Electronic Supplementary Material (ESI) for CrystEngComm.

Host compounds based on the rigid 9,10-dihydro-9,10-ethanoanthracene framework: selectivity behaviour in mixed isomeric dichlorobenzenes

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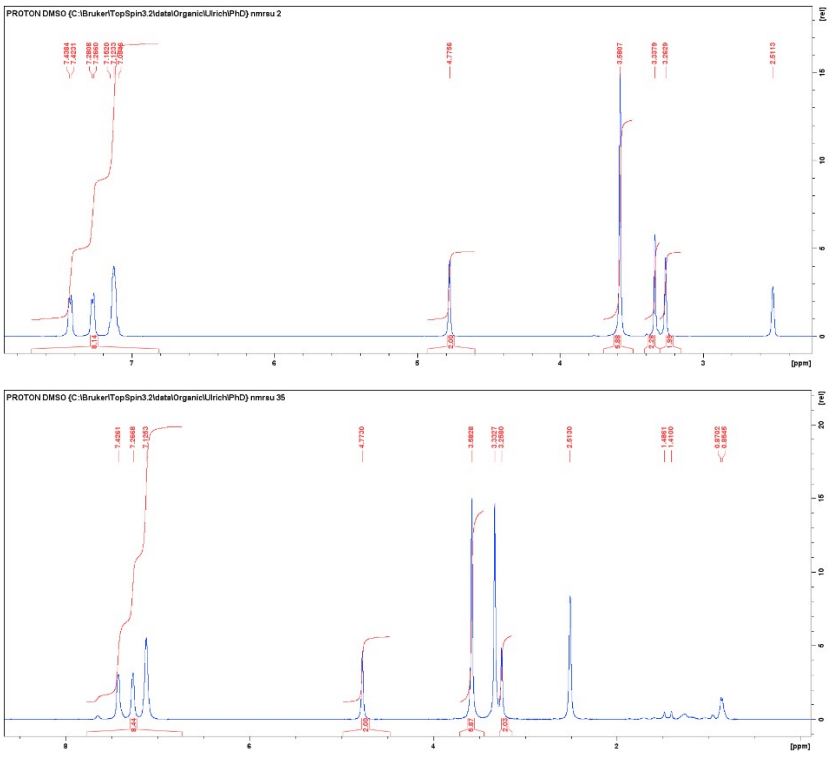
a)



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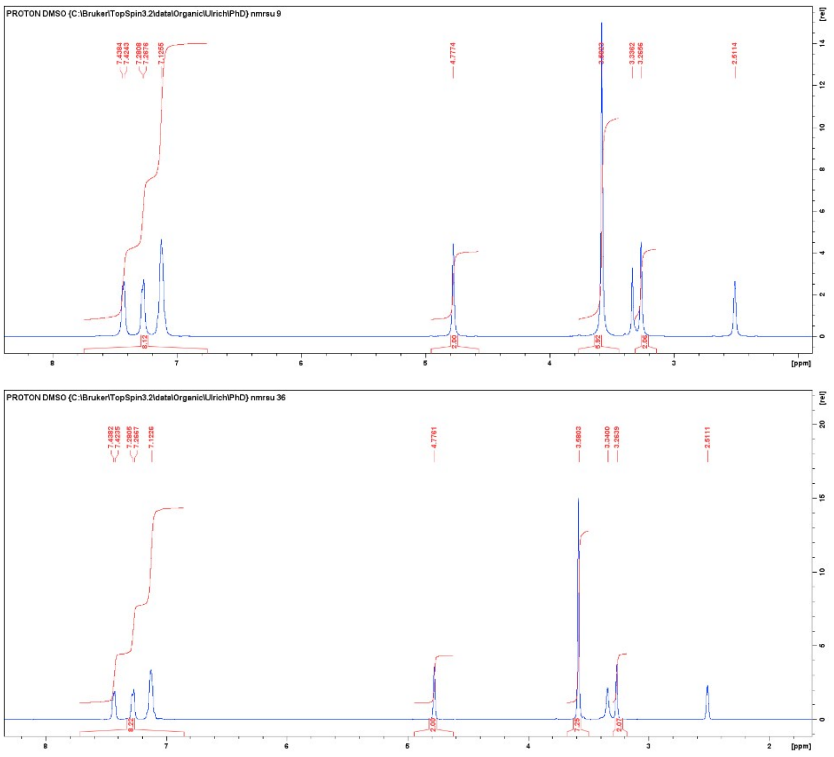
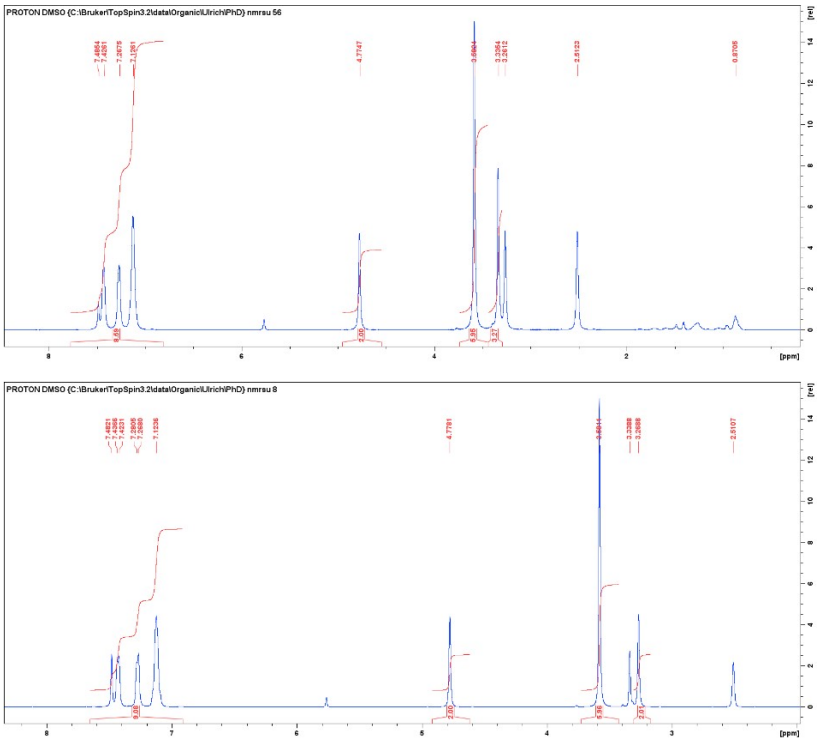


Figure S1. ^{1}H-NMR spectra of the duplicated single solvent experiments of *o*-DCB (a) and *m*-DCB (b) with H1

a)



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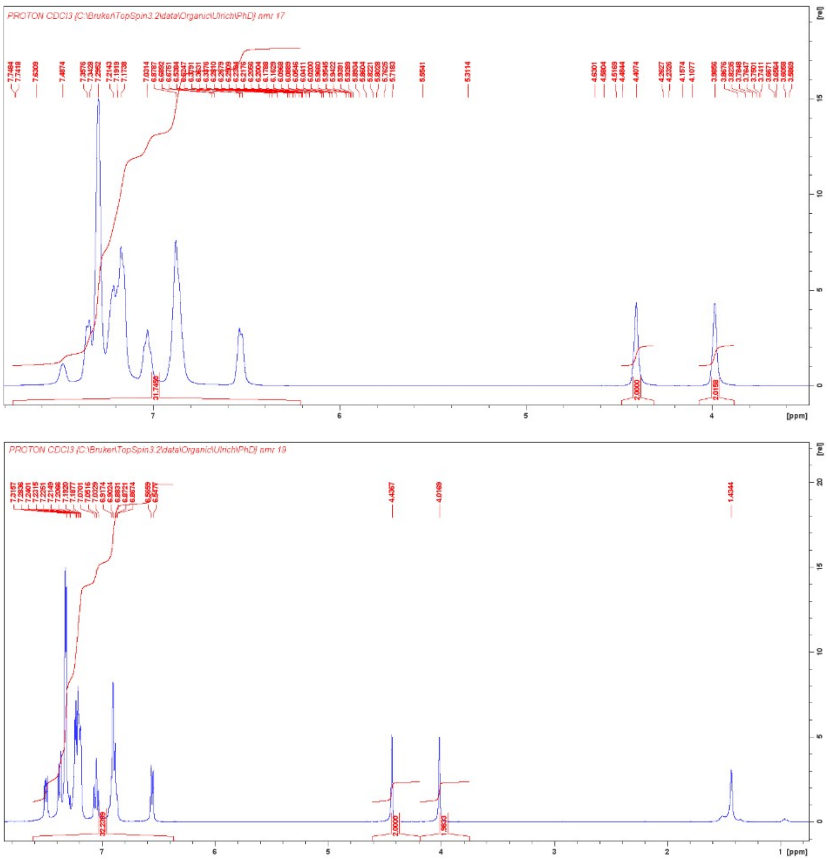
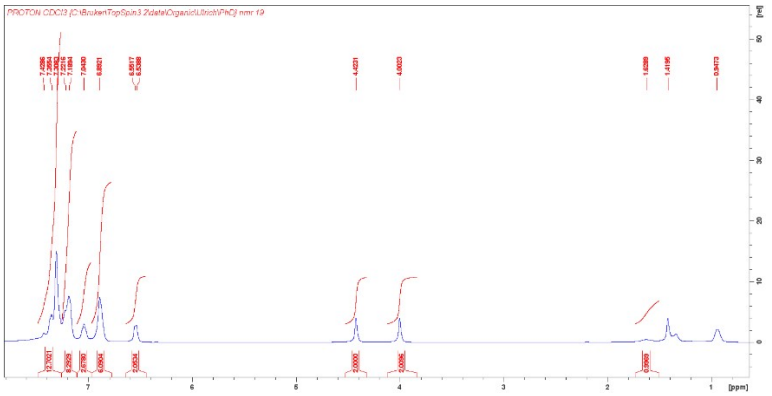
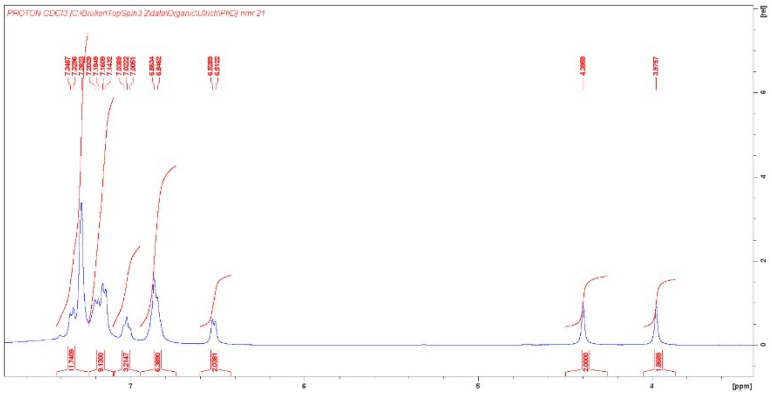


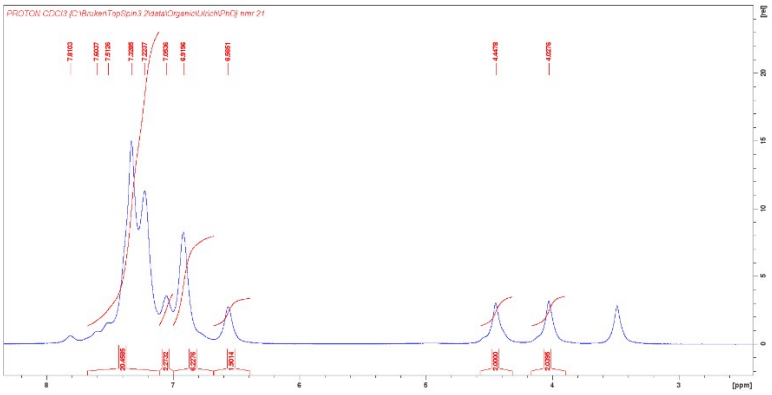
Figure S2. ^{1}H-NMR spectra of the duplicated single solvent experiments of *p*-DCB (a) with H1 and *o*-DCB (b) with H2

a)





b)



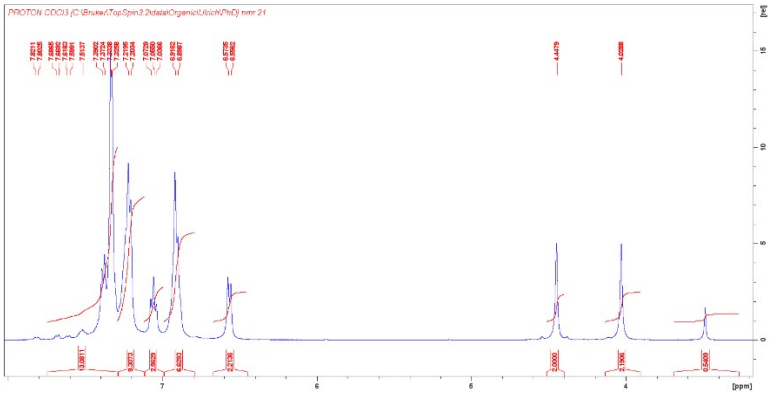


Figure S3. ^{1}H-NMR spectra of the duplicated single solvent experiments of *m*-DCB (a) and *p*-DCB (b) with H2

a)

b)

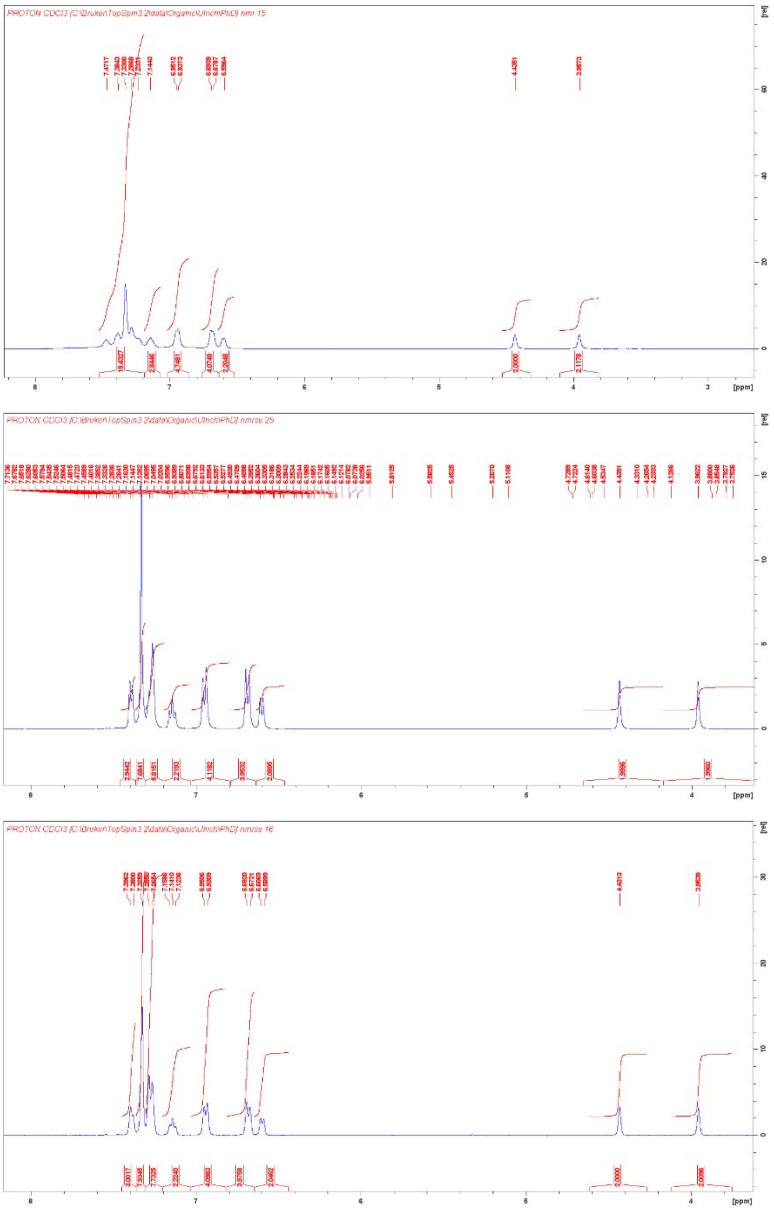


Figure S4. ^{1}H-NMR spectra of the duplicated single solvent experiments of *o*-DCB (a) and *m*-DCB (b) with H3

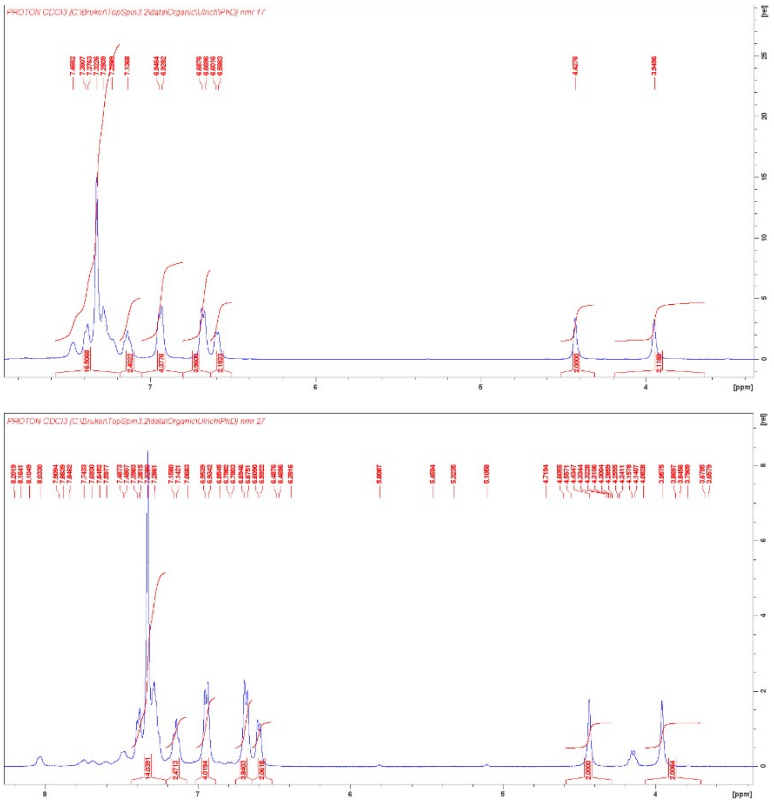


Figure S5. ^{1}H-NMR spectra of the duplicated single solvent experiment of *p*-DCB with H3

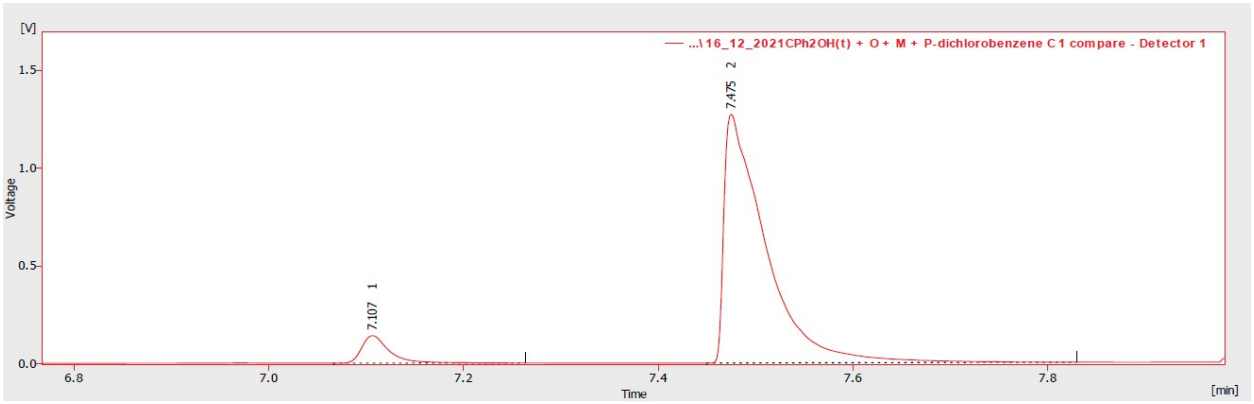
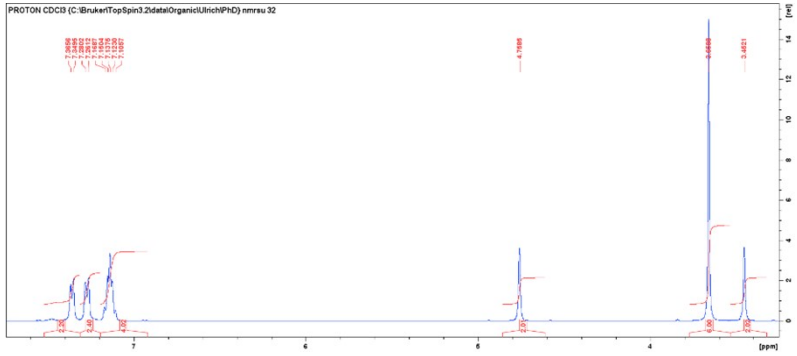


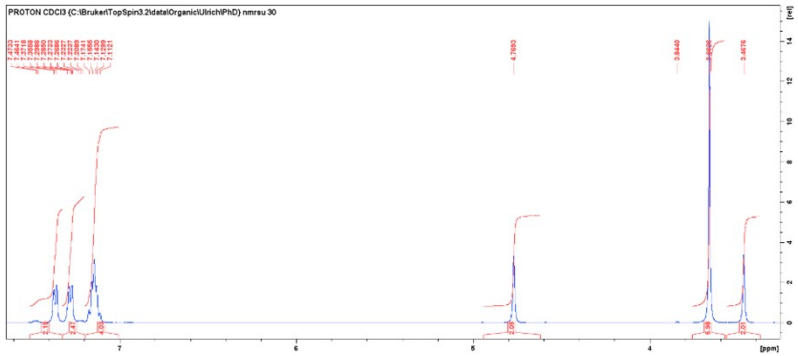
Figure S6. *o*-DCB/*m*-DCB/*p*-DCB ternary mixture of the three dichlorobenzene isomers; eluding in the order of *m*-DCB, *o*-DCB and *p*-DCB (the latter two peak overlapped)

a)

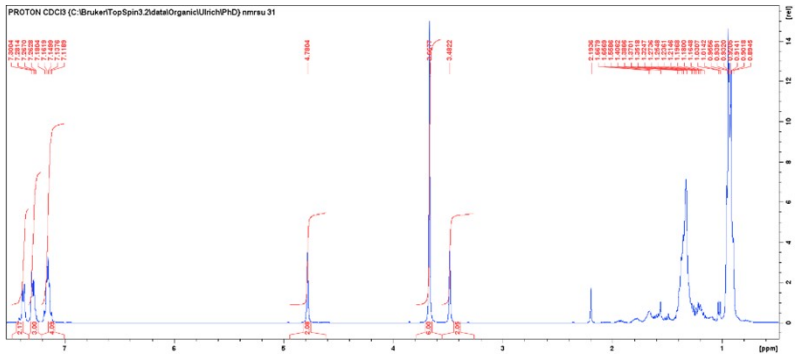

PROTON CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich\PhD) nmrsu 32
4.7999
3.4621
[ppm]

b)

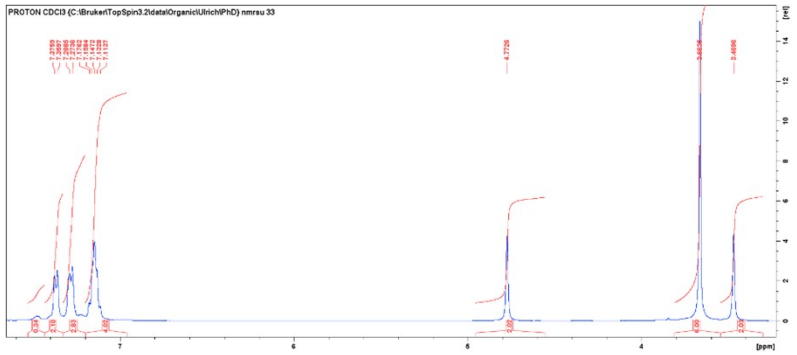
c)

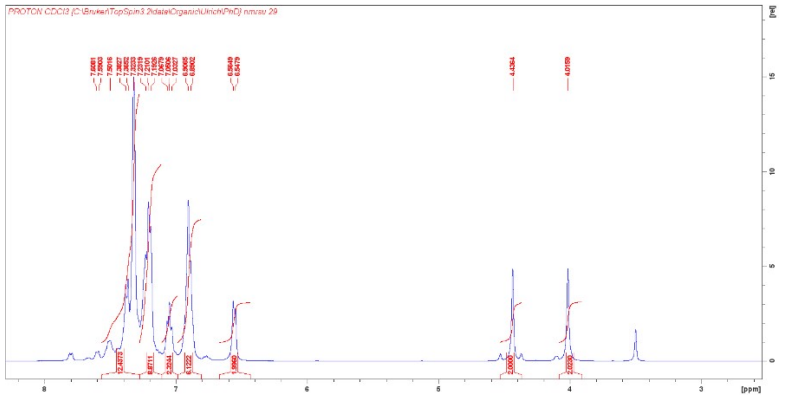

PROTON CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich\PhD) nmrsu 30
4.7993
3.8440
3.4076
[ppm]

d)



e)





f)

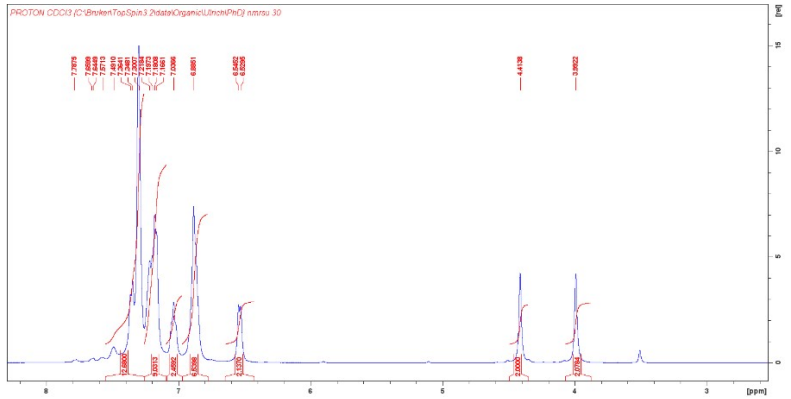


Figure S7. Overall H:G ratios for the *o*-DCB/*m*-DCB (a), *o*-DCB/*p*-DCB (b), *m*-DCB/*p*-DCB (c), *o*-DCB/*m*-DCB/*p*-DCB (d) with H1, *o*-DCB/*m*-DCB (e), *o*-DCB/*p*-DCB (f) competition experiments with H2

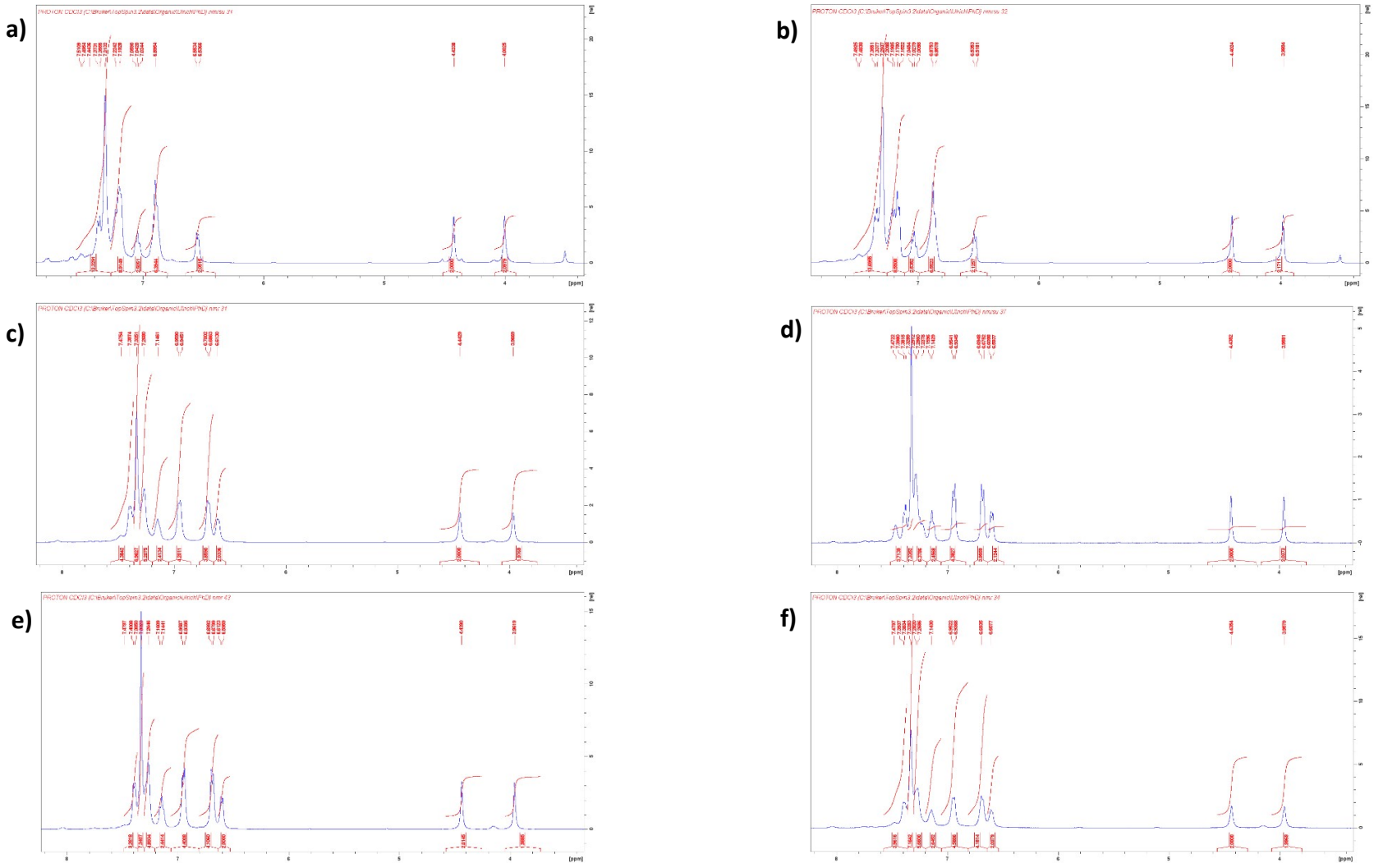
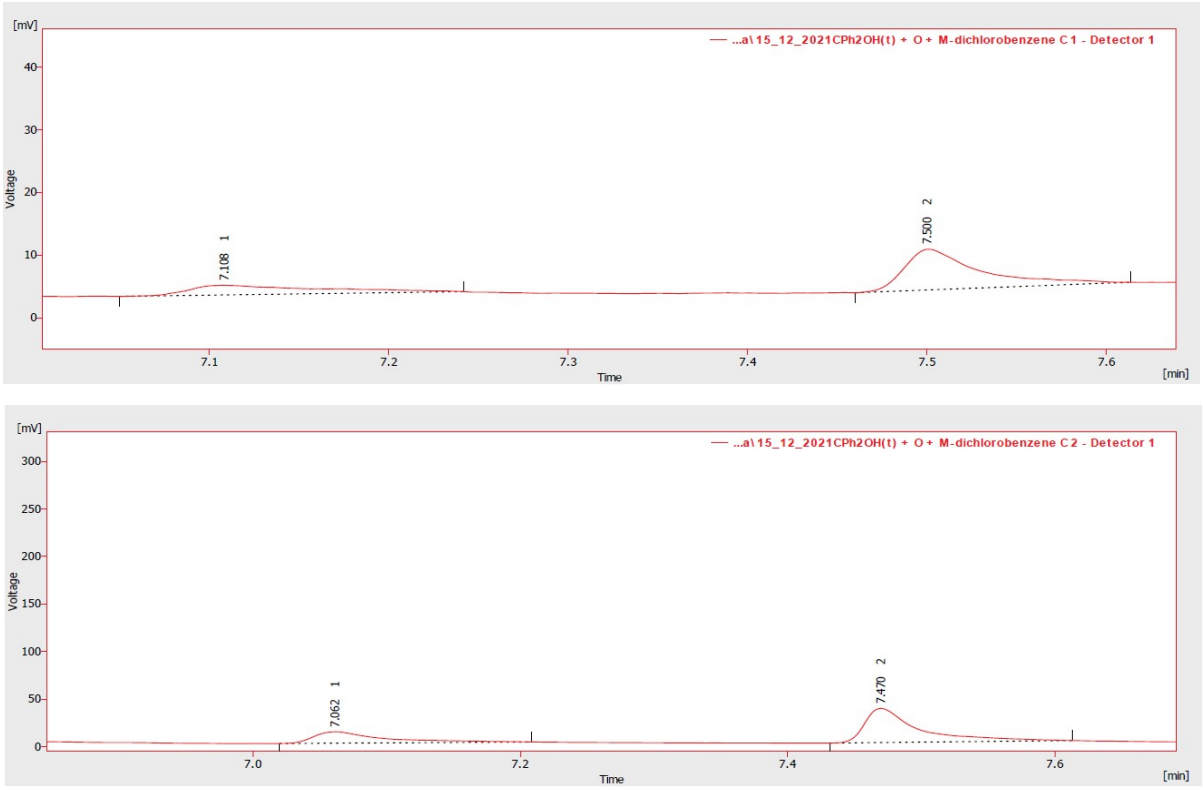


Figure S8. Overall H:G ratios for the *m*-DCB/*p*-DCB (a), *o*-DCB/*m*-DCB/*p*-DCB (b) with H2, *o*-DCB/*m*-DCB (c), *o*-DCB/*p*-DCB (d), *m*-DCB/*p*-DCB (e), *o*-DCB/*m*-DCB/*p*-DCB (f) competition experiments with H3

a)



b)

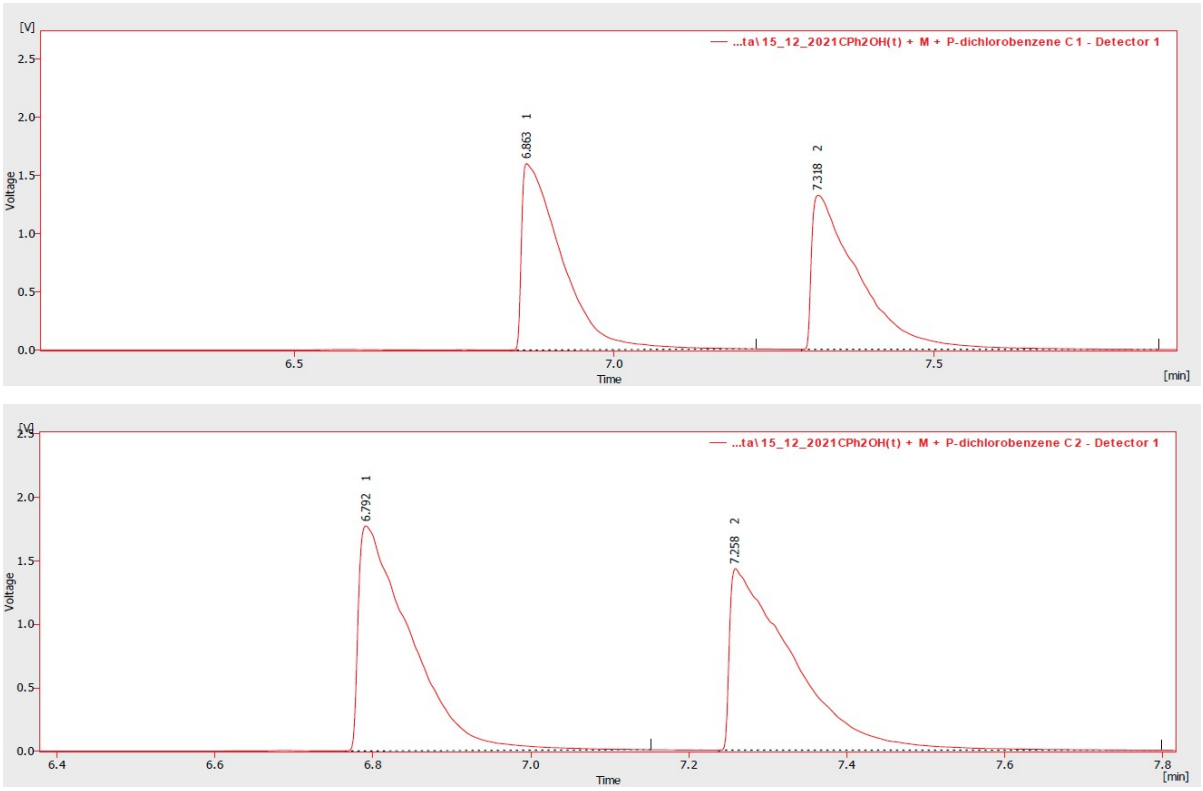


Figure S9. GC-FID chromatograms of the *o*-DCB/*m*-DCB (a) and *m*-DCB/*p*-DCB (b) binary guest mixtures with H2

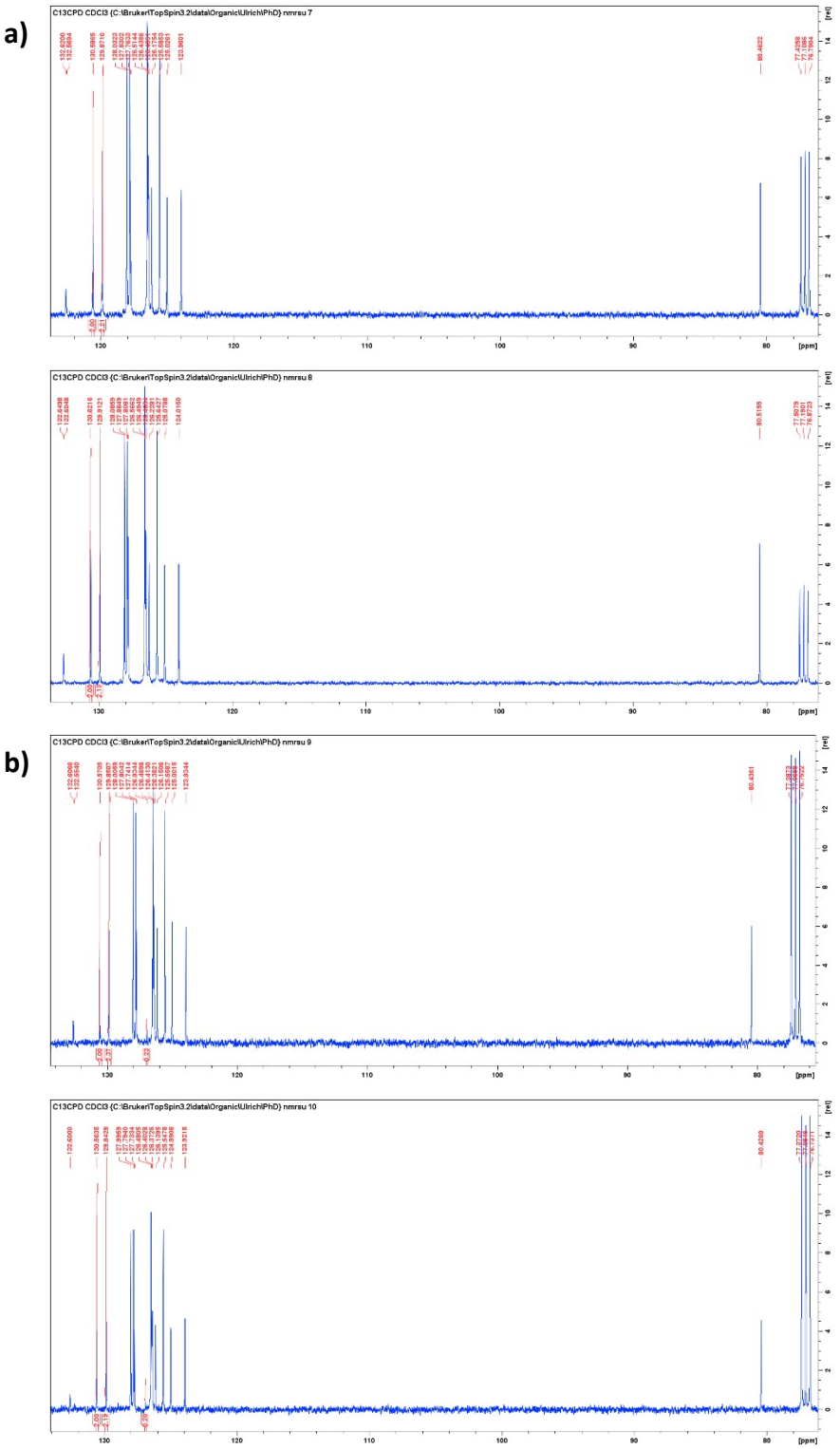
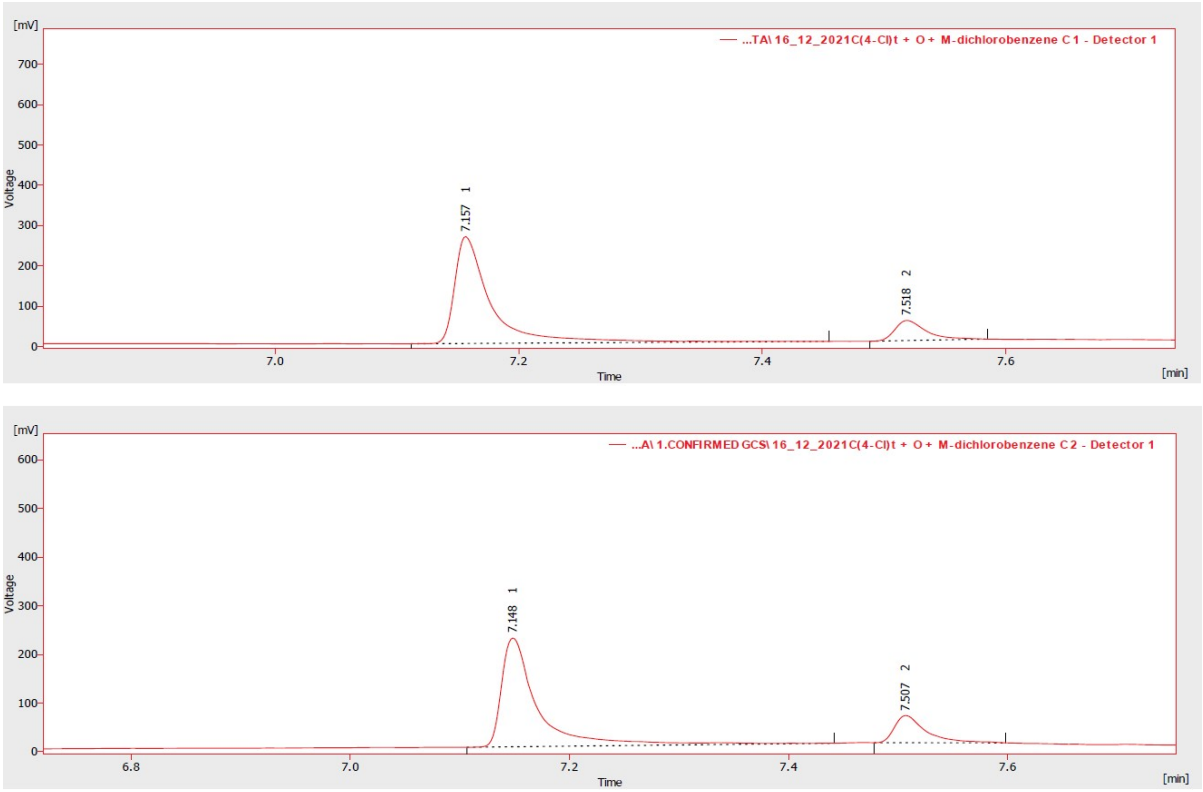


Figure S10. ^{13}C-NMR spectra of the *o*-DCB/*p*-DCB (a) binary and *o*-DCB/*m*-DCB/*p*-DCB ternary guest mixtures with H2

a)



b)

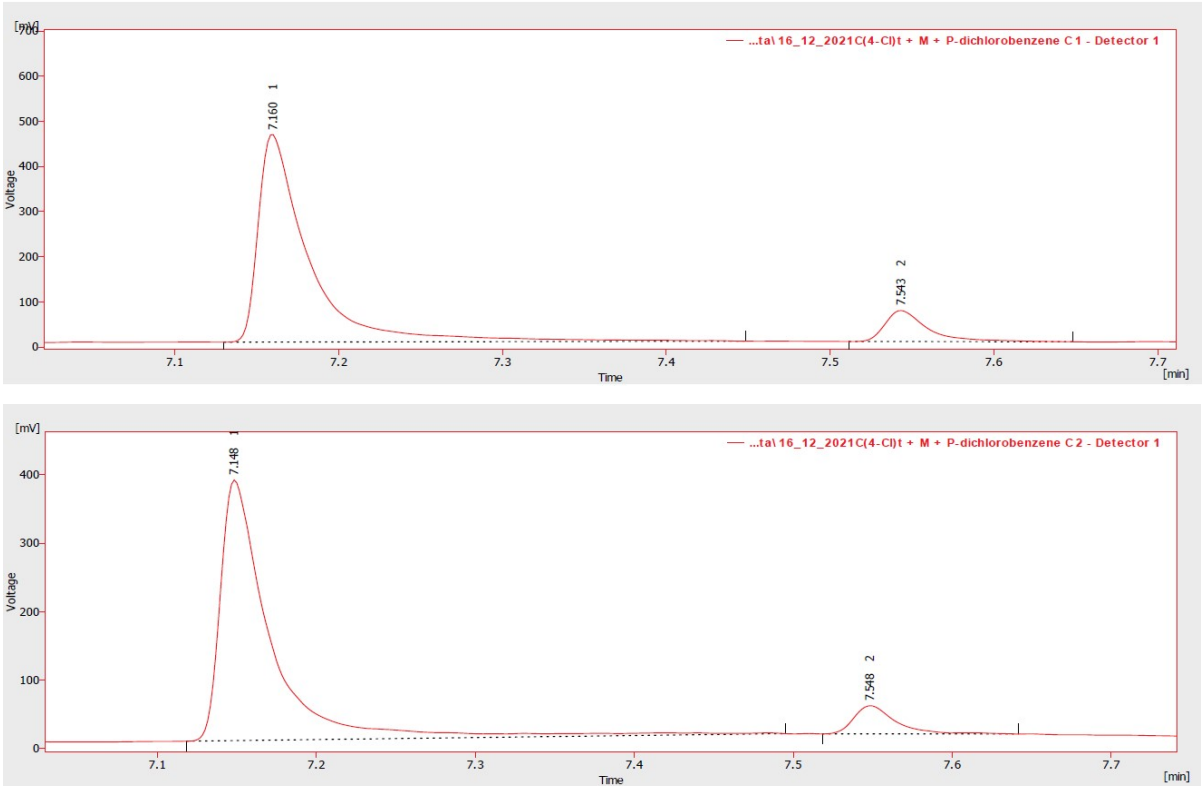
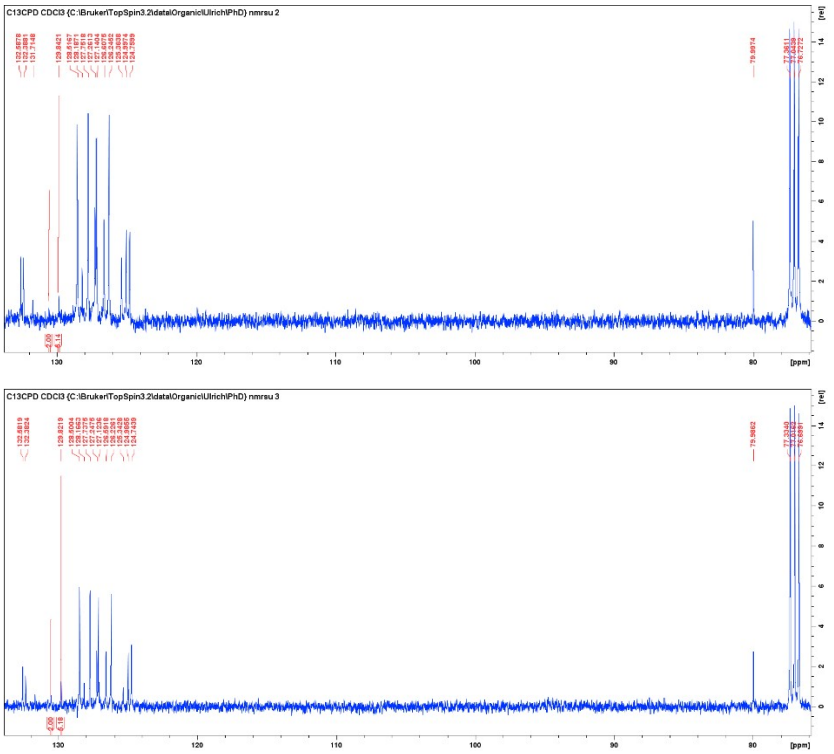


Figure S11. GC-FID chromatograms of the *o*-DCB/*m*-DCB (a) and *m*-DCB/*p*-DCB (b) binary guest mixtures with H3

a)



b)

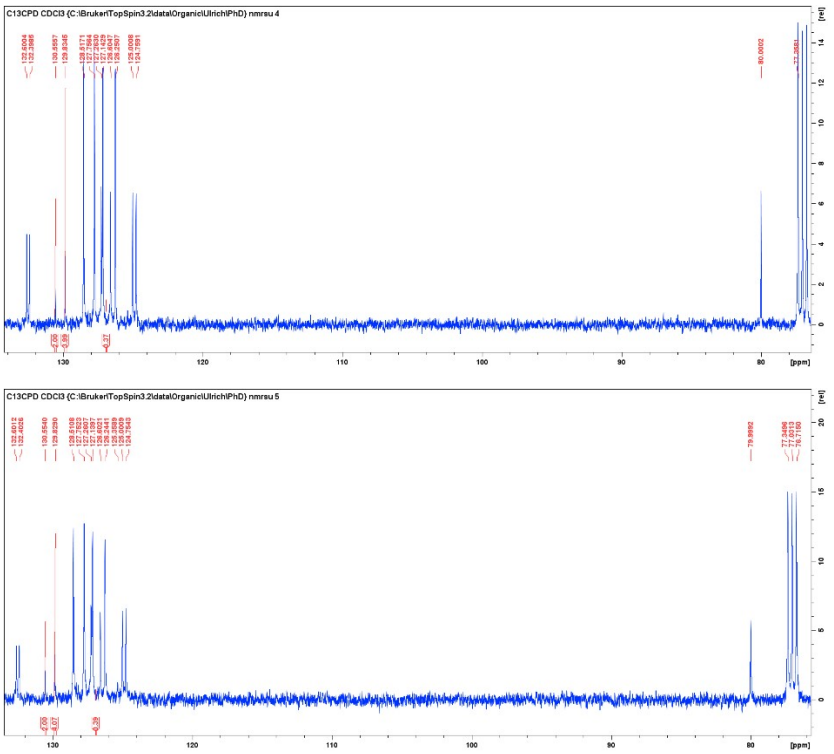
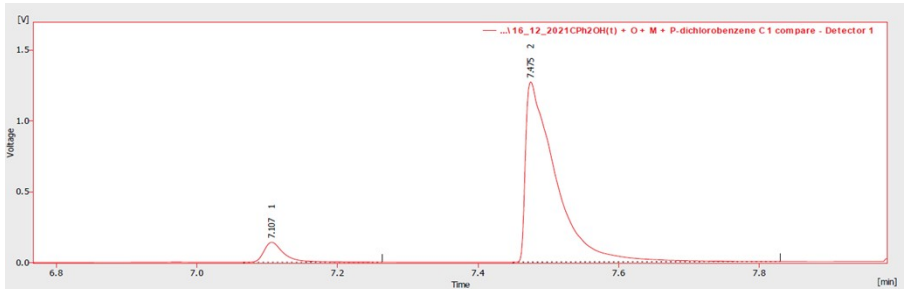


Figure S12. ^{13}C-NMR spectra of the *o*-DCB/*p*-DCB (a) binary and *o*-DCB/*m*-DCB/*p*-DCB ternary guest mixtures with H3

a)



b)

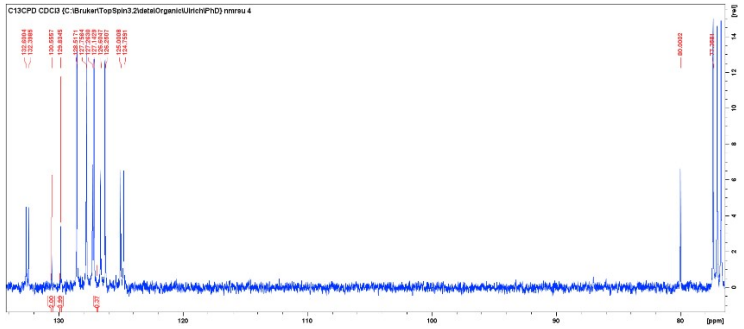


Figure S13. GC-FID chromatogram (a) and ^{13}C-NMR spectrum (b) of the *o*-DCB/*m*-DCB/*p*-DCB ternary guest mixtures with H2; showing the close agreement of the obtained G:G ratios [(6.8% *m*-DCB: 93.2% *o*-DCB/*p*-DCB from GC-FID) and (6.7% *m*-DCB: 58.6% *o*-DCB: 34.7% *p*-DCB from ^{13}C-NMR spectroscopy)

Table S1. Duplicate values obtained for the binary and ternary mixtures for H2 and H3, and toluene, ethylbenzene and cumene guests (H1 experiments resulted in the obtainment of vial containing only the apohost)

			H2			H3		
o-DCB	*m*-DCB	*p*-DCB	Duplicate #1	Duplicate #2	e.s.d.s (%)	Duplicate #1	Duplicate #2	e.s.d.s (%)
X	X[b]		71.1:28.9	70.0:30.0	(0.6)(0.6)	13.8:86.2	17.7:82.3	(2.0)(2.0)
X		X[c]	64.4:35.6	65.3:34.7	(0.5)(0.5)	43.8:56.2	43.6:56.4	(0.1)(0.1)

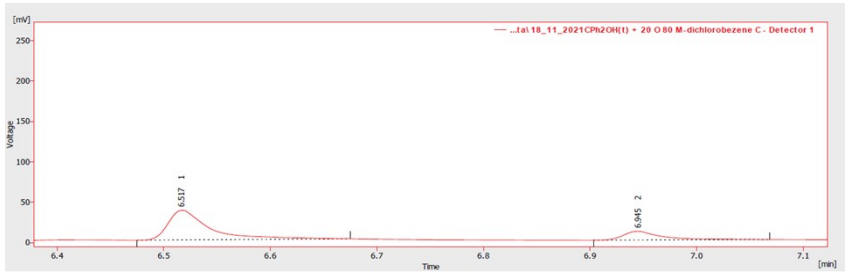
	X	X[b]	49.3:50.7	49.7:50.3	(0.2)(0.2)	88.8:11.2	91.7:8.3	(1.5)(1.5)
X	X	X[c]	58.6:6.7:34.7	60.7:6.1:33.2	(1.1)(0.3)(0.8)	45.8:45.7:8.5	45.2:46.0:8.8	(0.3)(0.1)(0.2)

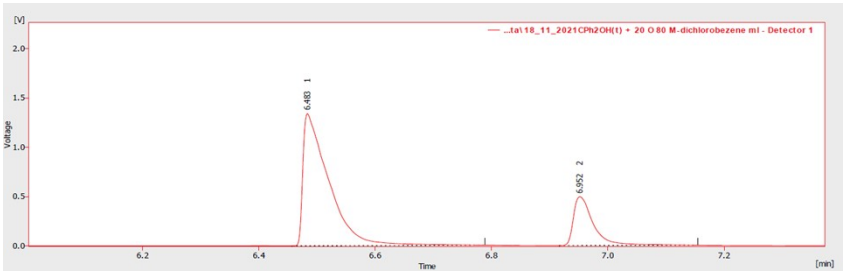
[a]Apohost was obtained, the guests were not included

[b]The *o*-DCB/*m*-DCB and *m*-DCB/*p*-DCB experiments were analyzed using GC-FID

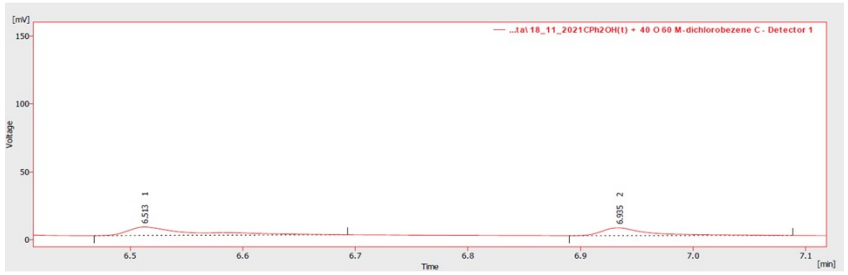
[c]The *o*-DCB/*p*-DCB and *o*-DCB/*m*-DCB/*p*-DCB experiments were analyzed using ^{13}C-NMR spectroscopy

a)

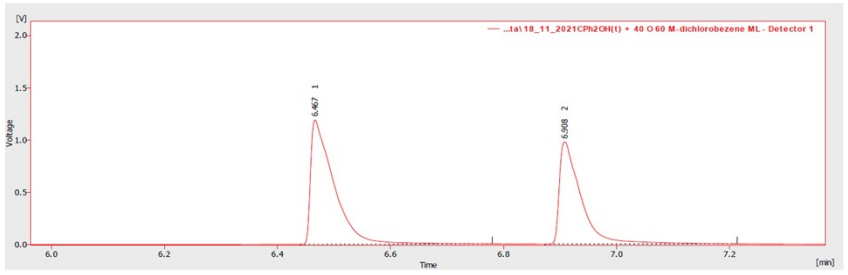

[mV]
...ta\18_11_2021CPh2OH(t) + 20 O 80 M-dichlorobezene C - Detector 1
Voltage
6.517 1
6.945 2
Time
[min]

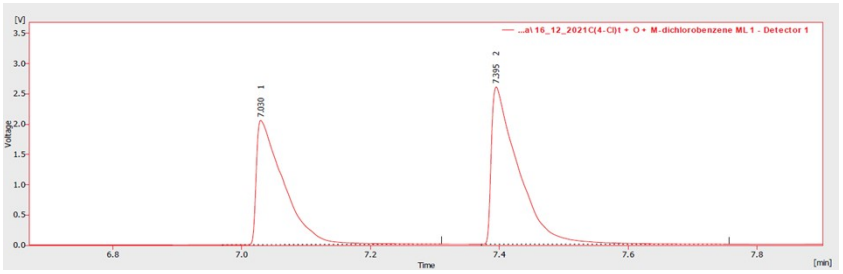

[V]
...ta\18_11_2021CPh2OH(t) + 20 O 80 M-dichlorobezene ml - Detector 1
Voltage
6.483 1
6.952 2
Time
[min]

b)


[mV]
...ta\18_11_2021CPh2OH(t) + 40 O 60 M-dichlorobezene C - Detector 1
Voltage
6.513 1
6.935 2
Time
[min]

c)


[V]
...ta\18_11_2021CPh2OH(t) + 40 O 60 M-dichlorobezene ML - Detector 1
Voltage
6.467 1
6.908 2
Time
[min]


[V]
...a\16_12_2021C(4-Cl)t + O + M-dichlorobenzene ML1 - Detector 1
Voltage
7.030 1
7.395 2
Time
[min]

d)

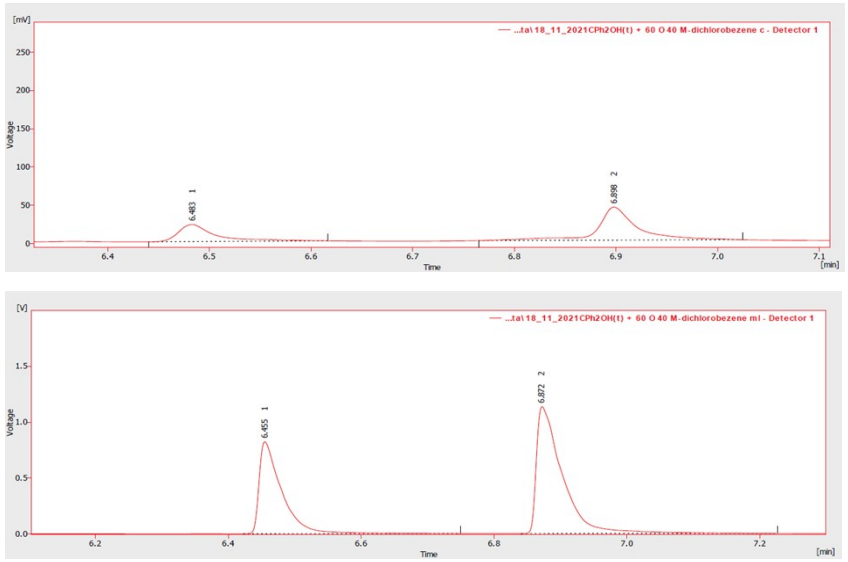
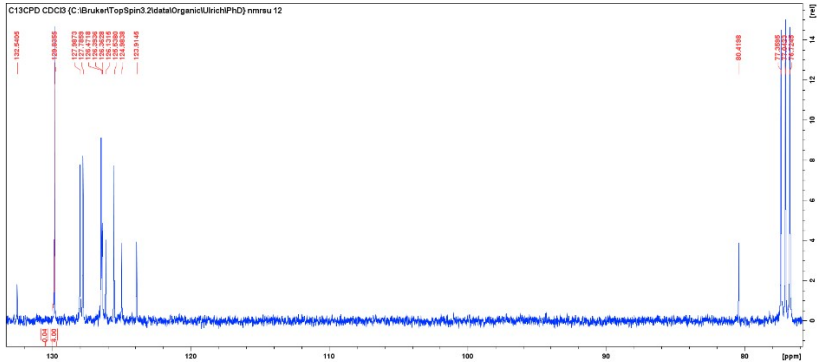
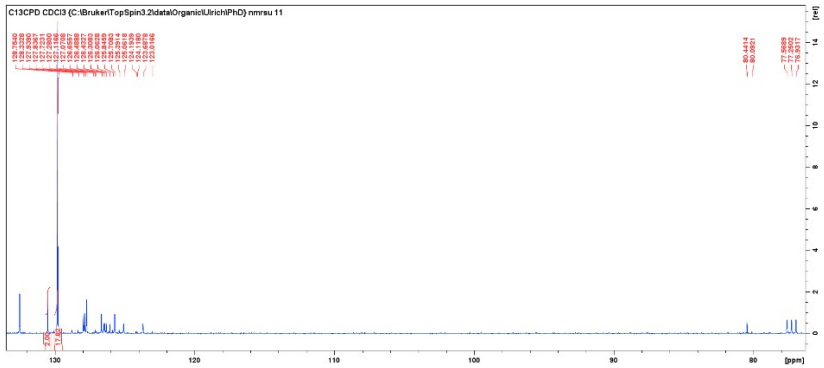


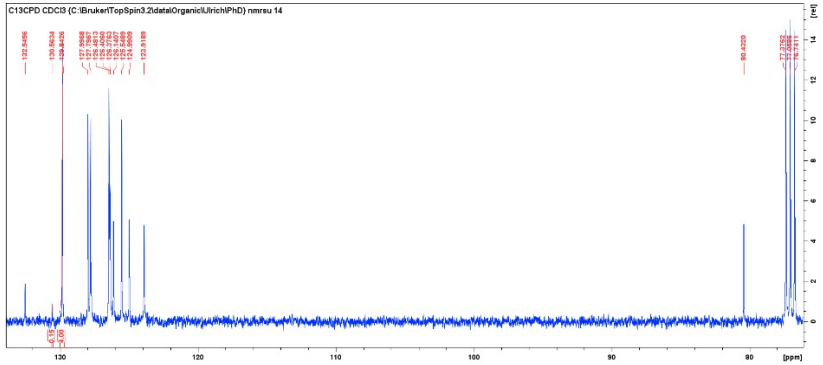
Figure S14. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 20:80 (a), 40:60 (b), 50:50 (c), and 60:40 (d) *o*-DCB/*m*-DCB binary experiments with H2

a)

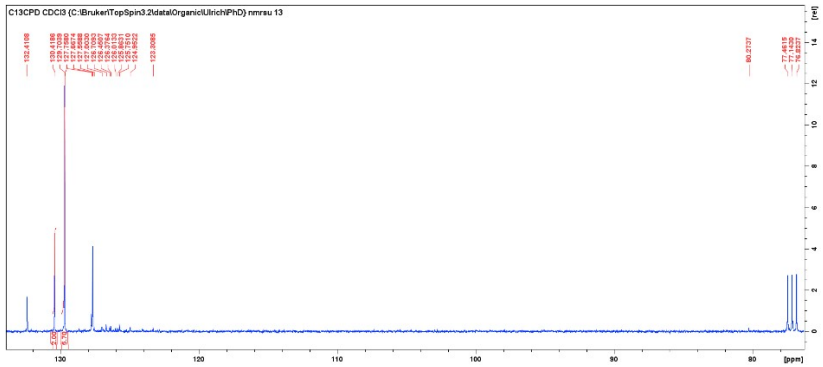

C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\OrganicIUlrichPhD) nmrsu 12
[ppm]
[rel]

b)


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\OrganicIUlrichPhD) nmrsu 11
[ppm]
[rel]


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich\PhD) nmrsu 14
[rel]
[ppm]

c)


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich\PhD) nmrsu 13
[rel]
[ppm]

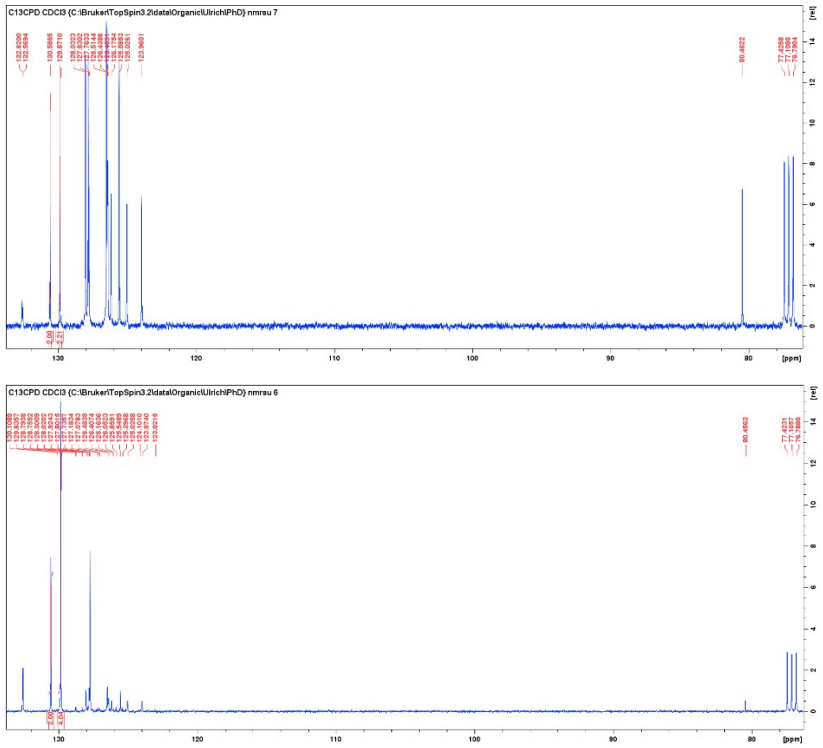
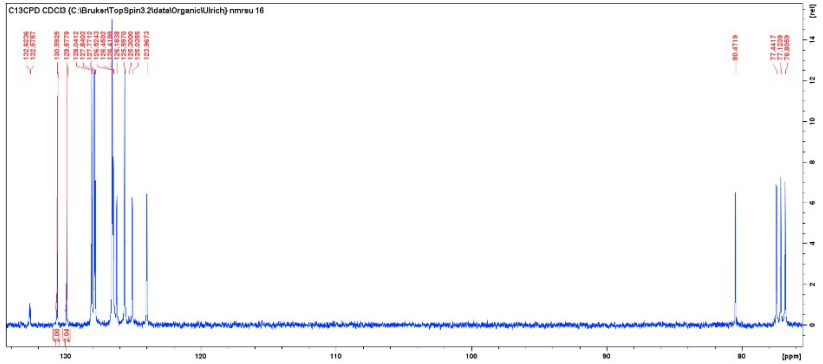
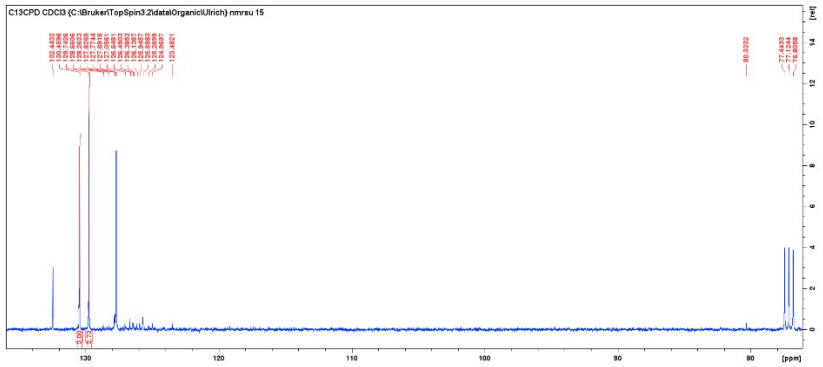


Figure S15. ^{13}C-NMR spectra of the crystals (left) and mother liquor (right) for the 20:80 (a), 40:60 (b), and 50:50 (c) *o*-DCB/*p*-DCB binary experiments with H2

a)


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich) nmrsu 16
[rel]
[ppm]

b)


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich) nmrsu 15
[rel]
[ppm]

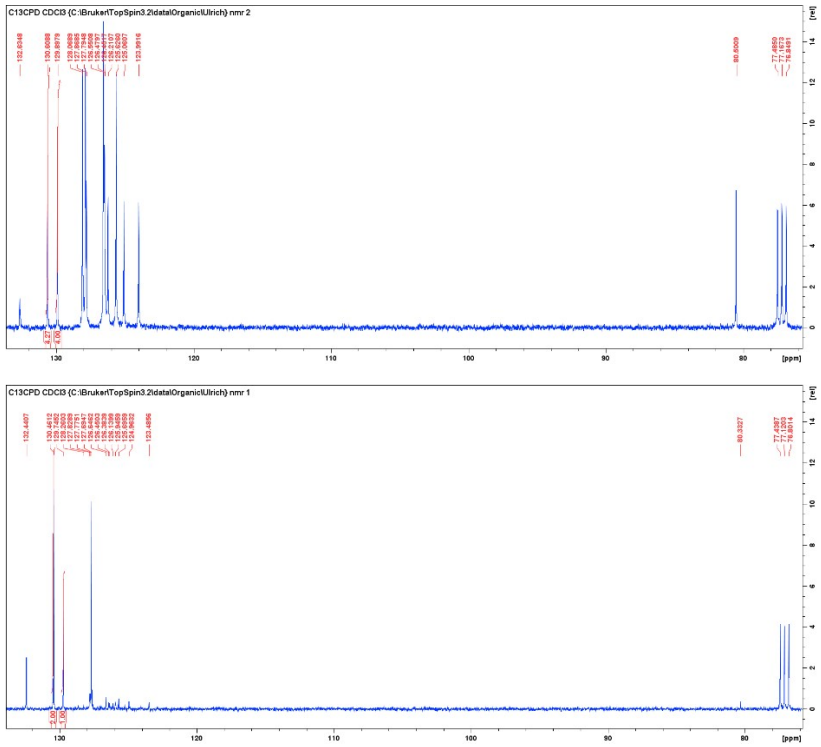
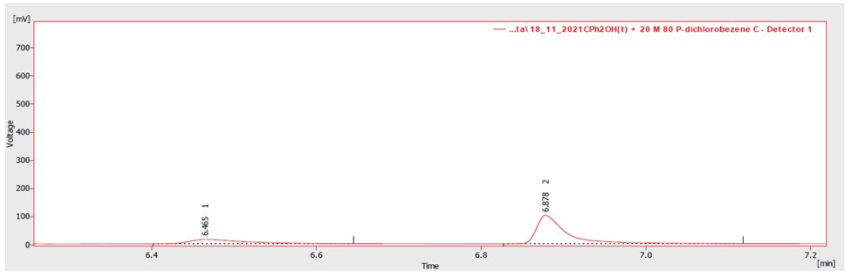
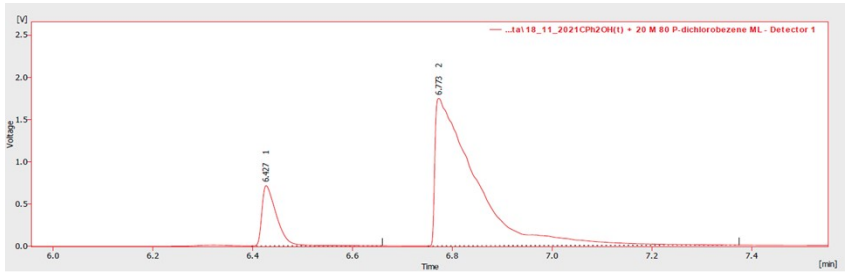


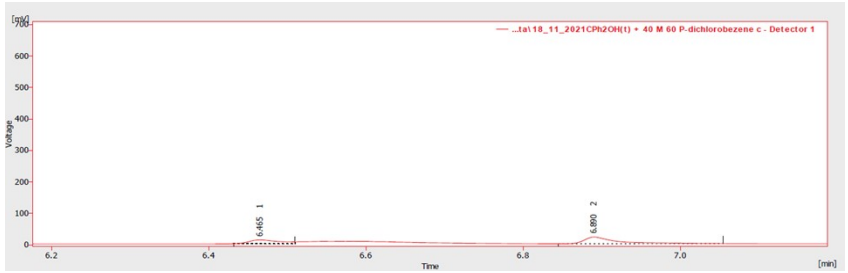
Figure S16. ^{13}C-NMR spectra of the crystals (left) and mother liquor (right) for the 60:40 (a) and 80:20 (b) *o*-DCB/*p*-DCB binary experiments with H2

a)

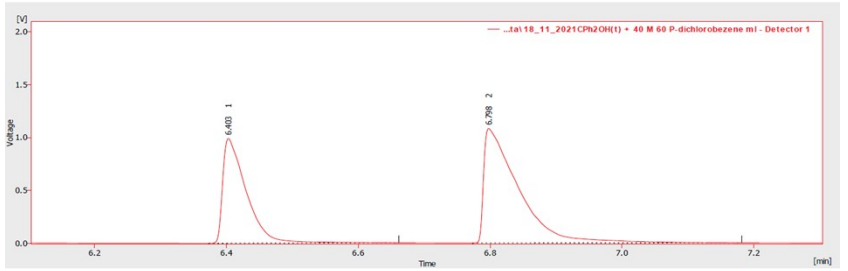

...ta\18_11_2021CPh2OH(t) + 20 M 80 P-dichlorobezene C - Detector 1
[mV]
Voltage
Time
[min]
6.465 1
6.878 2

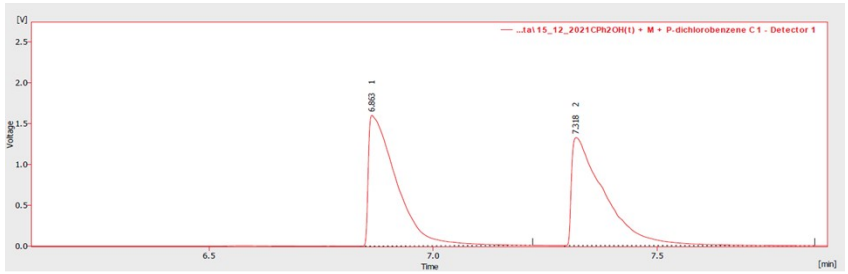
b)


...ta\18_11_2021CPh2OH(t) + 20 M 80 P-dichlorobezene ML - Detector 1
[V]
Voltage
Time
[min]
6.427 1
6.773 2

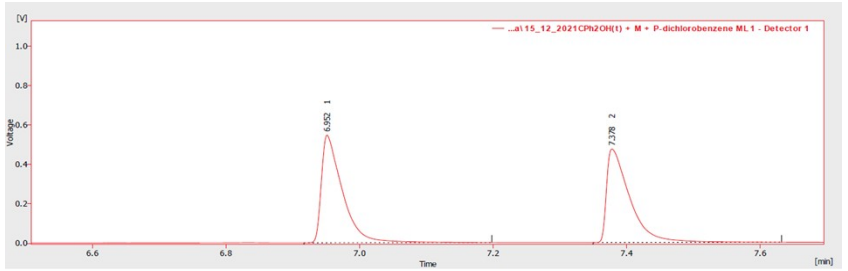

...ta\18_11_2021CPh2OH(t) + 40 M 60 P-dichlorobezene c - Detector 1
[mV]
Voltage
Time
[min]
6.465 1
6.890 2

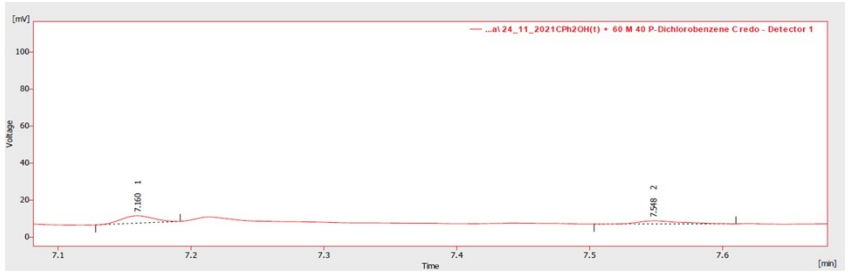
c)


...ta\18_11_2021CPh2OH(t) + 40 M 60 P-dichlorobezene mI - Detector 1
[V]
Voltage
Time
[min]
6.403 1
6.798 2


[V]
...ta\15_12_2021CPh2OH(t) + M + P-dichlorobenzene C1 - Detector 1
Voltage
6.863
7.318
Time
[min]

d)


[V]
...a\15_12_2021CPh2OH(t) + M + P-dichlorobenzene ML1 - Detector 1
Voltage
6.952
7.378
Time
[min]


[mV]
...a\24_11_2021CPh2OH(t) + 60 M 40 P-Dichlorobenzene Credo - Detector 1
Voltage
7.160
7.548
Time
[min]

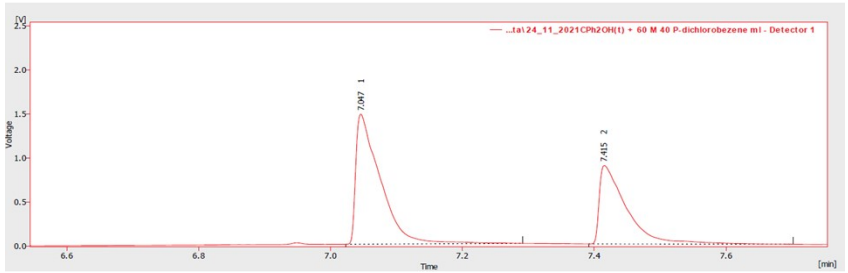

[V]
...ta\24_11_2021CPh2OH(t) + 60 M 40 P-dichlorobezene ml - Detector 1
Voltage
7.007
7.415
Time
[min]

Figure S17. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 20:80 (a), 40:60 (b), 50:50 (c), and 60:40 (d) *m*-DCB/*p*-DCB binary experiments with H2

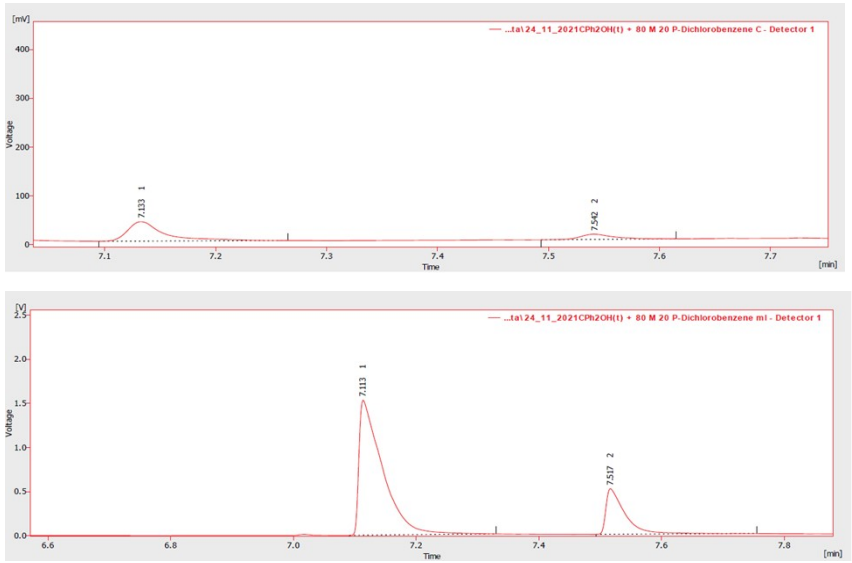
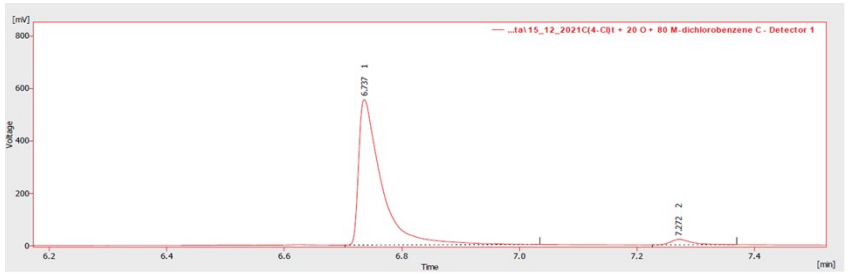
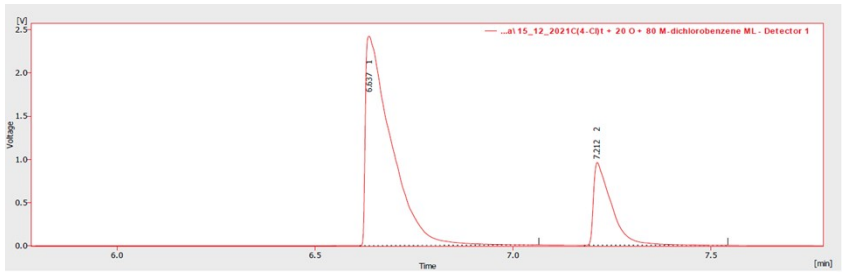


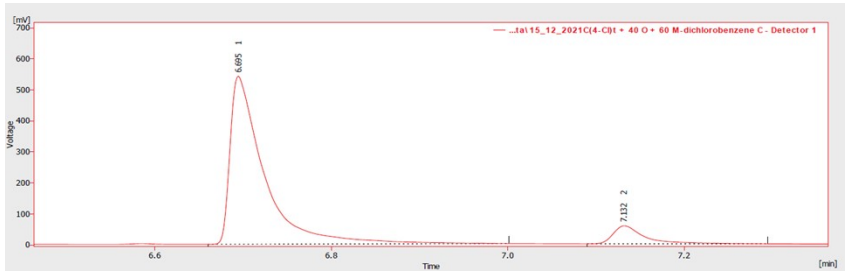
Figure S18. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 80:20 *m*-DCB/*p*-DCB binary experiments with H2

a)


[mV]
...ta\15_12_2021C(4-Cl)t + 20 O + 80 M-dichlorobenzene C - Detector 1
6.737 1
7.272 2
Voltage
Time
[min]

b)


[V]
...a\15_12_2021C(4-Cl)t + 20 O + 80 M-dichlorobenzene ML - Detector 1
6.637 1
7.212 2
Voltage
Time
[min]


[mV]
...ta\15_12_2021C(4-Cl)t + 40 O + 60 M-dichlorobenzene C - Detector 1
6.695 1
7.132 2
Voltage
Time
[min]

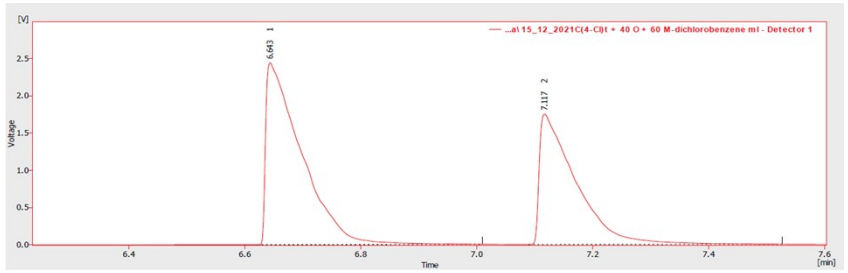
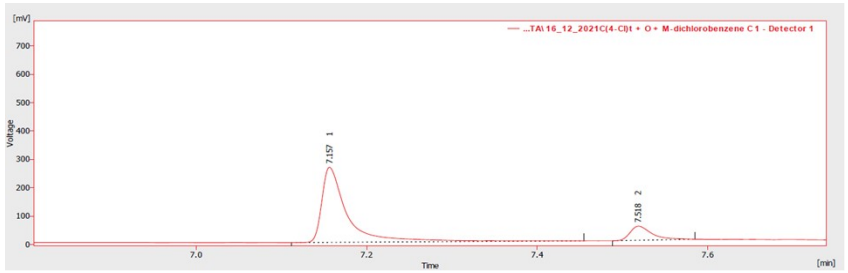
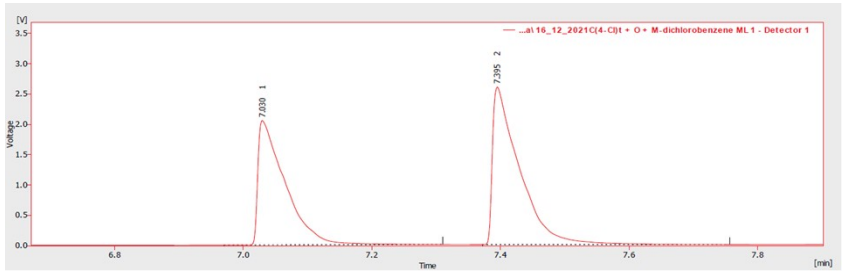

[V]
...a\15_12_2021C(4-Cl)t + 40 O + 60 M-dichlorobenzene mI - Detector 1
6.643 1
7.117 2
Voltage
Time
[min]

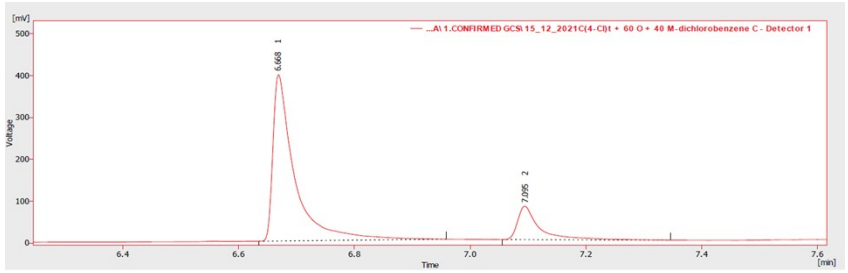
Figure S19. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 20:80 (a) and 40:60 (b) *o*-DCB/*m*-DCB binary experiments with H3

a)

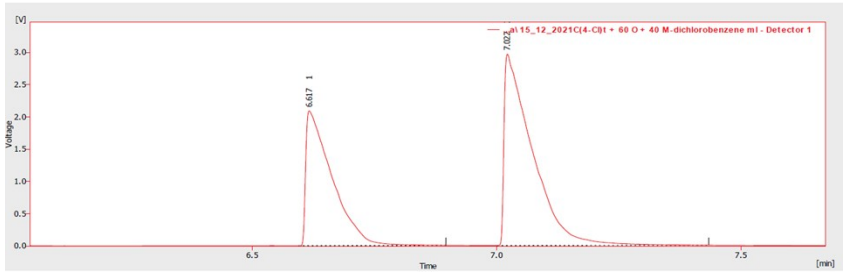

[mV]
...TA\16_12_2021C(4-Cl)t + O + M-dichlorobenzene C 1 - Detector 1
Voltage
Time
[min]
7.157
7.518

b)


[V]
...a\16_12_2021C(4-Cl)t + O + M-dichlorobenzene ML 1 - Detector 1
Voltage
Time
[min]
7.030
7.395


[mV]
...A\1.CONFIRMED GCS\15_12_2021C(4-Cl)t + 60 O + 40 M-dichlorobenzene C - Detector 1
Voltage
Time
[min]
6.668
7.095

c)


[V]
...a\15_12_2021C(4-Cl)t + 60 O + 40 M-dichlorobenzene mI - Detector 1
Voltage
Time
[min]
6.617
7.027

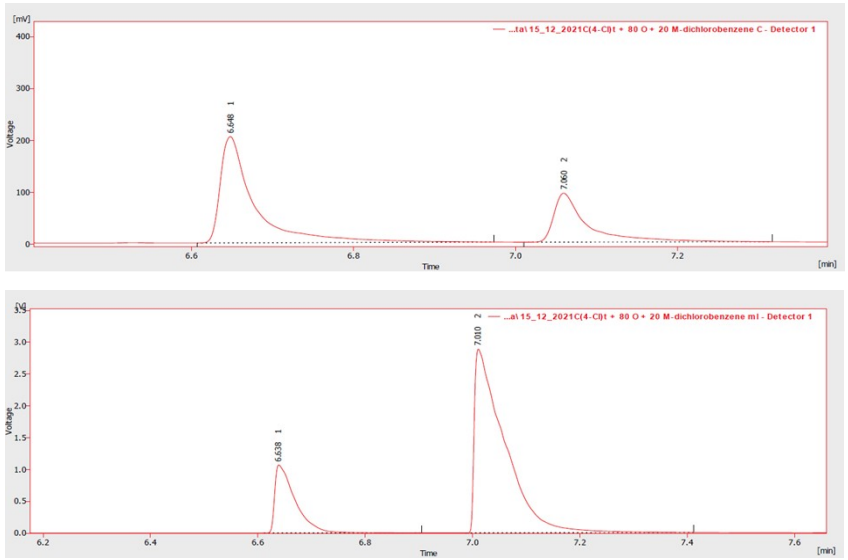
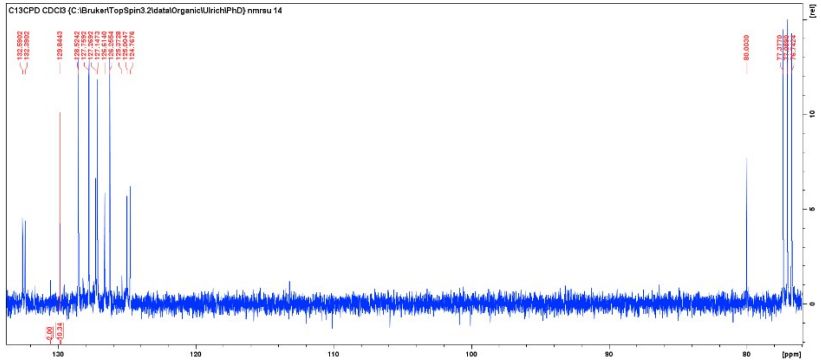
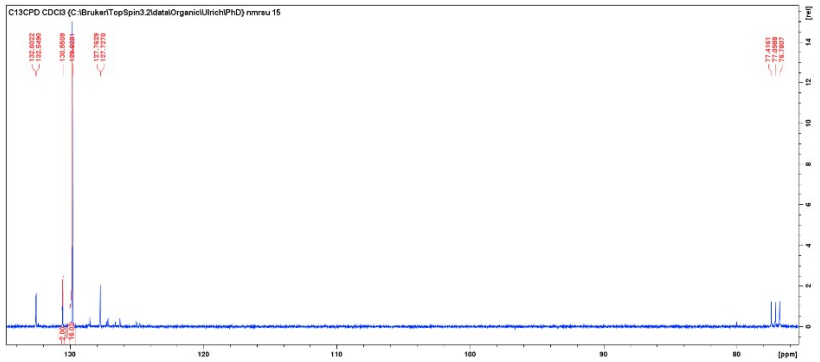


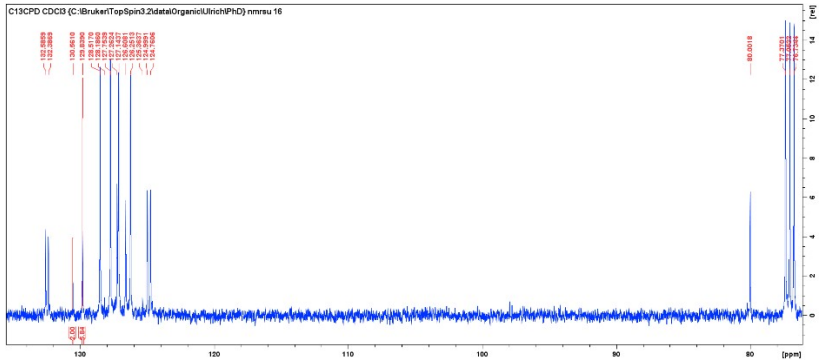
Figure S20. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 50:50 (a), 60:40 (a), and 80:20 (b) *o*-DCB/*m*-DCB binary experiments with H3

a)

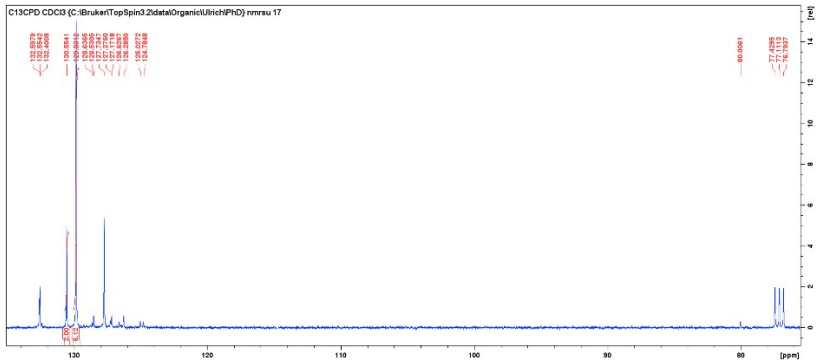

C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\OrganicIUlrichPhD) nmrsu 14
[rel]
[ppm]

b)


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\OrganicIUlrichPhD) nmrsu 15
[rel]
[ppm]


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich\PhD) nmrsu 16
[rel]
[ppm]

c)


C13CPD CDCl3 (C:\Bruker\TopSpin3.2\data\Organic\Ulrich\PhD) nmrsu 17
[rel]
[ppm]

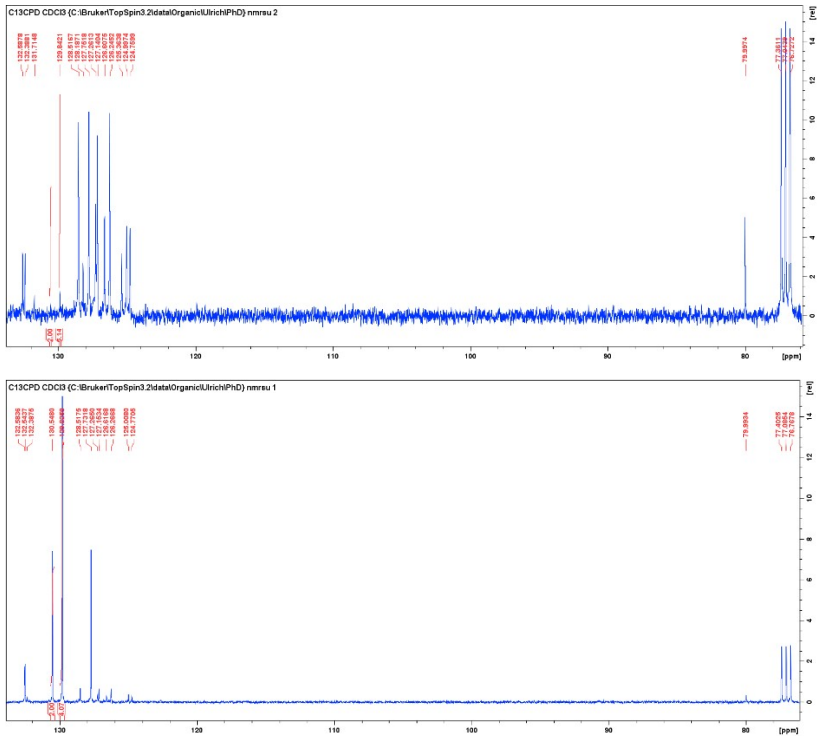
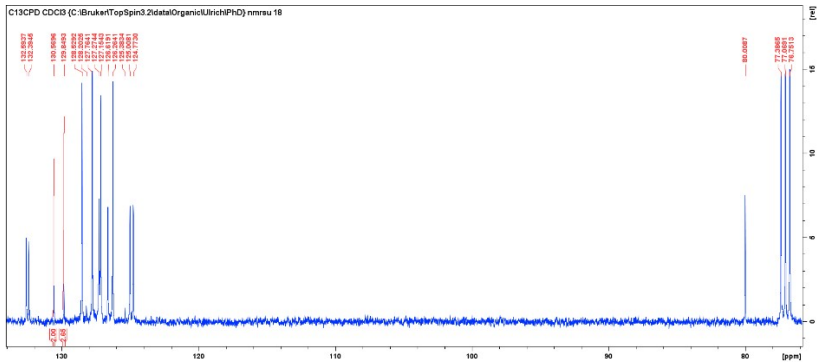
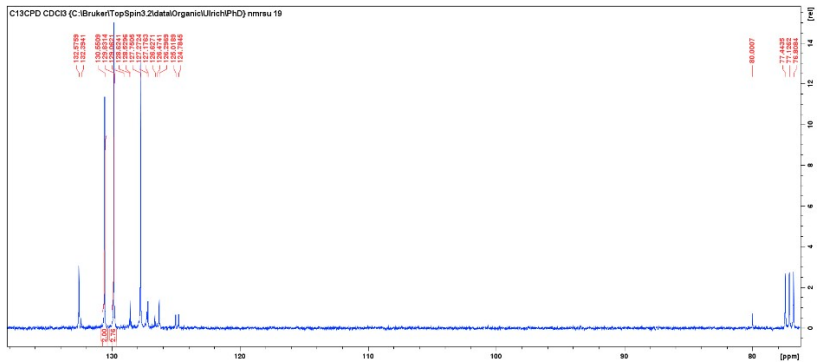


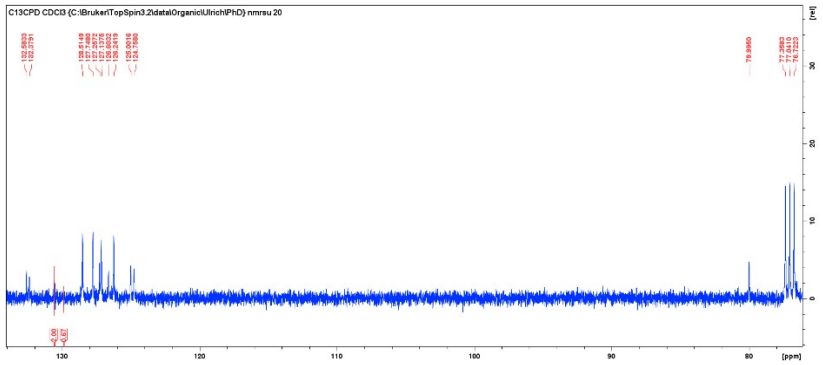
Figure S21. ^{13}C-NMR spectra of the crystals (left) and mother liquor (right) for the 20:80 (a), 40:60 (b), and 50:50 (c) *o*-DCB/*p*-DCB binary experiments with H3

a)





b)



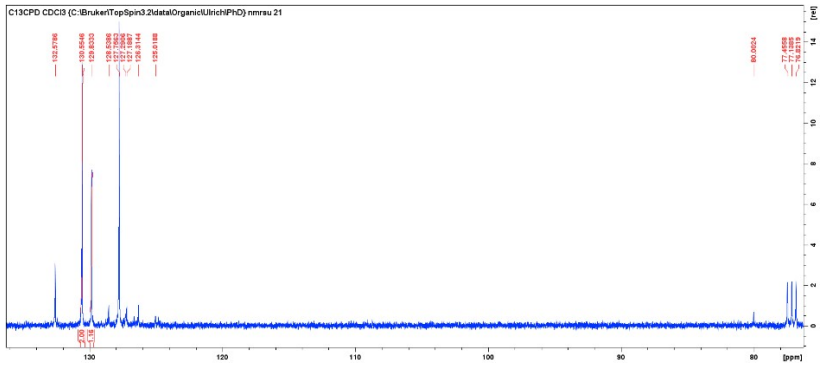
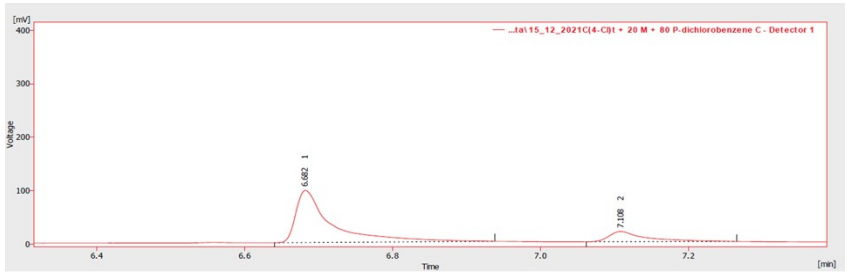
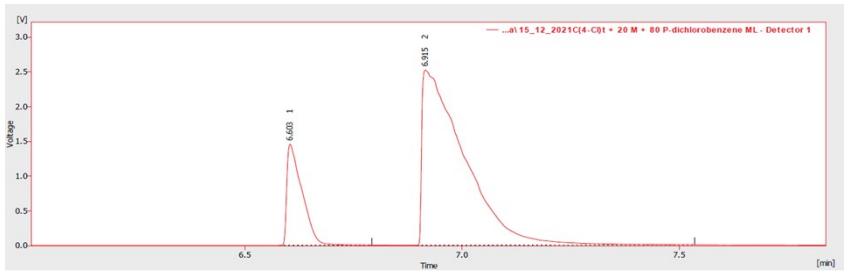


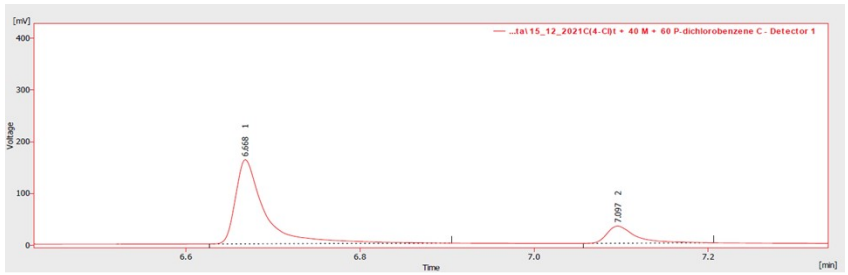
Figure S22. ^{13}C-NMR spectra of the crystals (left) and mother liquor (right) for the 60:40 (a) and 80:20 (b) *o*-DCB/*p*-DCB binary experiments with H3

a)

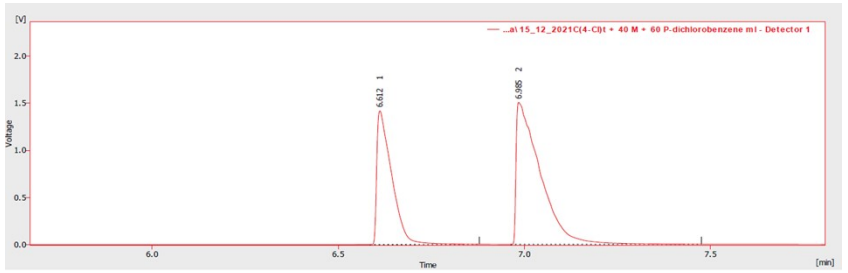

[mV]
...ta\15_12_2021C(4-Cl)t + 20 M + 80 P-dichlorobenzene C - Detector 1
Voltage
6.682 1
7.108 2
Time
[min]

b)


[V]
...a\15_12_2021C(4-Cl)t + 20 M + 80 P-dichlorobenzene ML - Detector 1
Voltage
6.603 1
6.915 2
Time
[min]


[mV]
...ta\15_12_2021C(4-Cl)t + 40 M + 60 P-dichlorobenzene C - Detector 1
Voltage
6.668 1
7.097 2
Time
[min]

c)


[V]
...a\15_12_2021C(4-Cl)t + 40 M + 60 P-dichlorobenzene ml - Detector 1
Voltage
6.612 1
6.985 2
Time
[min]

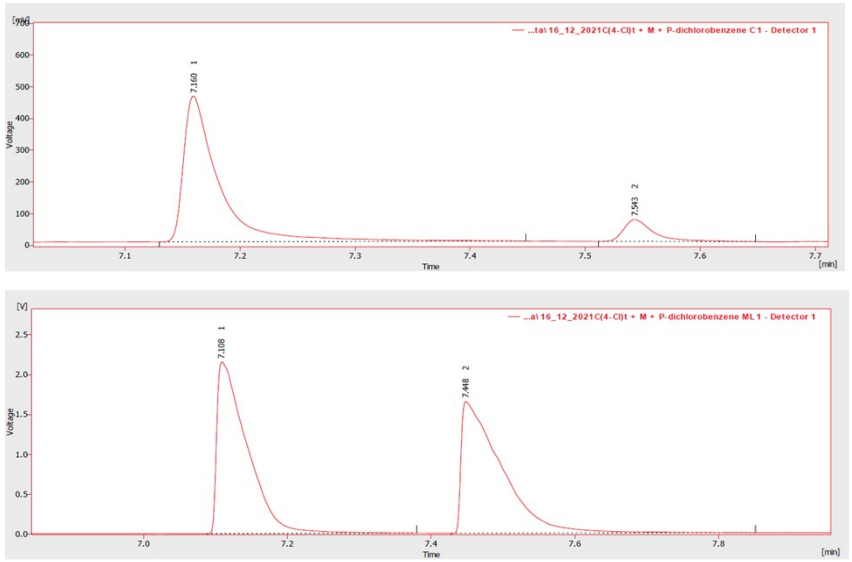
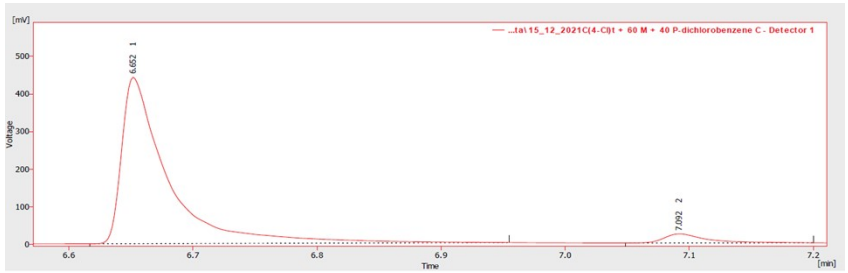
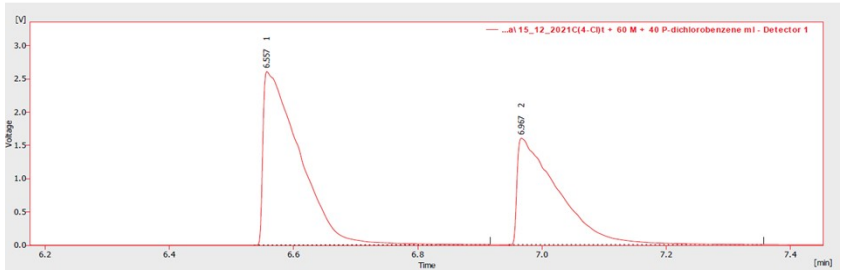


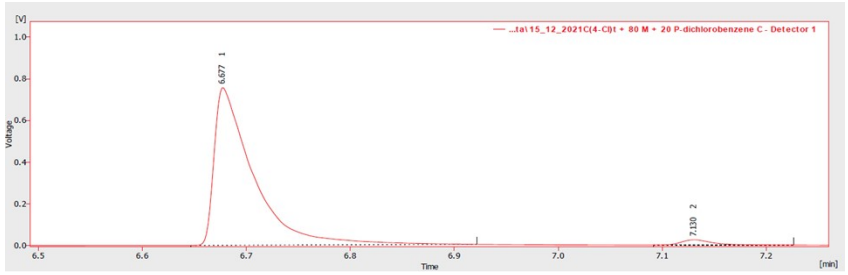
Figure S23. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 20:80 (a), 40:60 (b), and 50:50 (c) *m*-DCB/*p*-DCB binary experiments with H3

a)


[mV]
...ta\15_12_2021C(4-Cl)t + 60 M + 40 P-dichlorobenzene C - Detector 1
6.652 1
7.092 2
Voltage
Time
[min]

b)


[V]
...a\15_12_2021C(4-Cl)t + 60 M + 40 P-dichlorobenzene mI - Detector 1
6.557 1
6.967 2
Voltage
Time
[min]


[V]
...ta\15_12_2021C(4-Cl)t + 80 M + 20 P-dichlorobenzene C - Detector 1
6.677 1
7.130 2
Voltage
Time
[min]

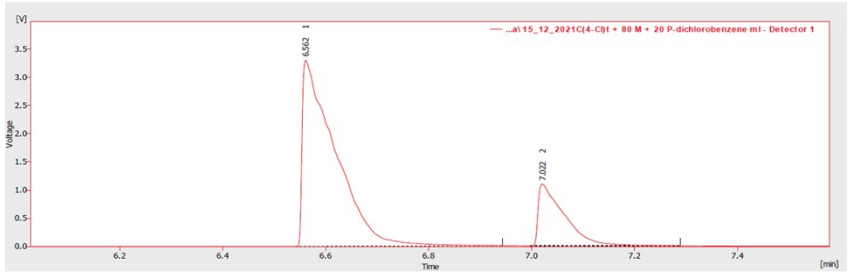

[V]
...a\15_12_2021C(4-Cl)t + 80 M + 20 P-dichlorobenzene mI - Detector 1
6.562 1
7.022 2
Voltage
Time
[min]

Figure S24. GC-FID chromatograms of the crystals (left) and mother liquor (right) for the 60:40 (a) and 80:20 (b) *m*-DCB/*p*-DCB binary experiments with H3

Table S2. Data points obtained for the guest/guest (dichlorobenzene) mixtures with corresponding K values for H2

Binary mixture	Crystal G_A:G_B	Mother liquor G_A:G_B	K values
20:80 *o*-DCB/*m*-DCB	0.21:0.79	0.22:0.78	1.04
40:60 *o*-DCB/*m*-DCB	0.41:0.59	0.43:0.57	1.12
50:50 *o*-DCB/*m*-DCB	0.68:0.32	0.61:0.39	1.31
60:40 *o*-DCB/*m*-DCB	0.71:0.29	0.62:0.38	1.51
80:20 *o*-DCB/*m*-DCB	[a]	[a]	–
20:80 *o*-DCB/*p*-DCB	0.02:0.98	0.18:0.82	10.98
40:60 *o*-DCB/*p*-DCB	0.07:0.93	0.41:0.59	9.31
50:50 *o*-DCB/*p*-DCB	0.64:0.36	0.50:0.50	1.82
60:40 *o*-DCB/*p*-DCB	0.66:0.34	0.59:0.41	1.34
80:20 *o*-DCB/*p*-DCB	0.68:0.32	0.80:0.20	1.87
20:80 *m*-DCB/*p*-DCB	0.22:0.78	0.13:0.87	1.91
40:60 *m*-DCB/*p*-DCB	0.36:0.64	0.38:0.62	1.11
50:50 *m*-DCB/*p*-DCB	0.49:0.51	0.49:0.51	1.01
60:40 *m*-DCB/*p*-DCB	0.62:0.38	0.60:0.40	1.10
80:20 *m*-DCB/*p*-DCB	0.80:0.20	0.79:0.21	1.12

[a]A gel remained in the vial

Table S3. Data points obtained for the guest/guest (dichlorobenzene) mixtures with corresponding K values for H3

Binary mixture	Crystal G_A:G_B	Mother liquor G_A:G_B	K values
20:80 *o*-DCB/*m*-DCB	0.03:0.97	0.22:0.78	7.83
40:60 *o*-DCB/*m*-DCB	0.10:0.90	0.42:0.58	6.80
50:50 *o*-DCB/*m*-DCB	0.14:0.86	0.56:0.44	7.89
60:40 *o*-DCB/*m*-DCB	0.17:0.83	0.61:0.39	7.53
80:20 *o*-DCB/*m*-DCB	0.31:0.69	0.80:0.20	8.90
20:80 *o*-DCB/*p*-DCB	0.35:0.65	0.20:0.80	2.19
40:60 *o*-DCB/*p*-DCB	0.41:0.59	0.40:0.60	1.05
50:50 *o*-DCB/*p*-DCB	0.44:0.56	0.50:0.50	1.26
60:40 *o*-DCB/*p*-DCB	0.60:0.40	0.59:0.41	1.04
80:20 *o*-DCB/*p*-DCB	0.86:0.14	0.78:0.22	1.74
20:80 *m*-DCB/*p*-DCB	0.83:0.17	0.17:0.83	24.01
40:60 *m*-DCB/*p*-DCB	0.83:0.17	0.37:0.63	8.63
50:50 *m*-DCB/*p*-DCB	0.89:0.11	0.50:0.50	8.09
60:40 *m*-DCB/*p*-DCB	0.95:0.05	0.59:0.41	13.97
80:20 *m*-DCB/*p*-DCB	0.97:0.03	0.79:0.21	9.78

Table S4. Host···host forces for the H2·*o*-DCB, 3(H2)·*m*-DCB and H3·*m*-DCB[a]

Interactions	**H2**·*o*-DCB	3(**H2**)·*m*-DCB	**H3**·*m*-DCB	Symmetry
(host)π···π(host)	3.511(1) – 3.733(1) Å (2 contacts)	3.572(2) Å (1 contact)	3.561(2) Å (1 contact)	
C–H···π	(H···Cg, X–H···Cg)	(H···Cg, X–H···Cg)	(H···Cg, X–H···Cg)	
(host)C–H···π(host)[b]	2.89 Å, 136°		None	–x, –y, 1–z
(host)C–H···π(host)[b]		2.79 Å, 137°		1–x, y, 1–z
(host)C–H···π(host)[b]		2.93 Å, 137°		1–x, y, 1–z
O–H···π				
(host)O–H···π(host)[c]	2.67 Å, 153°			x, y, z
(host)O–H···π(host)[c]	2.58 Å, 161°			x, y, z
(host)O–H···π(host)[c]		2.55 Å, 154°		x, y, z
(host)O–H···π(host)[c]		2.57 Å, 165°		x, y, z
(host)O–H···π(host)[c]			2.54 Å, 155°	x, y, z
(host)O–H···π(host)[c]			2.53 Å, 166°	x, y, z
C–Cl···π	(X···Cg, Y–X···Cg)	(X···Cg, Y–X···Cg)	(X···Cg, Y–X···Cg)	
(host)C–Cl···π(host)[b]	–	–	3.511(1) Å, 94.7(1)°	3/2–x, y, 1–z
(host)C–Cl···π(host)[b]			3.644(1) Å, 170.1(1)°	3/2–x, y, 1–z
(host)C–Cl···π(host)[b]			3.418(1) Å, 160.4(1)°	1/2+x, y, –z
(host)C–Cl···π(host)[b]			3.517(1) Å, 93.8(1)°	1/2+x, y, –z
Short contacts				
(host)C–H···O(host)[c]	2.33 Å, 112°, <<			
(host)C–H···O(host)[c]	2.55 Å, 106°, <<			
(host)C–H···O(host)[c]	2.41 Å, 103°, <<			
(host)C–H···O(host)[c]	2.29 Å, 102°, <<			
(host)C–H···O(host)[c]	2.41 Å, 102°, <<			
(host)C–H···O(host)[c]	2.29 Å, 102°, <<			
(host)C–H···O(host)[c]		2.38 Å, 111°, <<		
(host)C–H···O(host)[c]		2.48 Å, 109°, <<		
(host)C–H···O(host)[c]		2.43 Å, 103°, <<		
(host)C–H···O(host)[c]		2.32 Å, 102°, <<		
(host)C–H···O(host)[c]		2.38 Å, 103°, <<		
(host)C–H···O(host)[c]		2.30 Å, 103°, <<		
(host)C–C···Cl–C(host)[b]			3.443 Å, 103°, <	1/2–x, y, –z
(host)C–H···O–C(host)[b]			2.65 Å, 144°, <	1–x, 1/2+y, 1/2–z
(host)C–H···H–C(host)[b]			2.18 Å, 156°, <<	1/2+x, –1/2+y, 1/2+z
(host)C–H···O(host)[c]			2.34 Å, 111°, <<	
(host)C–H···O(host)[c]			2.44 Å, 108°, <<	
(host)C–H···O(host)[c]			2.37 Å, 103°, <<	
(host)C–H···O(host)[c]			2.29 Å, 102°, <<	
(host)C–H···O(host)[c]			2.32 Å, 102°, <<	
(host)C–H···O(host)[c]			2.35 Å, 104°, <<	
Hydrogen bonding	(H···A, D–H···A) None	(H···A, D–H···A) None	(H···A, D–H···A) None	

[a]< denotes contacts less than the sum of the van der Waals radii and << contacts less than this sum minus 0.2 Å
[b]Intermolecular interaction
[c]Intramolecular interaction

Table S5. Host···guest and guest···guest forces for the H2·*o*-DCB, 3(H2)·*m*-DCB and H3·*m*-DCB[a]

Interactions	**H2**·*o*-DCB	3(**H2**)·*m*-DCB	**H3**·*m*-DCB	**Symmetry**
(host)π···π(guest)	Not significant	Not significant	Not significant	
(guest)π···π(guest)	None	None	None	
C–H···π	(H···Cg, X–H···Cg)	(H···Cg, X–H···Cg)	(H···Cg, X–H···Cg)	
(host)C–H···π(guest)[b]	2.91 Å, 145°		None	1–x, 1–y, 1–z
(host)C–H···π(guest)[b]		2.75 Å, 160°		x, 1–y, 1–z
C–Cl···π	(X···Cg, Y–X···Cg)	(X···Cg, Y–X···Cg)	(X···Cg, Y–X···Cg)	
(guest)C–Cl···π(host)[b]	None	None	3.864(2) Å, 134.2(1)°	1/2+x, 1–y, z
Short contacts				
(host)C–H···C–Cl(guest)[b]	2.85 Å, 146°, <			x, y, z
(guest)C–H···C–C(host)[b]	2.74 Å, 133°, <			1/2–x, 1/2+y, 3/2–z
(host)C–H···H–C(guest)[b]		2.35 Å, 161°, <		x, y, z
(host)C–H···C–Cl(guest)[b]		2.61 Å, 154°, <<		1–x, y, 1–z
(host)C–H···Cl–C(guest)[b]		2.75 Å, 155°, <<		1–x, 1–y, z
(host)C–H···C–C(guest)[b]		2.84 Å, 134°, <		x, 1–y, 1–z
(guest)C–H···C–C(guest)[b]		2.45 Å, 154°, <<		x, 1–y, 1–z
(guest)C–Cl···C–Cl(guest)[b]		2.51(3) Å, 156(2)°, <<		1–x, y, 2–z
(guest)C–Cl···C–Cl(guest)[b]		2.65(3) Å, 141(2)°, <<		x, 1–y, 2–z
(guest)C–H···C–C(guest)[b]		2.52 Å, 144°, <<		1–x, y, 1–z
(host)C–H···Cl(guest)[b]		2.75 Å, 123°, <<		1–x, y, 1–z
(guest)C–H···H–C(guest)[b]			2.24 Å, 148°, <	3/2–x, y, 1–z

[a]< denotes contacts less than the sum of the van der Waals radii and << contacts less than this sum minus 0.2 Å
[b]Intermolecular interaction