Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

A new fan-like adaptive porous organic cage for the structure determination of perfume molecules

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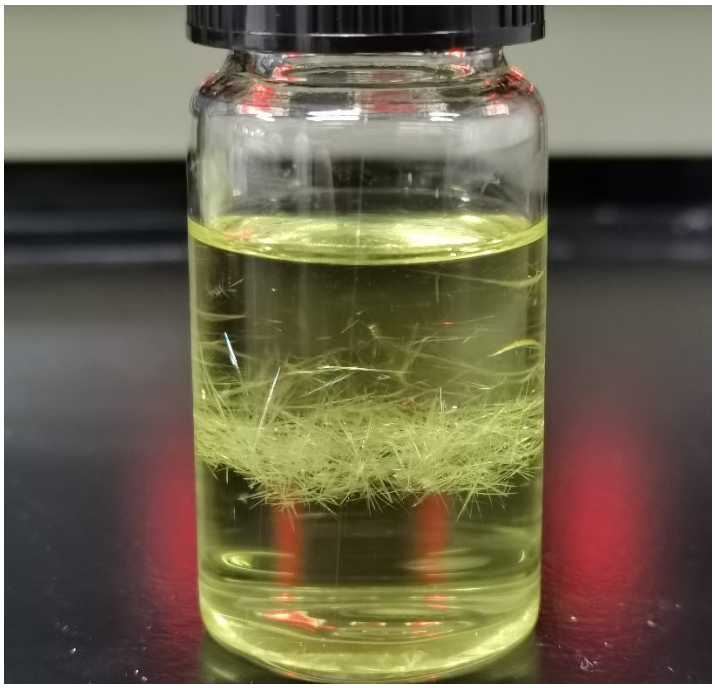
Outline

1. Materials and instrumentations

All reagents were commercially available and used as supplied without further purification. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker AV-400 spectrometer (400 MHz). The chemical shifts were measured relative to TMS (0.00 ppm) for $CDCl_3$ as indicated. All single-crystal measurements were performed on Rigaku Oxford Atals-CCD diffractometer using CuKα (λ= 1.54056 Å) radiation. The diffraction data were collected in the ω-scanning mode. The structures were solved by direct methods (SHELXTL-2014)[1], which yielded the positions of all nonhydrogen atoms and refined by full-matrix least-squares on F^2.

2. Synthesis and characterization of FPOC

Synthesis of FPOC. A solution of 1,3-bis[2-(4-aminophenyl)-2-propyl]benzene (0.032g, 0.09mmol) in acetonitrile (4 ml) was added slowly to a solution of 2,4,6-tris(4-formylphenyl)-1,3,5-triazine (0.023g, 0.06mmol in 8 ml $CHCl_3$) in a 20 ml glass vial. Then the solvent diffusion system was kept undisturbed at room temperature for 3 days. Light yellow and long rod crystals were form in the interphase between acetonitrile and chloroform. The crystals were filtered and then washed with ACN (73% yield).



The crystals of FPOC formed in the interphase between acetonitrile and chloroform

Activation of cage

Single crystals of cage FPOC⊃$CHCl_3$ were dried under vacuum at 60℃ for 24h to remove all solvents and obtain the cage **FPOC** without solvent.

characterization of FPOC

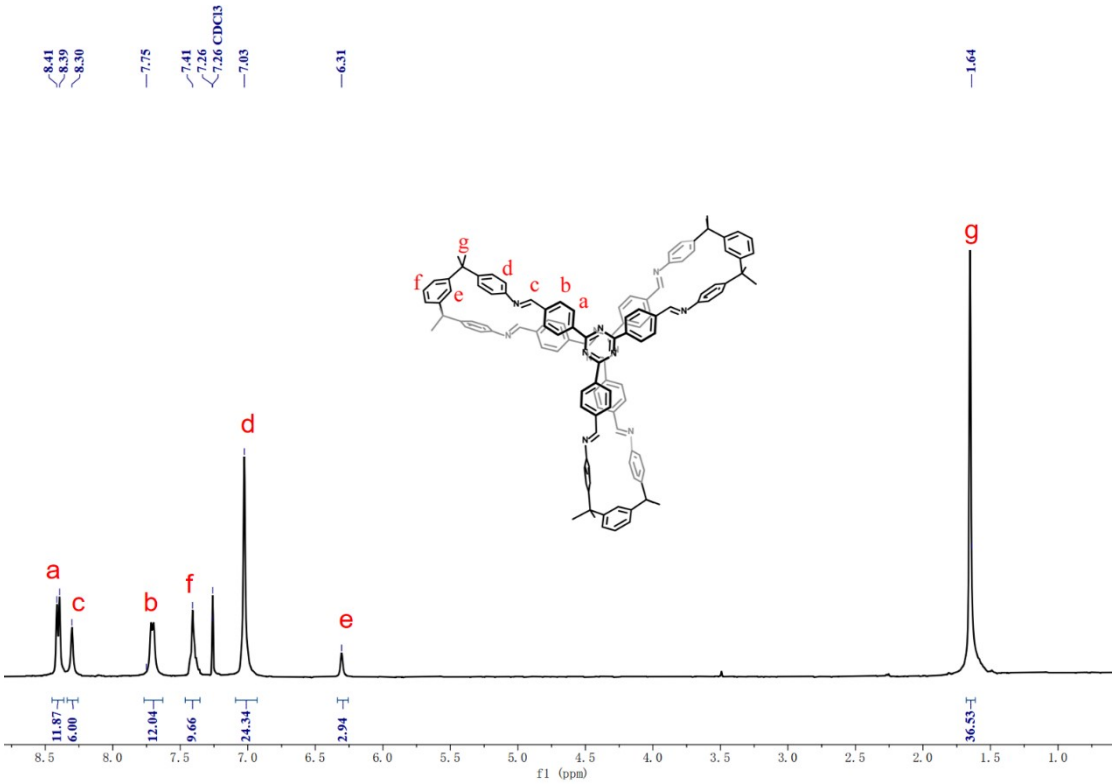


Fig. S1a ^{1}H-NMR spectrum of fan-like adaptive porous organic cage (FPOC) (400 MHz, 10 mg de-solvated FPOC 0.6 mL $CDCl_3$).

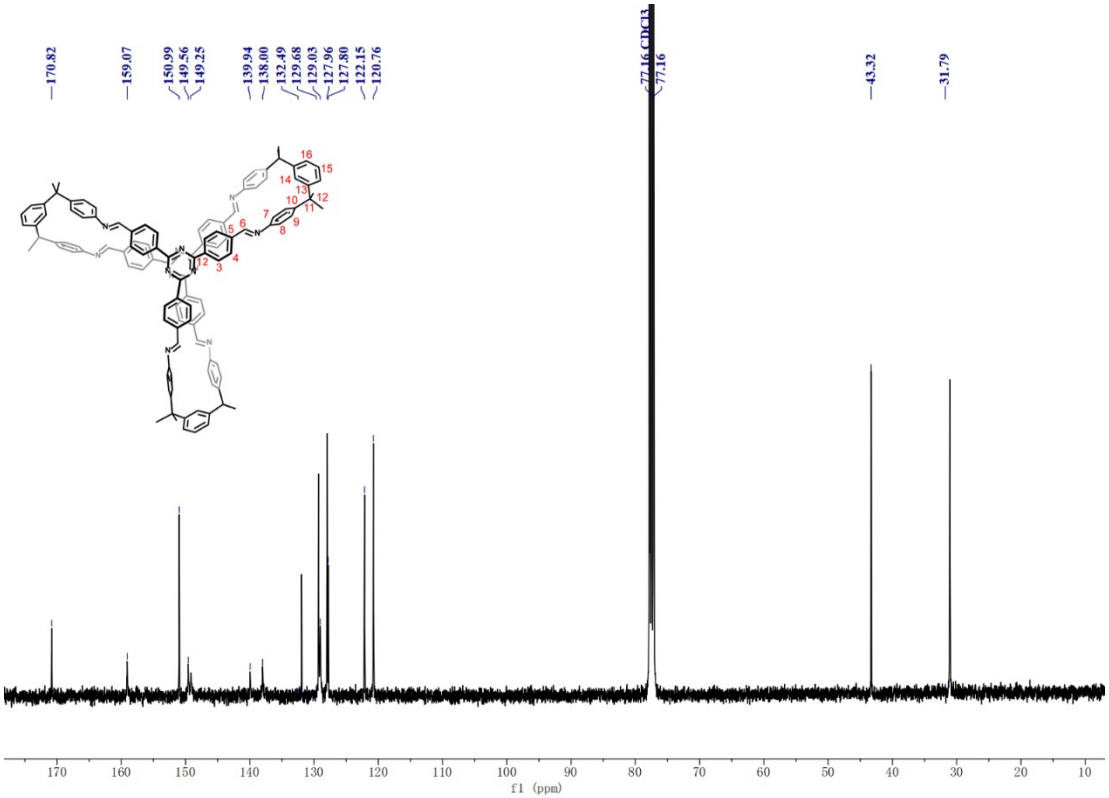


Fig. S1a ^{13}C-NMR spectrum of fan-like adaptive porous organic cage (FPOC) (400 MHz, 10 mg de-solvated FPOC in 0.6 mL $CDCl_3$).

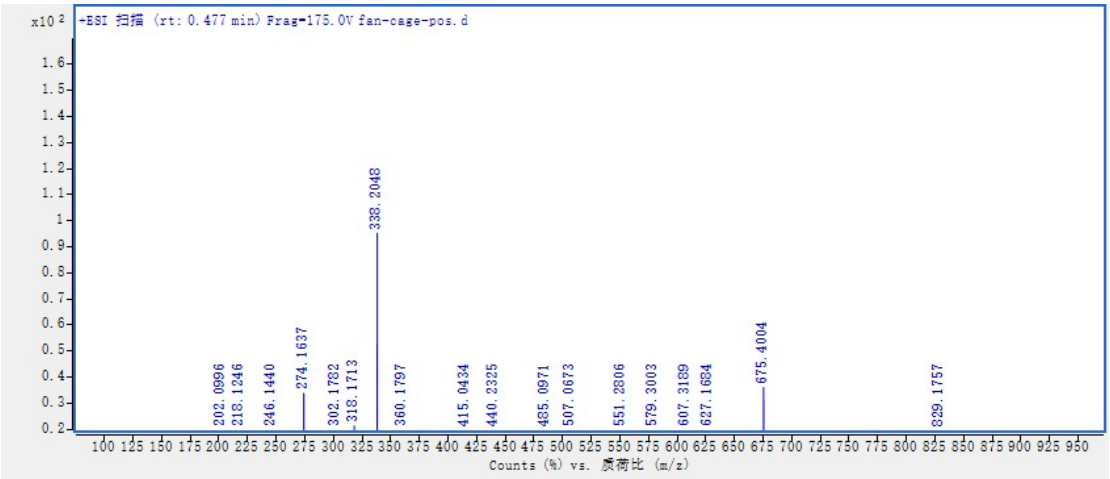


Figure S1c HR-MS

3. The crystallization methods of host-guest complexes.

Crystallization of FPOC ⊃1. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **1** (0.6 ml), and ether was diffused into the FPOC solution at 20℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃2. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **2** (0.6 ml), and ether was diffused into the FPOC solution at 8℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃3. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **3** (0.6 ml), and methanol was diffused into the FPOC solution at 20℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃4. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **4** (0.6 ml), and methanol was diffused into the FPOC solution at 20℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃5. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **5** (0.6 ml) and the resulting suspension was filtrated through a syringe filter (polytetrafluoroethylene, pore size 0.45um). Methanol was diffused into the FPOC solution at 8℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃6. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **6** (0.6 ml), and methanol was diffused into the FPOC solution at 8℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃7. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **7** (0.6 ml), and methanol was diffused into the FPOC solution at 8℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃8. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **8** (0.6 ml) and the resulting suspension was filtrated through a syringe filter (polytetrafluoroethylene, pore size 0.45um). Methanol was diffused into the FPOC solution at 8℃. Three days later, light yellow block-shaped single crystals were obtained.

Crystallization of FPOC ⊃9. FPOC (0.002 mmol, 3.4 mg) was dissolved in guest **8** (0.6 ml) and the resulting suspension was filtrated through a syringe filter (polytetrafluoroethylene, pore size 0.45um). Methanol-ethanol (1:1) was diffused into the FPOC solution at 8℃. Three days later, light yellow block-shaped single crystals were obtained.

4. Figures for the NMR and interactions of inclusion complexes

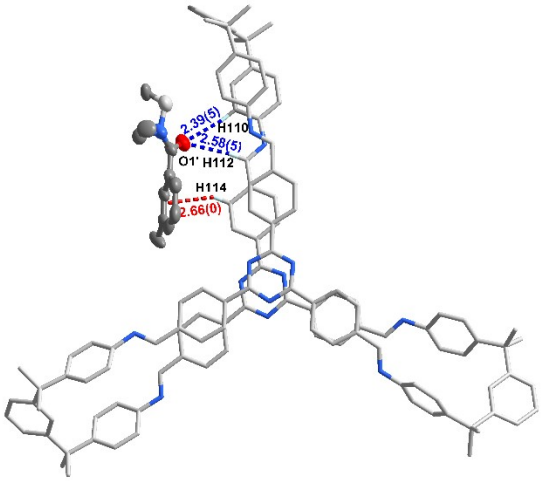


Fig. S1 the C–H···O and C–H···π interaction in FPOC ⊃ **1**

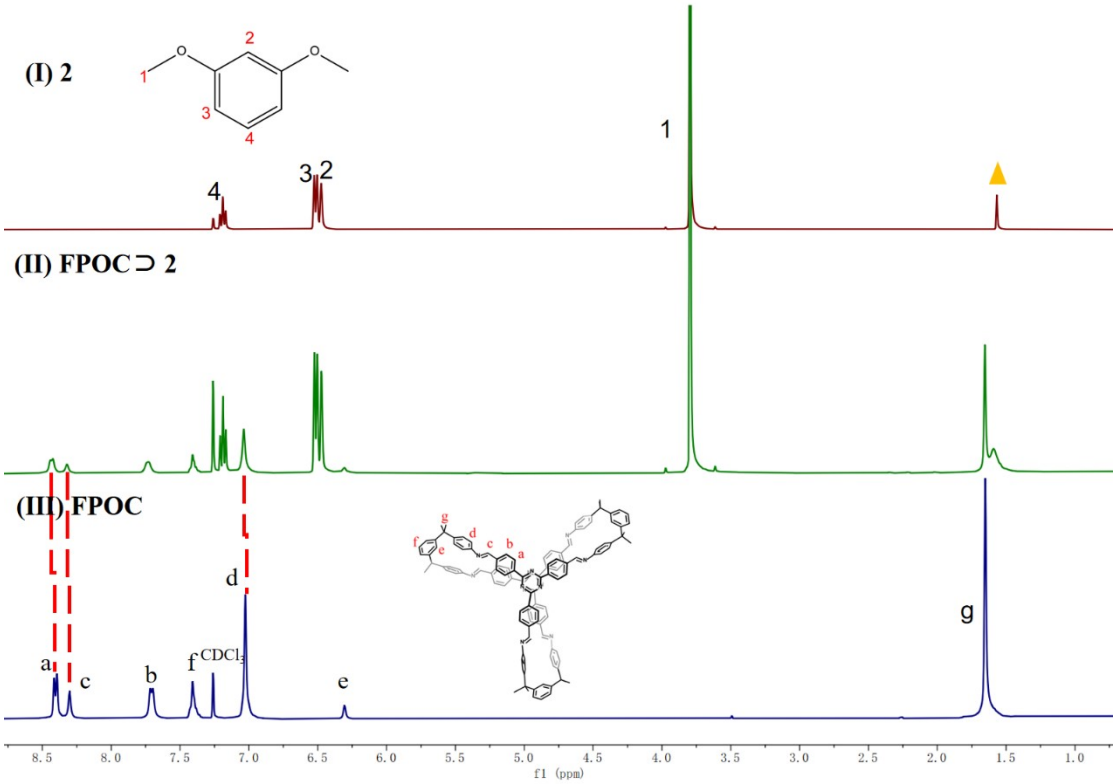


Fig. S2a ^{1}H-NMR of (I) **2**, (II) **FPOC⊃2** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃2** crystals in 0.6 mL $CDCl_3$) (▲ is from residual water)

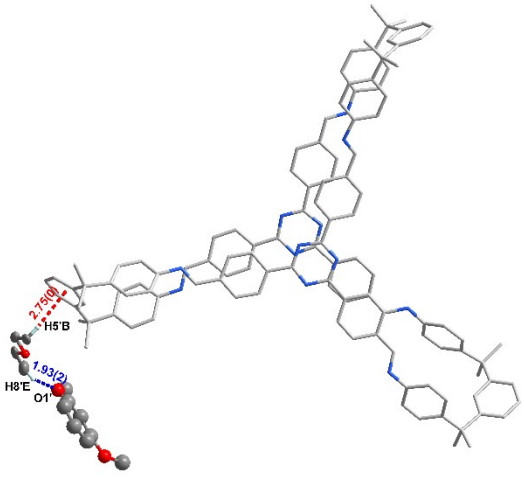


Fig. S2b the C–H···O and C–H···π interaction in FPOC ⊃ **2**

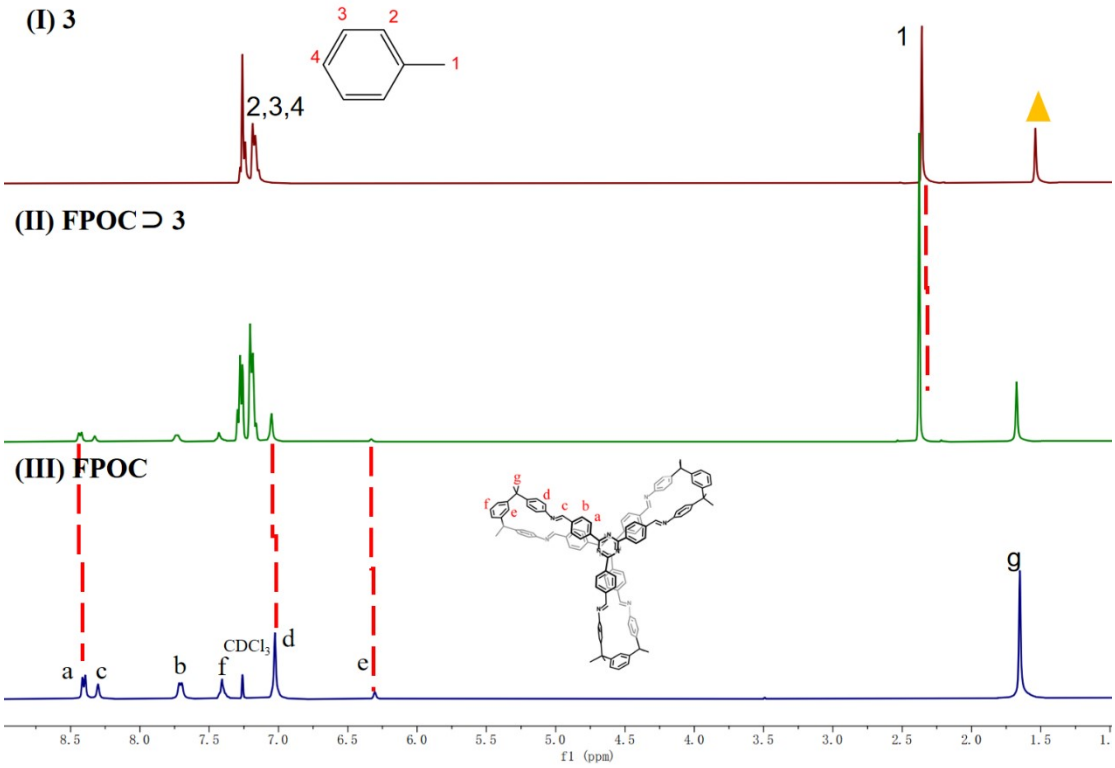


Fig. S3a ^{1}H-NMR of (I) **3**, (II) **FPOC⊃3** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃3** crystals in 0.6 mL $CDCl_3$) (▲ is from residual water.)

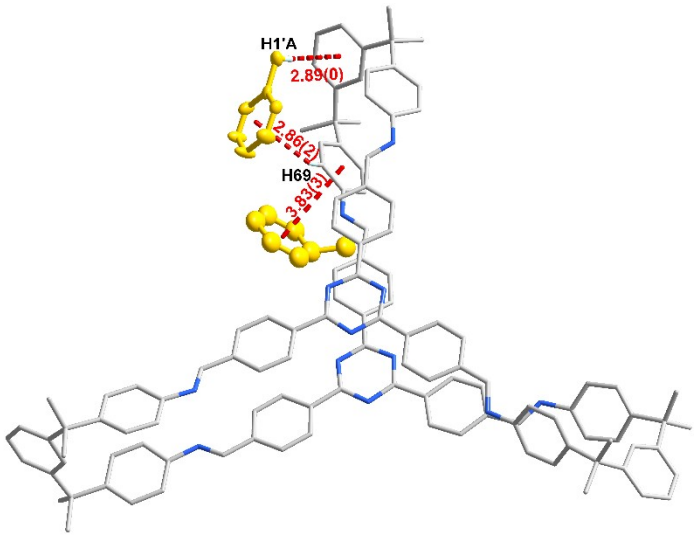


Fig. S3b the C–H···π interactions in FPOC ⊃ **3**

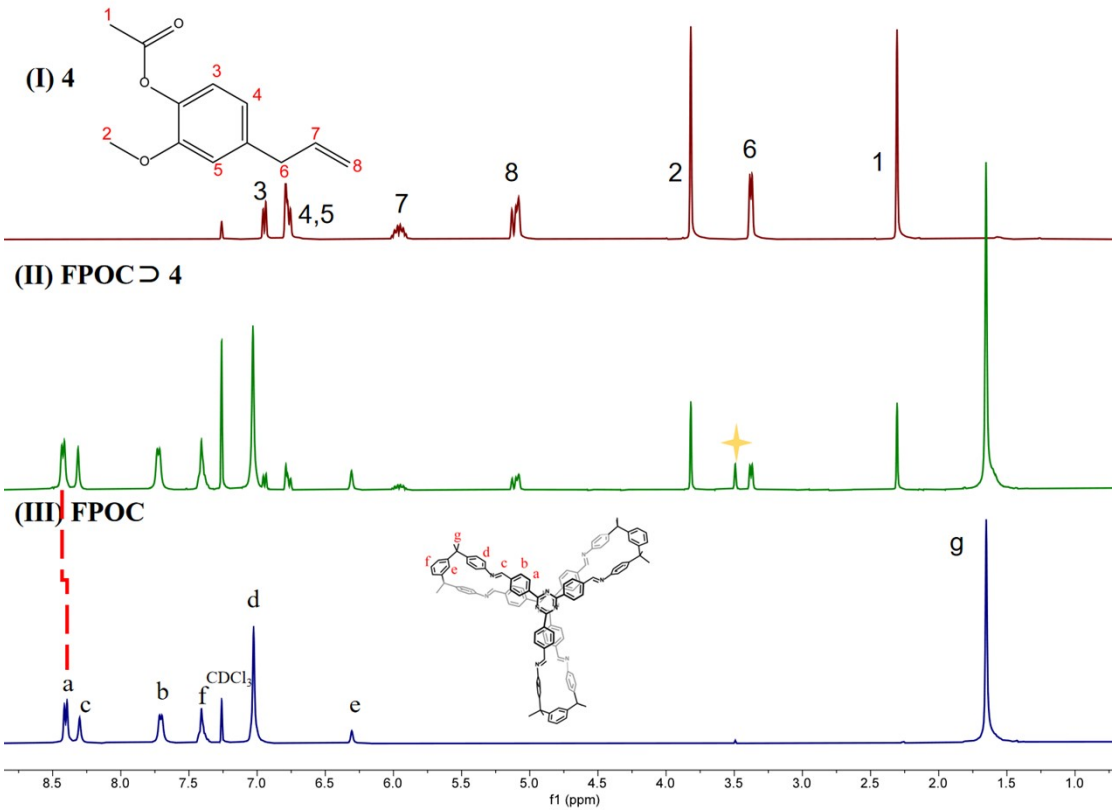


Fig. S4a ^{1}H-NMR of (I) **4**, (II) **FPOC⊃4** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃4** crystals in 0.6 mL $CDCl_3$) (✨ comes from residual methanol in the host-guest complex.)

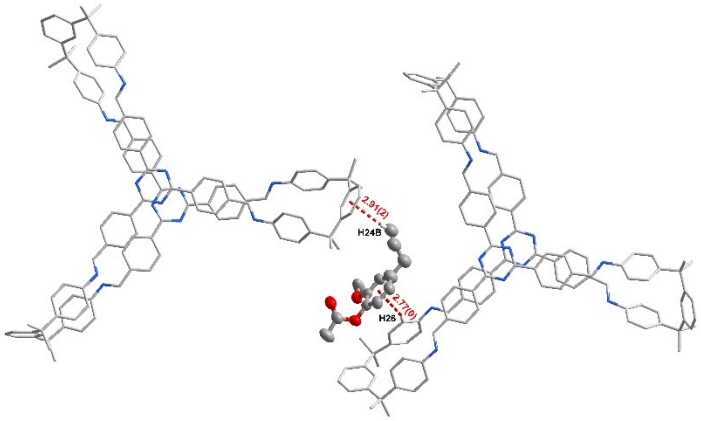


Fig. S4b the C–H···π interactions in FPOC ⊃ **4**

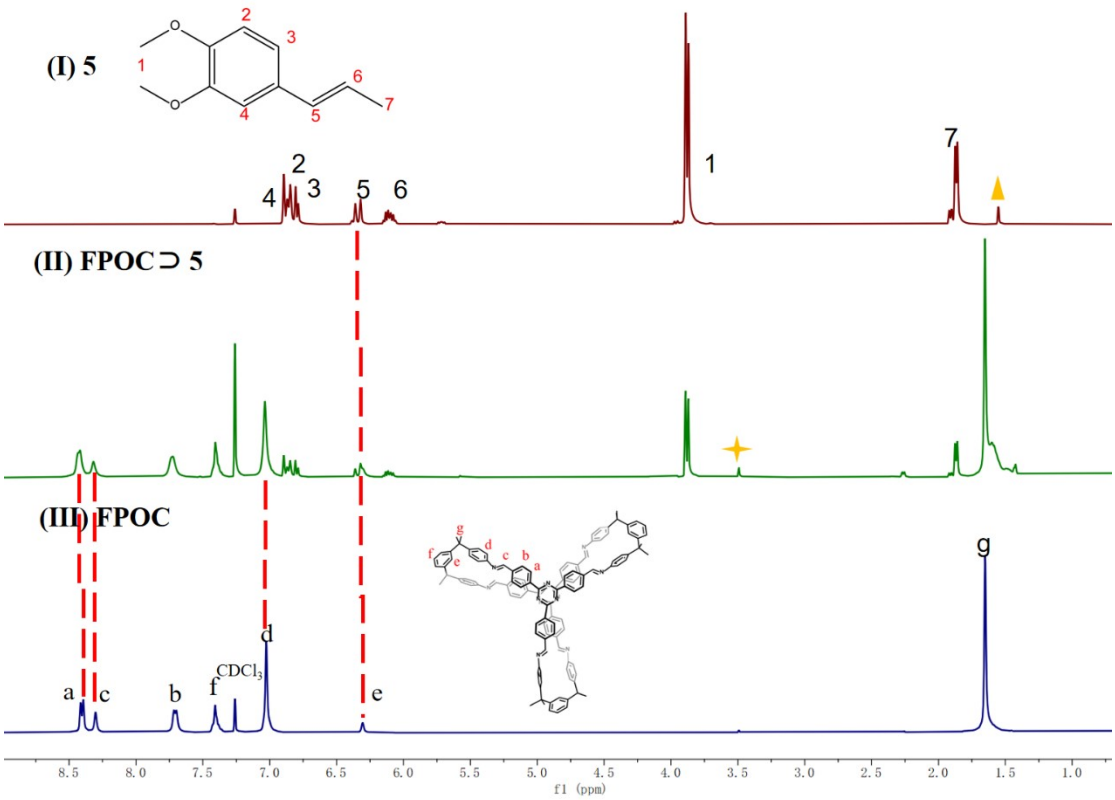


Fig. S5a ^{1}H-NMR of (I) **5**, (II) **FPOC⊃5** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃5** crystals in 0.6 mL $CDCl_3$) (▲ is from residual water.) (✦ is from residual methanol in the host-guest complex.)

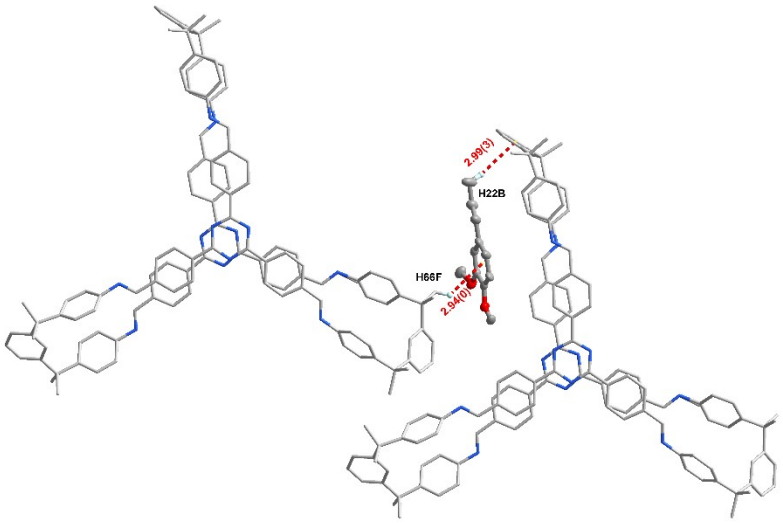


Fig. S5b the C–H···π interactions in FPOC ⊃ **5**

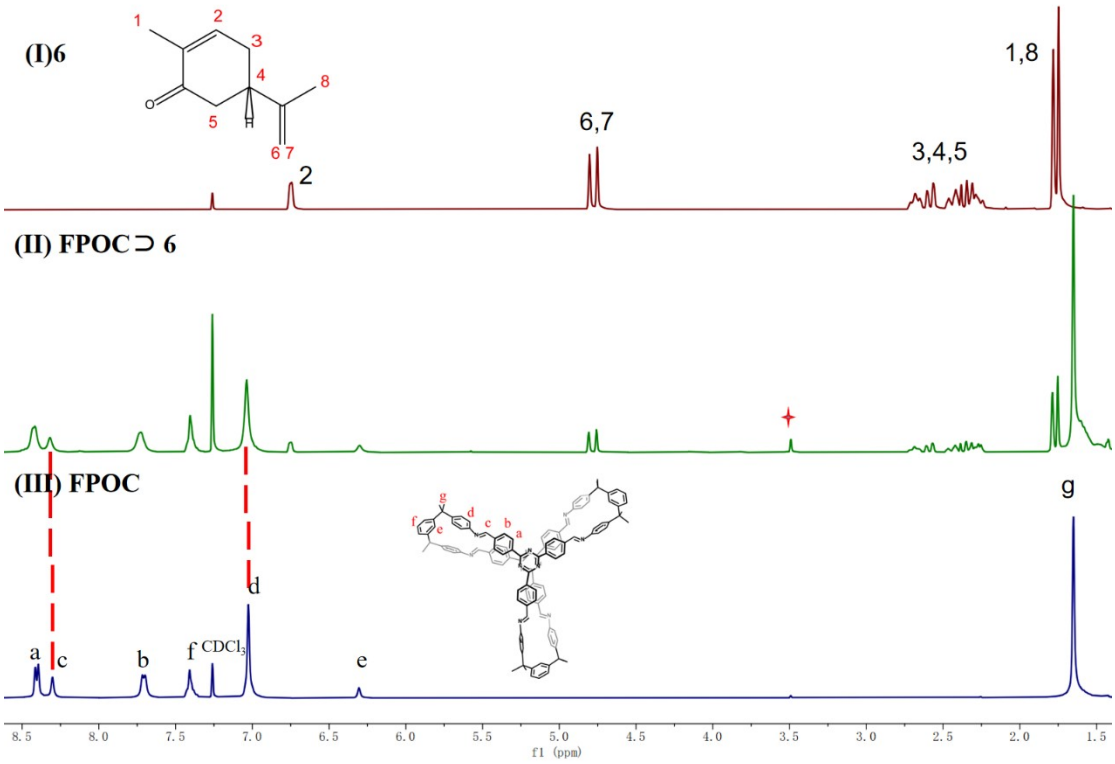


Fig. S6a ^{1}H-NMR of (I) **6**, (II) **FPOC⊃6** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃6** crystals in 0.6 mL $CDCl_3$)

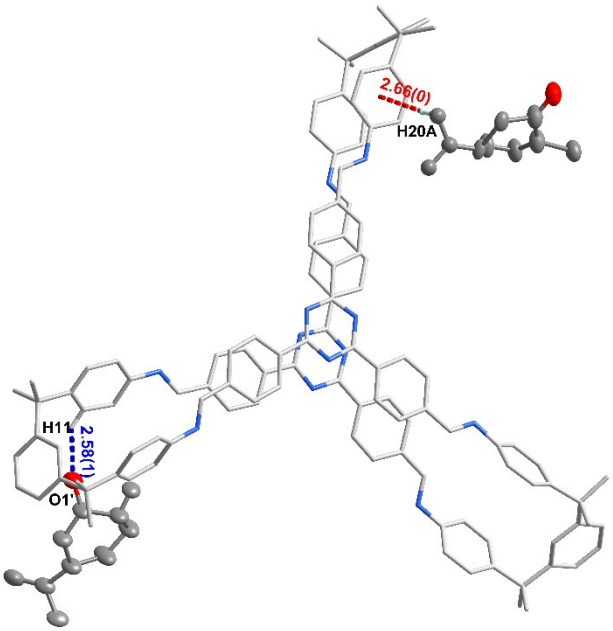


Fig. S6b the C–H···O and C–H···π interactions in FPOC ⊃ **6**

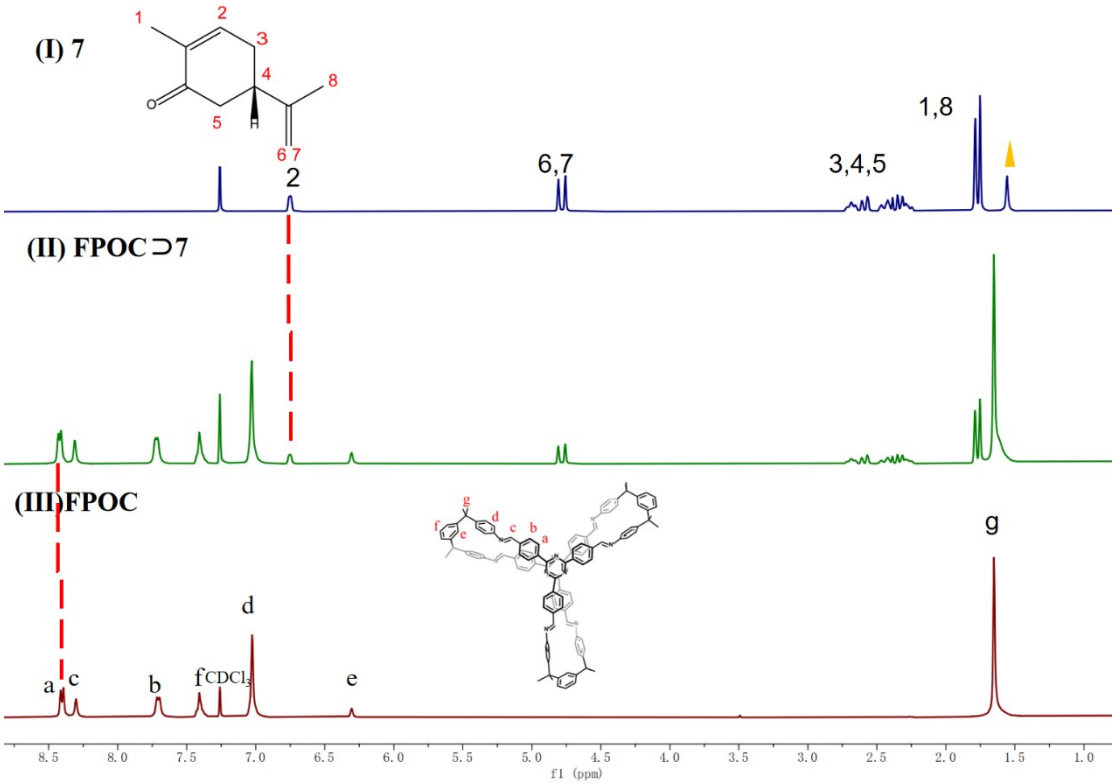


Fig. S7a ^{1}H-NMR of (I) **7**, (II) **FPOC⊃7** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃7** crystals in 0.6 mL $CDCl_3$) (⚠ is from residual water.)

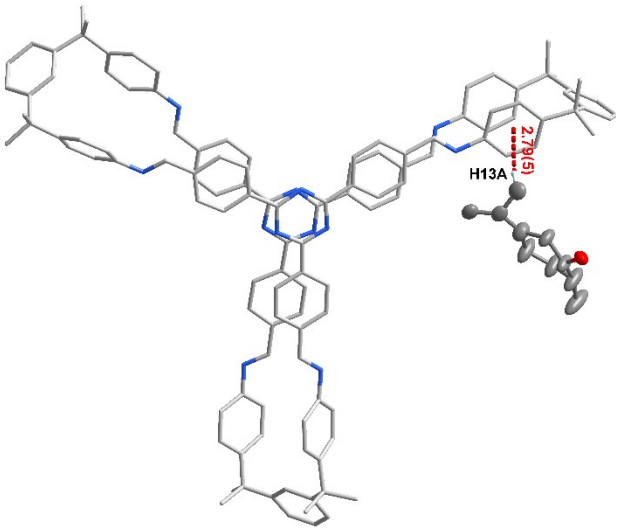


Fig. S7b the C–H···π interactions in FPOC ⊃ **7**

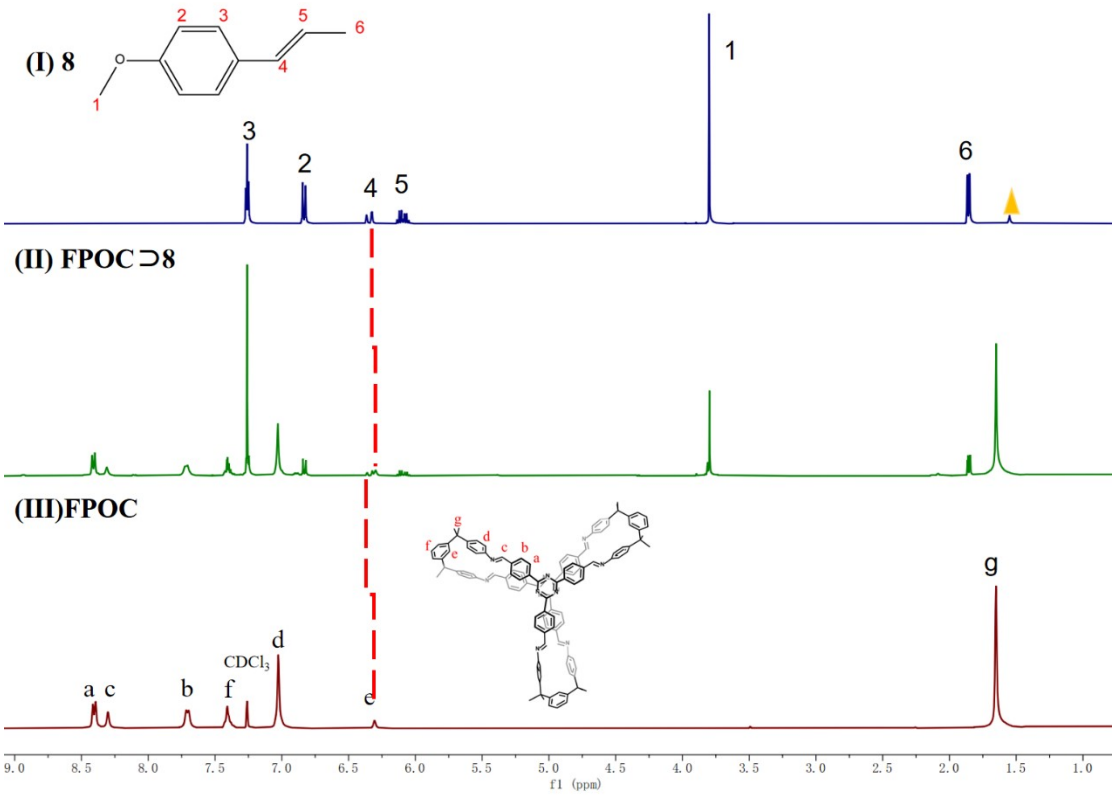


Fig. S8a ^{1}H-NMR of (I) **8**, (II) **FPOC⊃8** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃8** crystals in 0.6 mL $CDCl_3$) (is from residual water.)

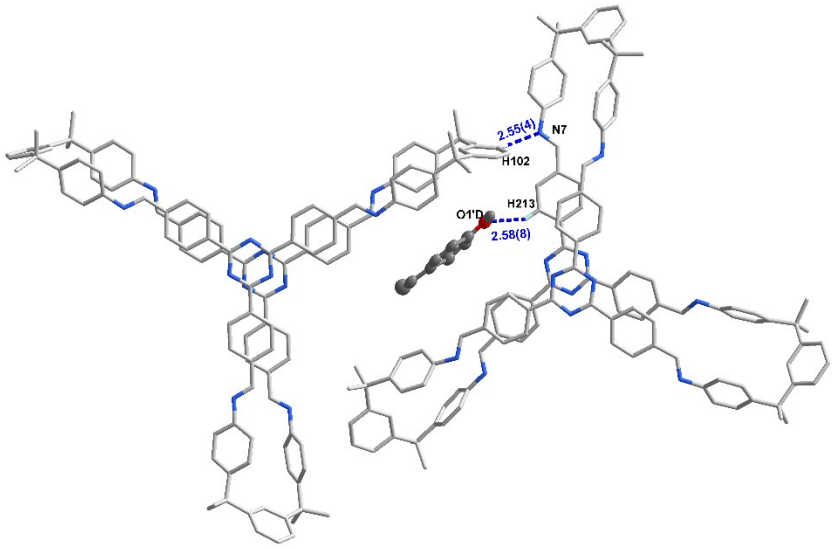


Fig. S8b the C–H···N and C–H···O interactions in FPOC ⊃**8**

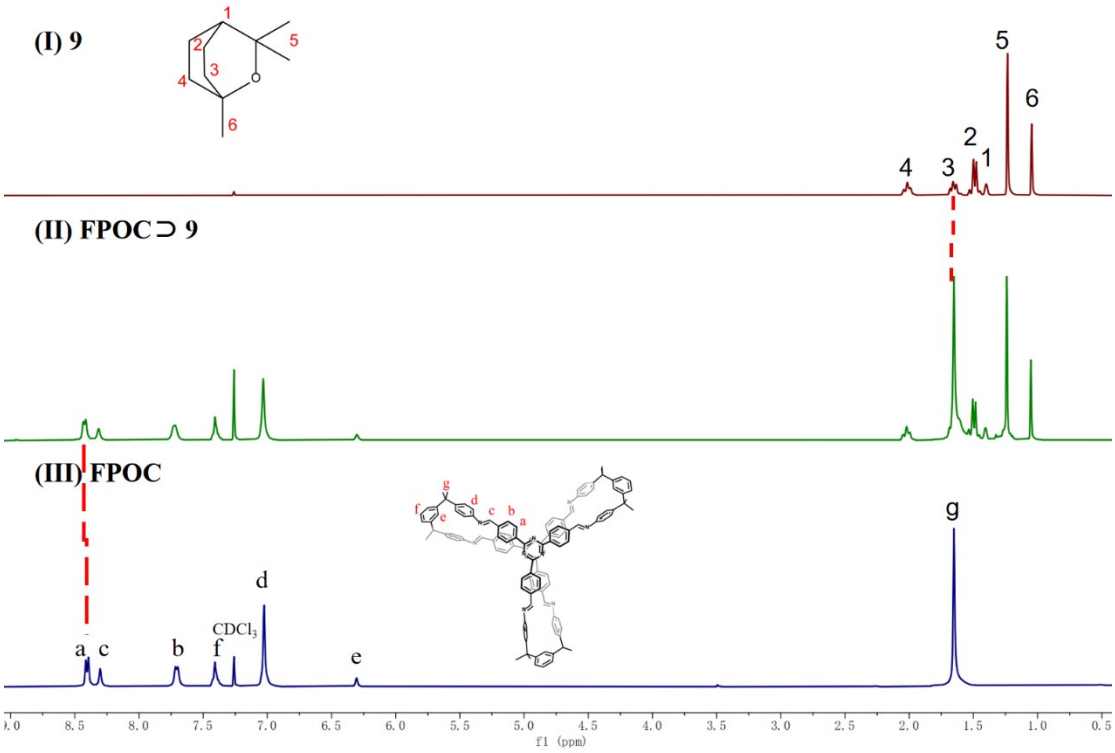


Fig. S9a ^{1}H-NMR of (I) **9**, (II) **FPOC⊃9** and (III)**FPOC** (400 MHz, 5 mg **FPOC⊃9** crystals in 0.6 mL $CDCl_3$)

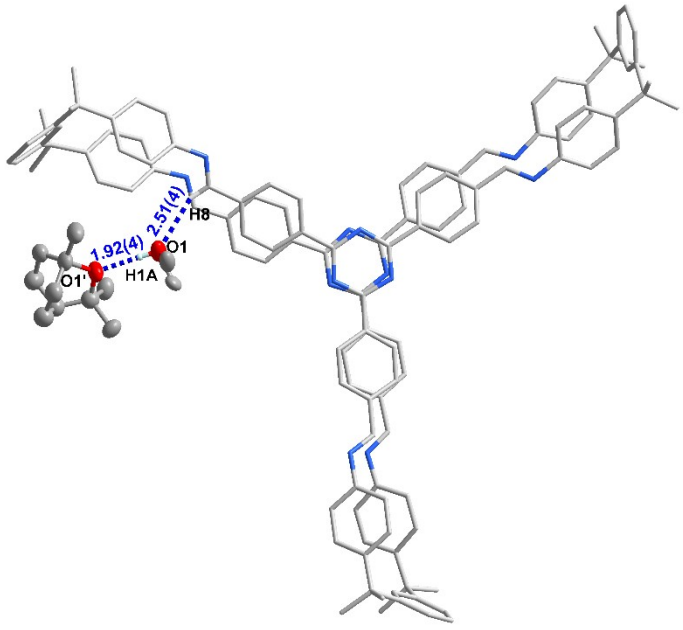


Fig. S9b the O–H···O and C–H···O interactions in FPOC ⊃**9**

5. Supplementary Tables

Table S1. Changes of ^{1}H-NMR chemical shifts of FPOC

δ/ppm	FPOC	FPOC⊃1	FPOC⊃2	FPOC⊃3	FPOC⊃4	FPOC⊃5	FPOC⊃6	FPOC⊃7	FPOC⊃8	FPOC⊃9
Ha	8.41	8.44(0.03)	8.44(0.03)	8.44(0.03)	8.43(0.02)	8.44(0.03)	8.42(0.01)	8.43(0.02)	8.42(0.01)	8.43(0.02)
Hb	7.72	7.72(0.00)	7.73(0.01)	7.74(0.02)	7.72(0.00)	7.73(0.01)	7.73(0.01)	7.73(0.01)	7.72(0.00)	7.73(0.01)
Hc	8.30	8.31(0.01)	8.32(0.02)	8.32(0.02)	8.31(0.01)	8.32(0.02)	8.32(0.02)	8.31(0.01)	8.31(0.01)	8.31(0.01)
Hd	7.02	7.03(0.01)	7.04(0.02)	7.05(0.03)	7.03(0.01)	7.04(0.02)	7.04(0.02)	7.03(0.01)	7.03(0.01)	7.03(0.01)
He	6.30	6.30(0.00)	6.31(0.01)	6.33(0.03)	6.31(0.01)	6.32(0.02)	6.30(0.00)	6.31(0.01)	6.36(0.06)	6.30(0.00)
Hf	7.41	7.41(0.00)	7.41(0.00)	7.43(0.02)	7.41(0.00)	7.41(0.00)	7.41(0.00)	7.41(0.00)	7.41(0.00)	7.41(0.00)
Hg	1.66	1.65(0.01)	1.65(0.01)	1.67(0.01)	1.65(0.01)	1.65(0.01)	1.65(0.01)	1.65(0.01)	1.65(0.01)	1.65(0.01)

Table S2. C-H···π intermolecular interactions in host and guest

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC⊃1	C114 -H114- Cg35[a]	2.655(0)	134	3.367(4)

Symmetry codes: [a] X, Y, Z; Cg35 is the centroid of C2', C3', C4', C5', C6', C7'.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC⊃2	C5'A -H5'B-Cg5[a]	2.748(0)	156	3.646(9)

Symmetry codes: [a] 1-X, -Y,1-Z; Cg5 is the centroid of C13, C14, C18, C19, C20, C21.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC ⊃3	C1' -H1'A··Cg9[a]	2.886(0)	168	3.851(7)
	C69-H69··Cg20[b]	2.855(2)	131	3.548(9)

Symmetry codes: [a] X,3/2-Y,1/2+Z; [b] X,3/2-Y, -1/2+Z; Cg9 is the centroid of C58, C59, C60, C61, C62 and C63. Cg20 is the centroid of C2', C3', C4', C5', C6' and C7'.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC ⊃4	C24'-H24B··Cg12[a]	2.906(2)	154	3.763(12)
	C26-H26··Cg18[b]	2.774(0)	145	3.576(5)

Symmetry codes: [a] 1+X, Y, Z; [b]X,1/2-Y, -1/2+Z; Cg12 is the centroid of C89, C90, C91, C92, C93

and C94. Cg18 is the centroid of C16', C17', C18', C19', C20'and C21'.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC ⊃5	C22' -H22B·Cg15[a]	2.987(3)	157	3.887(6)
	C66A-H66F·Cg20[b]	2.943(0)	121	3.535(11)

Symmetry codes: [a] X, Y, Z; [b] 1+X, Y, Z; Cg15 is the centroid of C98, C99, C100, C101, C102 and C103. Cg20 is the centroid of C14', C15', C16', C17', C18' and C19'.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC ⊃6	C20' -H20A ··Cg9[a]	2.644(0)	176	3.645(16)

Symmetry codes: [a] X, Y, Z; Cg9 is the centroid of C49, C50, C51, C52, C53 and C54.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
FPOC ⊃7	C13'-H13A··Cg12[a]	2.793(5)	169	3.74(3)

Symmetry codes: [a] 3/2-X,1/2+Y, Z; Cg12 is the centroid of C67, C68, C69, C70, C71 and C72.

Table S3. Geometric parameters of the O–H···O and C–H···O hydrogen bonding interactions in the co-crystals

H-G	Interactions	D−H(Å)	H···A(Å)	D···A(Å)	D-H···A(deg)	Symmetry code
FPOC⊃1	C110-H110-O1'	0.93	2.393(5)	3.304(5)	167	X, Y, Z
	C112-H112-O1'	0.93	2.581(5)	3.304(5)	171	X, Y, Z
FPOC⊃2	C8'A-H8'E-O1'	0.96	1.933(2）	2.44(3)	110	1-x,1-y,1-z
FPOC⊃6	C11-H11-O1'	0.95	2.584(1）	3.415(15)	146	x,1-y,1/2+z
FPOC⊃8	C213-H213-O1'D	0.95	2.583(8）	3.330(7)	138	X, Y, Z
FPOC⊃9	C8-H8-O1	0.95	2.512(4）	3.368(7)	152	X, Y, Z
	O1-H1A- O1'	0.84	1.918(4)	2.733(8)	174	X, Y, Z

6. Guest volume calculations

All guest structures were fully optimized with Chem 3D at Minimize Energy level. The

length, width and height of the guests were calculated by Multiwfn.[2]

Table S4 The guest volume and three-dimensional values

Guest	Length(Å)	Width(Å)	Height(Å)	Volume(Å^3)	Standard Deviation (Å^3)
$CHCl_3$	6.246	6.281	4.593	180.189	4.291
1	11.486	7.521	7.652	661.027	38.947
2	10.375	7.594	4.252	335.006	11.405
3	7.128	7.644	4.130	225.029	15.102
4	12.500	8.819	5.464	602.337	9.540
5	12.694	8.493	4.433	477.922	34.373
6	9.579	7.104	6.940	472.262	10.192
7	10.672	7.116	6.442	489.218	7.864
8	6.813	12.914	4.549	400.235	5.976
9	7.467	7.993	6.680	398.687	28.445

Cartesian coordinates(Å) for the optimized geometry of $CHCl_3$

C	-0.4005	0.5760	0.2585
Cl	-0.4135	-1.1720	0.2825
Cl	1.2425	1.1720	0.2825
Cl	-1.2425	1.1710	-1.1535
H	-0.9175	0.9420	1.1535

Cartesian coordinates(Å) for the optimized geometry of guest **1**

C	2.9394	0.6271	0.7672
C	3.5768	-0.2513	1.8426
C	2.9598	-1.6480	1.8375
C	1.4417	-1.5931	1.9890
C	0.8343	-0.6968	0.9146
C	1.4279	0.7085	0.9663
C	3.5706	2.0163	0.6959
C	-0.6871	-0.7187	0.9397
N	-1.2959	-0.0751	-0.2178
O	-1.0673	-0.1304	2.1507
C	-2.7200	-0.3883	-0.3114
C	-3.5937	0.2193	0.7979
C	-0.6057	-0.4414	-1.4543
C	-0.5693	-1.9461	-1.7690
H	4.6734	-0.3320	1.6631
H	3.3978	-2.2566	2.6621
H	1.0206	-2.6205	1.8959
H	1.1858	1.2123	1.9295
H	4.6521	1.9396	0.4435
H	3.0783	2.6205	-0.0992
H	3.4707	2.5552	1.6652
H	-3.1205	0.0132	-1.2749
H	-2.8842	-1.4916	-0.3222
H	-4.6734	0.1630	0.5262
H	-3.4937	-0.3232	1.7639
H	-3.3474	1.2935	0.9614
H	-1.0661	0.0958	-2.3182
H	0.4412	-0.0567	-1.4300
H	0.0676	-2.1437	-2.6621
H	-0.1469	-2.5392	-0.9270
H	-1.5793	-2.3505	-2.0029

Cartesian coordinates(Å) for the optimized geometry of guest **2**

C	1.8522	0.1442	0.3521
C	2.3343	-1.0703	0.6759
C	1.5244	-2.1021	0.9447
C	0.1974	-1.9305	0.8922
C	-0.3522	-0.7433	0.5745
C	0.5080	0.2637	0.3128
O	-1.7244	-0.6515	0.5435
O	2.7527	1.1506	0.0897
C	-2.3222	0.5835	0.2234
C	2.2714	2.4274	-0.2612
H	3.4262	-1.2222	0.7218
H	1.9471	-3.0863	1.2076
H	-0.4613	-2.7871	1.1156
H	0.0870	1.2437	0.0510
H	-3.4262	0.4449	0.2570
H	-2.0479	1.3543	0.9779
H	-2.0444	0.8929	-0.8088
H	3.1519	3.0863	-0.4336
H	1.6883	2.3755	-1.2076
H	1.6749	2.8597	0.5730

Cartesian coordinates(Å) for the optimized geometry of guest **3**

C	1.3030	1.0319	-0.0244
C	1.8260	-0.1617	0.2944
C	1.0111	-1.1918	0.5676
C	-0.3202	-1.0266	0.5216
C	-0.8572	0.1651	0.2033
C	-0.0291	1.1897	-0.0685
C	-2.3533	0.3658	0.1476
H	1.9678	1.8825	-0.2501
H	2.9200	-0.2953	0.3316
H	1.4365	-2.1751	0.8302
H	-0.9741	-1.8845	0.7493
H	-0.4487	2.1751	-0.3316
H	-2.9200	-0.5599	0.3932
H	-2.6648	1.1512	0.8735
H	-2.6622	0.6862	-0.8735

Cartesian coordinates(Å) for the optimized geometry of guest **4**

C	1.0316	1.9270	-0.9550
C	1.4974	0.6992	-0.6591
C	0.6534	-0.2022	-0.0997
C	-0.6065	0.1997	0.1679
C	-1.0668	1.4316	-0.1074
C	-0.2263	2.2998	-0.6880
O	2.8025	0.4010	-0.9649
O	1.1271	-1.4649	0.1708
C	-2.4959	1.8125	0.2097
C	-3.4225	1.2002	-0.8088
C	-4.3499	0.2778	-0.5158
C	0.3090	-2.3856	0.8525
C	3.5423	-0.1953	0.0149
O	3.6004	0.1946	1.1605
C	4.2952	-1.3924	-0.5338
H	1.7092	2.6575	-1.4298
H	-1.3274	-0.4933	0.6281
H	-0.5623	3.3174	-0.9459
H	-2.7482	1.4771	1.2419
H	-2.6352	2.9179	0.1993
H	-3.3098	1.5351	-1.8544
H	-4.9988	-0.1435	-1.2992
H	-4.4897	-0.0878	0.5125
H	0.8999	-3.3174	0.9999
H	0.0318	-1.9884	1.8544
H	-0.5849	-2.6382	0.2399
H	3.5905	-2.1463	-0.9515
H	4.9988	-1.0699	-1.3343
H	4.8874	-1.8853	0.2698

Cartesian coordinates(Å) for the optimized geometry of guest **5**

C	0.9350	1.1580	-0.2373 C
C	1.4070	-0.0700	0.0851 C
C	0.5193	-1.0527	0.3447 C
C	-0.8182	-0.8938	0.3033 C
C	-1.2610	0.3324	-0.0198 C
C	-0.4004	1.3261	-0.2819 C
O	1.8502	2.1529	-0.5000 O
O	2.7750	-0.2304	0.1278 O
C	-1.6245	-1.9408	0.5796 C
C	-2.9685	-1.9665	0.5873 C
C	-3.7754	-3.1983	0.9126 C
C	1.3890	3.4377	-0.8487 C
C	3.3182	-1.4846	0.4696 C
H	0.9035	-2.0508	0.6077 H
H	-2.3341	0.5710	-0.0825 H
H	-0.8399	2.3030	-0.5393 H
H	-1.1481	-2.9049	0.8332 H
H	-3.5716	-1.0755	0.3530 H
H	-3.1418	-4.0824	1.1471 H
H	-4.4272	-3.0048	1.7949 H
H	-4.4257	-3.4666	0.0489 H
H	2.2800	4.0824	-1.0211 H
H	0.8047	3.3968	-1.7949 H
H	0.8009	3.8791	-0.0134 H
H	4.4272	-1.3903	0.4482 H
H	3.0177	-1.7700	1.5025 H
H	3.0246	-2.2529	-0.2801 H

Cartesian coordinates(Å) for the optimized geometry of guest **6**

C	1.3235	0.5792	0.8393
C	0.9761	-0.7029	1.1353
C	-0.4582	-0.9991	1.5525
C	-1.4842	-0.0844	0.8717
C	-1.0597	1.3616	1.1628
C	0.4038	1.5591	0.8735
C	2.7597	0.8907	0.4790
O	1.7757	-1.6140	1.1073
C	-1.6555	-0.4366	-0.5992
C	-2.4292	-1.7044	-0.8892
C	-1.1670	0.2967	-1.6132
H	-2.4886	-0.2332	1.3429
H	-0.6987	-2.0705	1.3684
H	-0.5034	-0.8585	2.6592
H	-1.6832	2.0690	0.5681
H	-1.2208	1.6137	2.2379
H	0.7138	2.5968	0.6623
H	2.9257	1.9691	0.2607
H	3.4413	0.6182	1.3167
H	3.0650	0.3241	-0.4302
H	-3.4413	-1.6541	-0.4282
H	-2.5750	-1.8790	-1.9784
H	-1.9019	-2.5968	-0.4861
H	-1.3194	-0.0083	-2.6592
H	-0.5981	1.2230	-1.4644

Cartesian coordinates(Å) for the optimized geometry of guest **7**

C	1.9336	0.3842	-0.4569
C	1.5245	-0.7726	0.1323
C	0.0835	-0.9041	0.6145
C	-0.8990	-0.0225	-0.1664
C	-0.3515	1.4095	-0.1427
C	1.0819	1.4143	-0.5990
C	3.3652	0.5061	-0.9326
O	2.2753	-1.7115	0.2937
C	-2.3298	-0.1880	0.3187
C	-3.0117	-1.4846	-0.0584
C	-2.9829	0.7311	1.0484
H	-0.8891	-0.3513	-1.2370
H	0.0585	-0.6387	1.6975
H	-0.2168	-1.9742	0.5255
H	-0.9631	2.0524	-0.8195
H	-0.3631	1.8535	0.8792
H	1.4425	2.3548	-1.0493
H	3.5826	1.4926	-1.3991
H	4.0721	0.3853	-0.0803
H	3.5903	-0.2718	-1.6975
H	-3.0113	-1.6149	-1.1641
H	-2.4921	-2.3548	0.3999
H	-4.0721	-1.5250	0.2762
H	-4.0183	0.5620	1.3798
H	-2.5310	1.6838	1.3530

Cartesian coordinates(Å) for the optimized geometry of guest **8**

C	1.8850	1.1986	-0.2486
C	2.3267	-0.0301	0.0782
C	1.4977	-1.0500	0.3472
C	0.1597	-0.9014	0.3048
C	-0.2920	0.3237	-0.0217
C	0.5458	1.3392	-0.2896
O	2.8032	2.1874	-0.5095
C	-0.6307	-1.9588	0.5840
C	-1.9741	-2.0024	0.5927
C	-2.7641	-3.2442	0.9209
C	2.3367	3.4701	-0.8589
H	3.4158	-0.2042	0.1266
H	1.9532	-2.0220	0.6061
H	-1.3692	0.5450	-0.0832
H	0.0900	2.3085	-0.5483
H	-0.1371	-2.9139	0.8389
H	-2.5883	-1.1194	0.3567
H	-2.1181	-4.1197	1.1541
H	-3.4158	-3.0586	1.8049
H	-3.4131	-3.5217	0.0592
H	3.2244	4.1197	-1.0298
H	1.7523	3.4249	-1.8049
H	1.7430	3.9066	-0.0250

Cartesian coordinates(Å) for the optimized geometry of guest **9**

C	-1.9155	0.5280	-0.7324
C	-1.7803	-0.2816	0.5654
C	-0.4816	-1.0989	0.5255
O	0.6075	-0.2273	0.4654
C	0.6052	0.6000	-0.6632
C	-0.6255	0.3070	-1.5427
C	0.6247	2.0613	-0.1830
C	1.9187	0.3653	-1.4286
C	-0.3373	-1.9276	1.8065
C	-0.6221	-1.1699	-1.9767
C	-0.4619	-2.0160	-0.7053
H	-2.8042	0.1959	-1.3184
H	-2.0879	1.6077	-0.5223
H	-1.7704	0.4005	1.4481
H	-2.6563	-0.9604	0.6893
H	-0.6300	0.9648	-2.4449
H	0.5715	2.7671	-1.0428
H	1.5544	2.2920	0.3850
H	-0.2158	2.2986	0.5048
H	2.0728	-0.7020	-1.6990
H	1.9485	0.9630	-2.3677
H	2.8042	0.6531	-0.8177
H	-1.1777	-2.6495	1.9186
H	0.6115	-2.5110	1.8054
H	-0.3283	-1.2764	2.7101
H	-1.5706	-1.4218	-2.5061
H	0.1889	-1.3797	-2.7101
H	0.4969	-2.5851	-0.7374
H	-1.2833	-2.7671	-0.6360

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