Alternative separation strategy for *o-/p*-dichlorobenzene mixtures through supramolecular chemistry protocols

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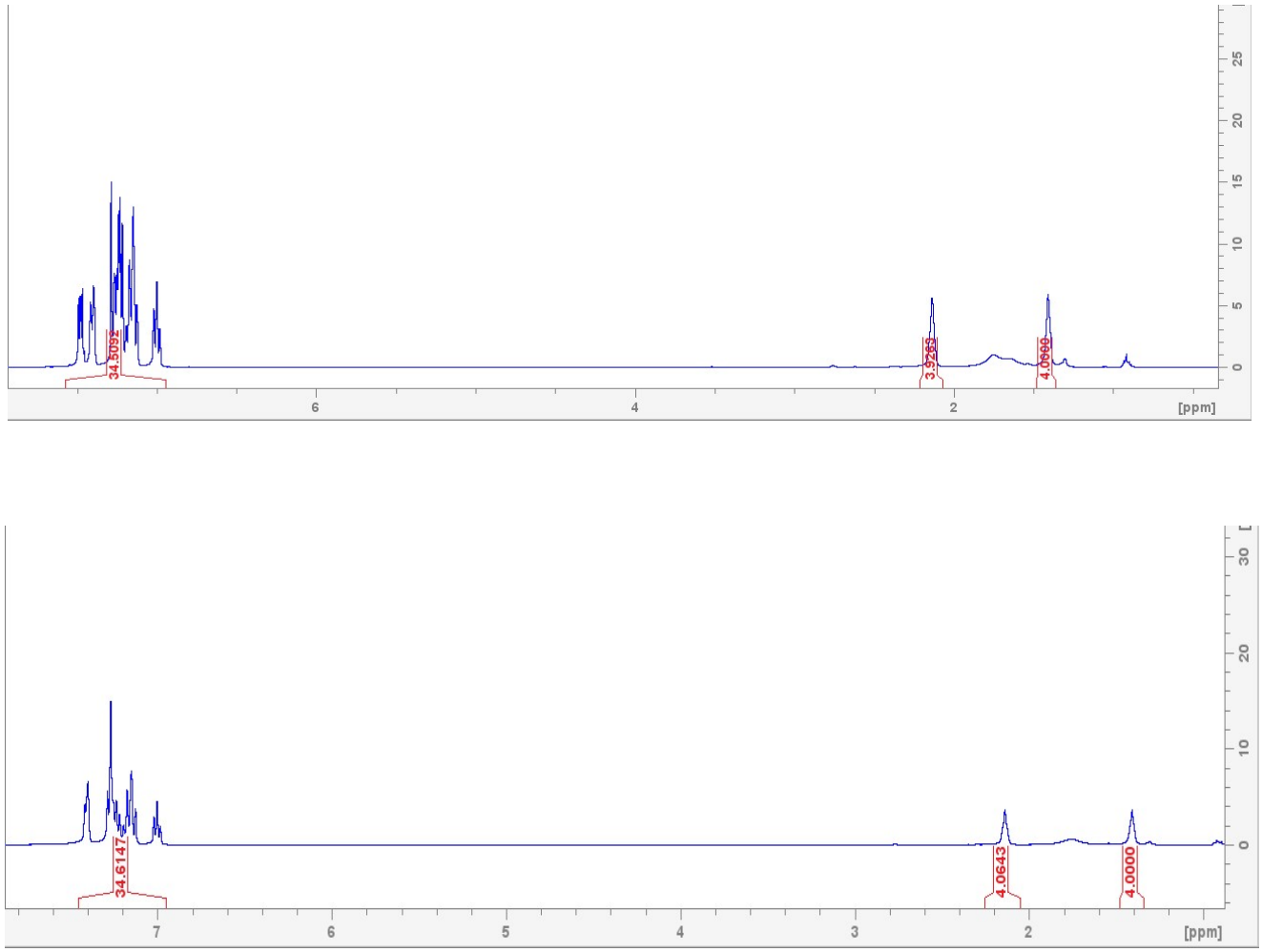

Figure S1 ^{1}H-NMR spectra of **H**·1.5(*o*DCB)(top) and **H**·1.5(*m*DCB) (bottom).

Table S1 Selectivity coefficients (K) and guest:guest ratios when **H** was crystallized from the various binary mixtures.

o/*m*DCB			*o*/*p*DCB			*m*/*p*DCB		
Molar concentration of *o*DCB	G:G	K_A	Molar concentration of *o*DCB	G:G	K_A	Molar concentration of *m*DCB	G:G	K_A
20	16.6	0.8	20	65.8	7.7	20	41.1	2.8
40	59.4	2.2	40	89.3	12.5	40	57.7	2.0
60	78.8	2.5	60	90.9	6.7	60	73.1	1.8
80	95.6	5.4	80	100	[a]	80	90.1	2.3

[a] K value is infinitive due to only *o*DCB being measured in the complex

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **H**·1.5(*o*DCB). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3469(2)	1541(1)	2571(1)	42(1)
O(2)	910(2)	9376(1)	2468(1)	39(1)
N(1)	4411(2)	3511(1)	3743(1)	33(1)
N(2)	970(2)	6829(1)	1619(1)	35(1)
C(1)	4738(2)	2479(1)	3772(1)	26(1)
C(2)	3661(3)	3956(1)	3023(1)	41(1)
C(3)	3027(3)	4990(1)	3110(1)	38(1)
C(4)	2349(3)	5449(1)	2337(1)	40(1)
C(5)	1690(3)	6485(1)	2373(1)	40(1)
C(6)	514(2)	7851(1)	1502(1)	29(1)
C(11)	3185(2)	2169(1)	3907(1)	27(1)
C(12)	2654(2)	1728(1)	3323(1)	32(1)
C(13)	1238(2)	1436(2)	3458(1)	40(1)
C(14)	339(2)	1590(2)	4193(2)	44(1)
C(15)	839(2)	2029(2)	4792(1)	43(1)
C(16)	2243(2)	2316(2)	4647(1)	36(1)
C(21)	5653(2)	2081(1)	2991(1)	29(1)
C(22)	4982(2)	1674(1)	2439(1)	33(1)
C(23)	5803(3)	1356(2)	1702(1)	42(1)
C(24)	7322(3)	1451(2)	1517(1)	45(1)
C(25)	8028(3)	1851(2)	2059(1)	46(1)
C(26)	7198(2)	2162(2)	2784(1)	39(1)
C(31)	5656(2)	2088(1)	4503(1)	30(1)
C(32)	6085(2)	2639(2)	5036(1)	40(1)
C(33)	6885(3)	2213(2)	5703(1)	53(1)
C(34)	7247(3)	1260(2)	5825(1)	55(1)
C(35)	6826(3)	707(2)	5294(2)	50(1)
C(36)	6031(2)	1120(2)	4639(1)	38(1)
C(41)	-626(2)	8269(1)	2206(1)	31(1)
C(42)	-390(2)	8988(1)	2632(1)	32(1)
C(43)	-1464(3)	9366(2)	3265(1)	45(1)
C(44)	-2798(3)	9021(2)	3473(2)	51(1)
C(45)	-3073(3)	8307(2)	3054(2)	51(1)
C(46)	-1994(3)	7939(2)	2426(1)	44(1)
C(51)	1966(2)	8264(1)	1428(1)	30(1)
C(52)	2105(2)	8965(1)	1909(1)	31(1)
C(53)	3460(3)	9307(2)	1862(1)	40(1)
C(54)	4701(3)	8958(2)	1309(2)	48(1)
C(55)	4596(3)	8267(2)	808(2)	53(1)
C(56)	3244(3)	7925(2)	869(2)	45(1)
C(61)	-286(2)	8094(1)	710(1)	31(1)
C(62)	-462(3)	7428(2)	204(1)	42(1)
C(63)	-1222(3)	7697(2)	-500(1)	48(1)
C(64)	-1804(3)	8622(2)	-698(1)	43(1)
C(65)	-1648(3)	9290(2)	-195(2)	48(1)
C(66)	-886(3)	9025(2)	504(1)	44(1)
Cl(71)	9291(1)	4004(1)	2011(1)	85(1)
Cl(72)	6598(1)	5827(1)	2067(1)	78(1)
C(71)	8561(3)	4512(2)	2919(2)	54(1)
C(72)	7396(3)	5319(2)	2938(2)	51(1)
C(73)	6856(3)	5713(2)	3678(2)	57(1)
C(74)	7456(4)	5311(2)	4389(2)	61(1)
C(75)	8598(4)	4508(2)	4362(2)	63(1)
C(76)	9153(3)	4114(2)	3629(2)	64(1)
Cl(81)	4774(4)	3555(2)	804(2)	103(1)
Cl(82)	1899(3)	4864(1)	52(1)	90(1)
C(81)	4988(10)	4575(4)	249(3)	74(2)
C(82)	3711(19)	5143(16)	-90(20)	77(3)
C(83)	3839(10)	5995(5)	-579(4)	78(2)
C(84)	5403(14)	6130(8)	-590(7)	101(3)
C(85)	6642(11)	5626(6)	-273(5)	95(2)
C(86)	6400(20)	4819(17)	150(20)	86(3)

Table S3 Bond lengths [Å] and angles [°] for **H**·1.5(*o*DCB)

O(1)-C(12)	1.376(2)
O(1)-C(22)	1.381(2)
O(2)-C(42)	1.379(2)
O(2)-C(52)	1.384(2)
N(1)-C(2)	1.468(3)
N(1)-C(1)	1.479(2)
N(1)-H(1)	0.89(3)
N(2)-C(5)	1.470(3)
N(2)-C(6)	1.471(2)
N(2)-H(2)	0.87(4)
C(1)-C(11)	1.523(2)
C(1)-C(21)	1.525(2)
C(1)-C(31)	1.538(2)
C(2)-C(3)	1.514(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.521(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.510(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(41)	1.520(3)
C(6)-C(51)	1.522(3)
C(6)-C(61)	1.541(3)
C(11)-C(12)	1.383(3)
C(11)-C(16)	1.398(3)
C(12)-C(13)	1.396(3)
C(13)-C(14)	1.376(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.383(3)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(21)-C(22)	1.382(3)
C(21)-C(26)	1.395(3)
C(22)-C(23)	1.401(3)
C(23)-C(24)	1.374(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.383(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.383(3)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(31)-C(32)	1.380(3)
C(31)-C(36)	1.395(3)
C(32)-C(33)	1.409(3)
C(32)-H(32)	0.9500
C(33)-C(34)	1.370(4)
C(33)-H(33)	0.9500
C(34)-C(35)	1.377(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.387(3)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(41)-C(42)	1.379(3)
C(41)-C(46)	1.395(3)
C(42)-C(43)	1.391(3)
C(43)-C(44)	1.378(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.380(4)
C(44)-H(44)	0.9500

C(45)-C(46)	1.382(3)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(51)-C(52)	1.384(3)
C(51)-C(56)	1.399(3)
C(52)-C(53)	1.387(3)
C(53)-C(54)	1.376(3)
C(53)-H(53)	0.9500
C(54)-C(55)	1.385(4)
C(54)-H(54)	0.9500
C(55)-C(56)	1.382(3)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(61)-C(62)	1.381(3)
C(61)-C(66)	1.386(3)
C(62)-C(63)	1.399(3)
C(62)-H(62)	0.9500
C(63)-C(64)	1.372(4)
C(63)-H(63)	0.9500
C(64)-C(65)	1.374(3)
C(64)-H(64)	0.9500
C(65)-C(66)	1.391(3)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500
Cl(71)-C(71)	1.723(3)
Cl(72)-C(72)	1.721(3)
C(71)-C(76)	1.376(4)
C(71)-C(72)	1.391(4)
C(72)-C(73)	1.383(4)
C(73)-C(74)	1.382(4)
C(73)-H(73)	0.9500
C(74)-C(75)	1.377(4)
C(74)-H(74)	0.9500
C(75)-C(76)	1.376(4)
C(75)-H(75)	0.9500
C(76)-H(76)	0.9500
Cl(81)-C(81)	1.728(6)
Cl(82)-C(82)	1.720(13)
C(81)-C(86)	1.359(14)
C(81)-C(82)	1.394(13)
C(82)-C(83)	1.455(13)
C(83)-C(84)	1.435(12)
C(83)-H(83)	0.9500
C(84)-C(85)	1.321(12)
C(84)-H(84)	0.9500
C(85)-C(86)	1.368(13)
C(85)-H(85)	0.9500
C(86)-H(86)	0.9500
C(12)-O(1)-C(22)	118.19(15)
C(42)-O(2)-C(52)	118.41(15)
C(2)-N(1)-C(1)	113.82(15)
C(2)-N(1)-H(1)	107.9(16)
C(1)-N(1)-H(1)	106.8(16)
C(5)-N(2)-C(6)	115.19(16)
C(5)-N(2)-H(2)	111(3)
C(6)-N(2)-H(2)	109(3)
N(1)-C(1)-C(11)	108.09(14)
N(1)-C(1)-C(21)	112.72(15)
C(11)-C(1)-C(21)	109.32(15)
N(1)-C(1)-C(31)	109.43(15)
C(11)-C(1)-C(31)	107.87(14)
C(21)-C(1)-C(31)	109.28(14)
N(1)-C(2)-C(3)	111.79(17)
N(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2A)	109.3
N(1)-C(2)-H(2B)	109.3
C(3)-C(2)-H(2B)	109.3

H(2A)-C(2)-H(2B)	107.9
C(2)-C(3)-C(4)	110.95(17)
C(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3B)	109.4
C(4)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
C(5)-C(4)-C(3)	114.37(18)
C(5)-C(4)-H(4A)	108.7
C(3)-C(4)-H(4A)	108.7
C(5)-C(4)-H(4B)	108.7
C(3)-C(4)-H(4B)	108.7
H(4A)-C(4)-H(4B)	107.6
N(2)-C(5)-C(4)	109.05(17)
N(2)-C(5)-H(5A)	109.9
C(4)-C(5)-H(5A)	109.9
N(2)-C(5)-H(5B)	109.9
C(4)-C(5)-H(5B)	109.9
H(5A)-C(5)-H(5B)	108.3
N(2)-C(6)-C(41)	111.54(15)
N(2)-C(6)-C(51)	109.16(15)
C(41)-C(6)-C(51)	109.69(15)
N(2)-C(6)-C(61)	108.71(15)
C(41)-C(6)-C(61)	108.33(15)
C(51)-C(6)-C(61)	109.38(15)
C(12)-C(11)-C(16)	117.36(17)
C(12)-C(11)-C(1)	122.43(16)
C(16)-C(11)-C(1)	120.20(16)
O(1)-C(12)-C(11)	123.10(17)
O(1)-C(12)-C(13)	114.97(18)
C(11)-C(12)-C(13)	121.93(18)
C(14)-C(13)-C(12)	119.3(2)
C(14)-C(13)-H(13)	120.4
C(12)-C(13)-H(13)	120.4
C(13)-C(14)-C(15)	120.2(2)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	119.8(2)
C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1
C(15)-C(16)-C(11)	121.4(2)
C(15)-C(16)-H(16)	119.3
C(11)-C(16)-H(16)	119.3
C(22)-C(21)-C(26)	117.02(18)
C(22)-C(21)-C(1)	122.25(16)
C(26)-C(21)-C(1)	120.64(17)
O(1)-C(22)-C(21)	123.12(17)
O(1)-C(22)-C(23)	114.87(18)
C(21)-C(22)-C(23)	122.01(19)
C(24)-C(23)-C(22)	119.3(2)
C(24)-C(23)-H(23)	120.3
C(22)-C(23)-H(23)	120.3
C(23)-C(24)-C(25)	120.0(2)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
C(26)-C(25)-C(24)	119.9(2)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.1
C(25)-C(26)-C(21)	121.8(2)
C(25)-C(26)-H(26)	119.1
C(21)-C(26)-H(26)	119.1
C(32)-C(31)-C(36)	118.84(19)
C(32)-C(31)-C(1)	123.75(18)
C(36)-C(31)-C(1)	117.38(17)
C(31)-C(32)-C(33)	119.4(2)
C(31)-C(32)-H(32)	120.3
C(33)-C(32)-H(32)	120.3

C(34)-C(33)-C(32)	121.0(2)
C(34)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	119.9(2)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	119.6(2)
C(34)-C(35)-H(35)	120.2
C(36)-C(35)-H(35)	120.2
C(35)-C(36)-C(31)	121.3(2)
C(35)-C(36)-H(36)	119.3
C(31)-C(36)-H(36)	119.3
C(42)-C(41)-C(46)	117.72(19)
C(42)-C(41)-C(6)	122.67(17)
C(46)-C(41)-C(6)	119.58(18)
O(2)-C(42)-C(41)	123.09(17)
O(2)-C(42)-C(43)	115.45(18)
C(41)-C(42)-C(43)	121.46(19)
C(44)-C(43)-C(42)	119.5(2)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(43)-C(44)-C(45)	120.4(2)
C(43)-C(44)-H(44)	119.8
C(45)-C(44)-H(44)	119.8
C(44)-C(45)-C(46)	119.4(2)
C(44)-C(45)-H(45)	120.3
C(46)-C(45)-H(45)	120.3
C(45)-C(46)-C(41)	121.6(2)
C(45)-C(46)-H(46)	119.2
C(41)-C(46)-H(46)	119.2
C(52)-C(51)-C(56)	117.13(19)
C(52)-C(51)-C(6)	122.62(17)
C(56)-C(51)-C(6)	120.24(18)
O(2)-C(52)-C(51)	122.73(17)
O(2)-C(52)-C(53)	115.10(18)
C(51)-C(52)-C(53)	122.17(19)
C(54)-C(53)-C(52)	119.4(2)
C(54)-C(53)-H(53)	120.3
C(52)-C(53)-H(53)	120.3
C(53)-C(54)-C(55)	120.1(2)
C(53)-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9
C(56)-C(55)-C(54)	119.8(2)
C(56)-C(55)-H(55)	120.1
C(54)-C(55)-H(55)	120.1
C(55)-C(56)-C(51)	121.4(2)
C(55)-C(56)-H(56)	119.3
C(51)-C(56)-H(56)	119.3
C(62)-C(61)-C(66)	118.35(19)
C(62)-C(61)-C(6)	123.19(18)
C(66)-C(61)-C(6)	118.44(17)
C(61)-C(62)-C(63)	120.2(2)
C(61)-C(62)-H(62)	119.9
C(63)-C(62)-H(62)	119.9
C(64)-C(63)-C(62)	120.7(2)
C(64)-C(63)-H(63)	119.6
C(62)-C(63)-H(63)	119.6
C(63)-C(64)-C(65)	119.6(2)
C(63)-C(64)-H(64)	120.2
C(65)-C(64)-H(64)	120.2
C(64)-C(65)-C(66)	119.8(2)
C(64)-C(65)-H(65)	120.1
C(66)-C(65)-H(65)	120.1
C(61)-C(66)-C(65)	121.3(2)
C(61)-C(66)-H(66)	119.3
C(65)-C(66)-H(66)	119.3
C(76)-C(71)-C(72)	120.2(2)

C(76)-C(71)-Cl(71)	119.1(2)
C(72)-C(71)-Cl(71)	120.7(2)
C(73)-C(72)-C(71)	118.9(3)
C(73)-C(72)-Cl(72)	119.4(2)
C(71)-C(72)-Cl(72)	121.7(2)
C(74)-C(73)-C(72)	120.7(3)
C(74)-C(73)-H(73)	119.6
C(72)-C(73)-H(73)	119.6
C(75)-C(74)-C(73)	119.7(3)
C(75)-C(74)-H(74)	120.2
C(73)-C(74)-H(74)	120.2
C(76)-C(75)-C(74)	120.1(3)
C(76)-C(75)-H(75)	119.9
C(74)-C(75)-H(75)	119.9
C(75)-C(76)-C(71)	120.3(3)
C(75)-C(76)-H(76)	119.8
C(71)-C(76)-H(76)	119.8
C(86)-C(81)-C(82)	120.6(10)
C(86)-C(81)-Cl(81)	119.7(7)
C(82)-C(81)-Cl(81)	119.8(7)
C(81)-C(82)-C(83)	122.0(10)
C(81)-C(82)-Cl(82)	121.6(8)
C(83)-C(82)-Cl(82)	116.5(9)
C(84)-C(83)-C(82)	108.1(9)
C(84)-C(83)-H(83)	125.9
C(82)-C(83)-H(83)	125.9
C(85)-C(84)-C(83)	132.2(11)
C(85)-C(84)-H(84)	113.9
C(83)-C(84)-H(84)	113.9
C(84)-C(85)-C(86)	114.4(12)
C(84)-C(85)-H(85)	122.8
C(86)-C(85)-H(85)	122.8
C(81)-C(86)-C(85)	122.6(13)
C(81)-C(86)-H(86)	118.7
C(85)-C(86)-H(86)	118.7

Symmetry transformations used to generate equivalent atoms:

Table S4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **H**·1.5(*o*DCB). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}
O(1)	36(1)	60(1)	35(1)	-15(1)
O(2)	39(1)	44(1)	36(1)	-12(1)
N(1)	41(1)	27(1)	31(1)	1(1)
N(2)	46(1)	26(1)	34(1)	1(1)
C(1)	26(1)	26(1)	25(1)	2(1)
C(2)	60(1)	28(1)	32(1)	2(1)
C(3)	51(1)	27(1)	34(1)	3(1)
C(4)	56(1)	27(1)	37(1)	2(1)
C(5)	57(1)	28(1)	34(1)	2(1)
C(6)	34(1)	24(1)	27(1)	1(1)
C(11)	24(1)	27(1)	29(1)	1(1)
C(12)	29(1)	34(1)	32(1)	-1(1)
C(13)	31(1)	44(1)	47(1)	-2(1)
C(14)	28(1)	51(1)	54(1)	5(1)
C(15)	29(1)	58(1)	39(1)	1(1)
C(16)	30(1)	45(1)	31(1)	-1(1)
C(21)	29(1)	30(1)	27(1)	2(1)
C(22)	32(1)	36(1)	30(1)	-1(1)
C(23)	47(1)	45(1)	34(1)	-9(1)
C(24)	47(1)	48(1)	34(1)	-2(1)
C(25)	35(1)	58(1)	41(1)	1(1)

C(26)	32(1)	51(1)	34(1)	0(1)
C(31)	24(1)	38(1)	26(1)	3(1)
C(32)	32(1)	56(1)	32(1)	-7(1)
C(33)	36(1)	93(2)	30(1)	-12(1)
C(34)	32(1)	94(2)	31(1)	15(1)
C(35)	33(1)	62(2)	46(1)	23(1)
C(36)	31(1)	41(1)	41(1)	9(1)
C(41)	32(1)	33(1)	27(1)	4(1)
C(42)	33(1)	34(1)	27(1)	1(1)
C(43)	47(1)	48(1)	37(1)	-8(1)
C(44)	45(1)	57(1)	42(1)	1(1)
C(45)	40(1)	63(2)	49(1)	7(1)
C(46)	42(1)	47(1)	44(1)	-1(1)
C(51)	30(1)	30(1)	27(1)	1(1)
C(52)	30(1)	33(1)	28(1)	3(1)
C(53)	39(1)	46(1)	39(1)	4(1)
C(54)	33(1)	59(1)	54(1)	10(1)
C(55)	35(1)	63(2)	56(2)	-3(1)
C(56)	41(1)	45(1)	44(1)	-8(1)
C(61)	32(1)	34(1)	26(1)	0(1)
C(62)	50(1)	40(1)	38(1)	-7(1)
C(63)	51(1)	57(1)	37(1)	-15(1)
C(64)	36(1)	65(2)	28(1)	4(1)
C(65)	54(1)	46(1)	43(1)	9(1)
C(66)	56(1)	35(1)	42(1)	3(1)
Cl(71)	87(1)	93(1)	80(1)	-47(1)
Cl(72)	107(1)	75(1)	61(1)	0(1)
C(71)	54(1)	52(1)	61(2)	-20(1)
C(72)	60(2)	46(1)	52(1)	-8(1)
C(73)	64(2)	47(1)	58(2)	-13(1)
C(74)	72(2)	57(2)	52(2)	-14(1)
C(75)	70(2)	56(2)	63(2)	-3(1)
C(76)	58(2)	51(2)	78(2)	-12(1)
Cl(81)	182(3)	57(1)	48(1)	-2(1)
Cl(82)	115(2)	73(1)	82(1)	-10(1)
C(81)	130(5)	49(3)	34(2)	-9(2)
C(82)	114(6)	66(5)	48(5)	-18(4)
C(83)	111(5)	65(3)	61(3)	-38(3)
C(84)	143(6)	84(6)	69(6)	-22(5)
C(85)	121(6)	88(5)	66(4)	-20(4)
C(86)	122(6)	76(6)	54(6)	-23(5)

Table S5 Summary of interactions identified in **H**·1.5(*o*DCB)

Interaction type	**Bond length/ Å**	**Associated bond angle/ °**	**Symmetry code**
(host)C−H···π(guest)	2.71[a], 3.647 (3)[b]	161	1+X, Y, Z
(host)C−Cl···π(guest)	3.615 (3)[c], 5.122 (6)[b]	144.7 (3)	X, Y, Z
(host)C−H···N(host)	2.46[d], 2.808 (3)[e]	102	1−X, 1−Y, 1−Z
(host)C−H···N(host)	2.42[d], 2.779 (3)[e]	102	1−X, 1−Y, 1−Z
(host)C−H···O(host)	2.46[f], 3.389 (3)[g]	167	1−X, 1−Y, 1−Z

[a]H···π bond distance
[b]C···π bond distance
[c]Cl···π bond distance
[d]H···N bond distance
[e]C···N bond distance
[f]H···O bond distance
[g]C···O bond distance