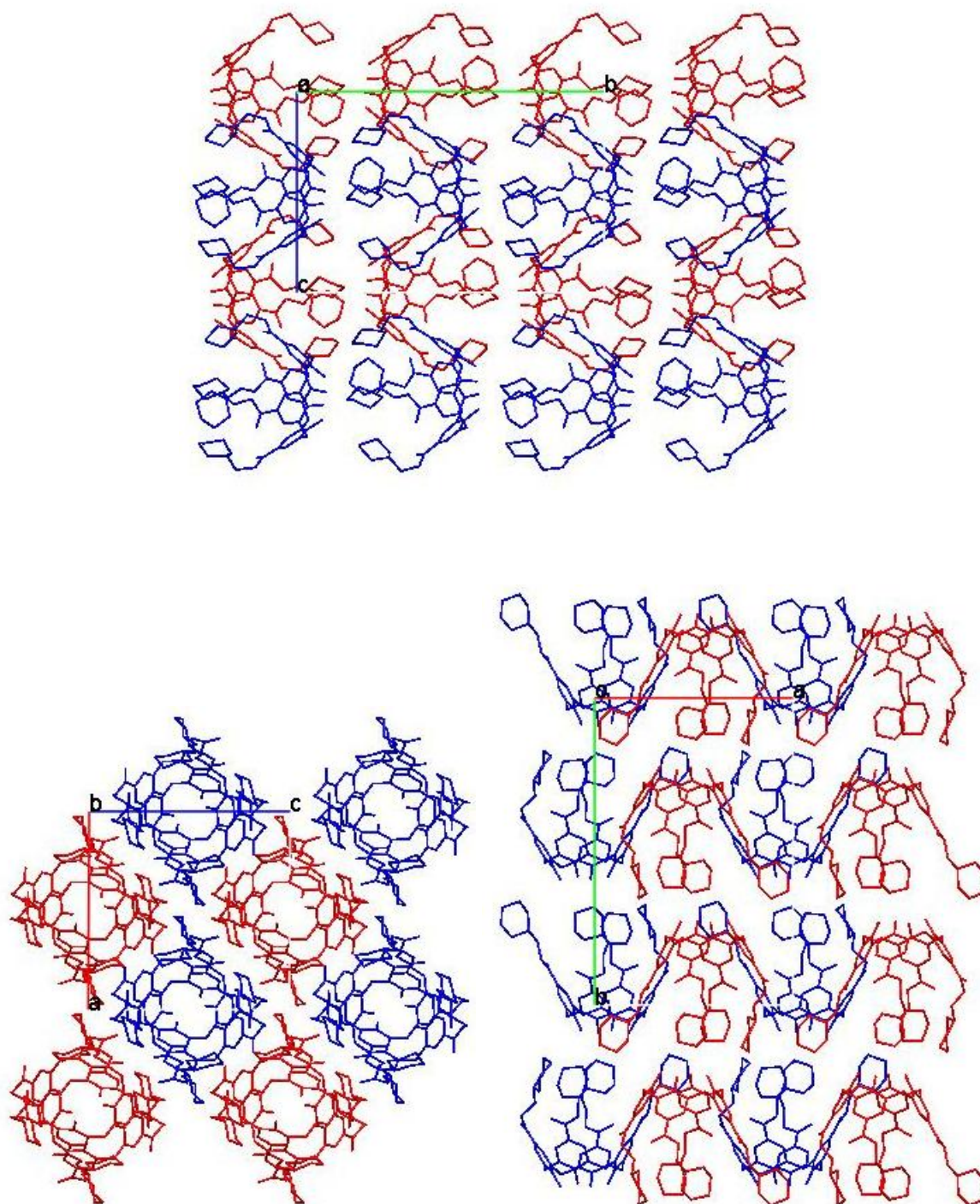


Fig. S5

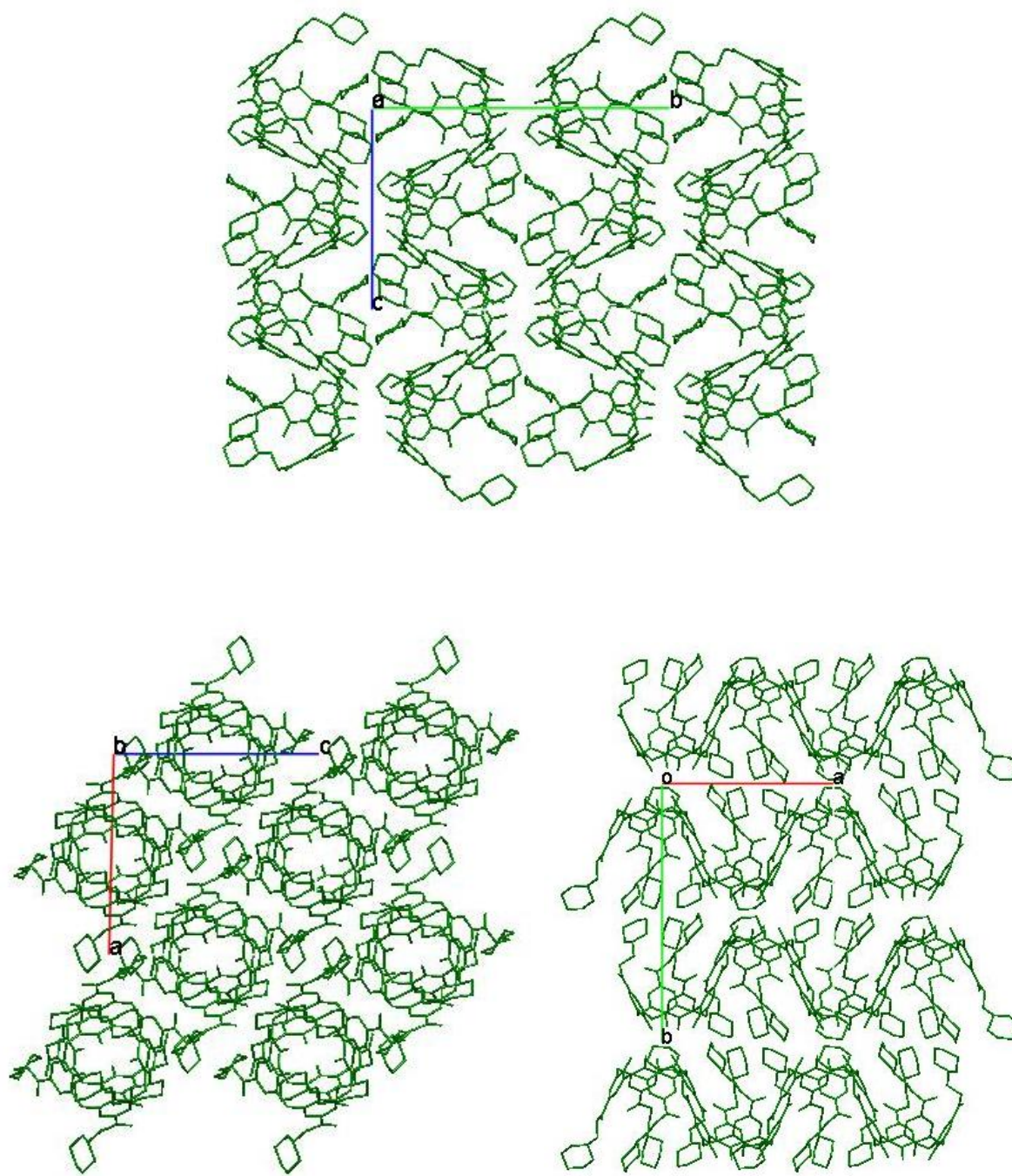


Fig. S6