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Separation of Lutidines by Enclathration

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Content

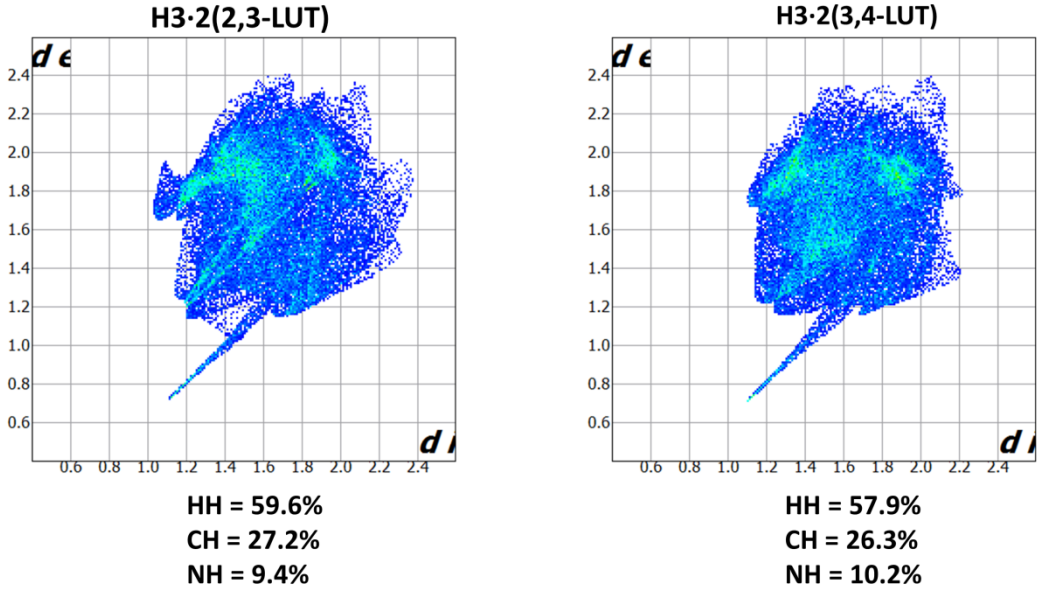

Figure S1 2D fingerprint plots generated from the Hirshfeld surface of the guest molecules in structures H3·2(2,3-LUT) and H3·2(3,4-LUT).

Table S1 ^{1}HNMR values for hosts and guest pairs

Experiment	Guest pair	H1.(2,3-LUT/ 3,4-LUT)	H2.(2,3-LUT/ 3,4-LUT)	H3.(2,3-LUT/ 3,4-LUT)
Solution concentration	$X_{2,3\text{-}LUT}$	0.5	0.5	0.5
	$X_{3,4\text{-}LUT}$	0.5	0.5	0.5
^{1}H NMR	$Z_{2,3\text{-}LUT}$	0.59	0.62	0.00
	$Z_{3,4\text{-}LUT}$	0.41	0.38	1.00
X-Ray	$Z_{2,3\text{-}LUI}$	0.63	0.69	0.00
	$Z_{3,4\text{-}LUT}$	0.37	0.31	1.00

Table S2 ^{1}H NMR values of additional Dutch resolution attempts carried out by the different combination of hosts (H1/H3 and H2/H3) with equimolar mixture of 2,3-LUT/3,4-LUT.

Name of Experiments	Solution concentration		^{1}H NMR		X-Ray		Comments
	$X_{2,3\text{-}LUT}$	$X_{3,4\text{-}LUT}$	$Z_{2,3\text{-}LUT}$	$Z_{3,4\text{-}LUT}$	$Z_{2,3\text{-}LUT}$	$Z_{3,4\text{-}LUT}$	
H1/H2. (2,3-LUT/ 3,4-LUT)	0.5	0.5	I = 0.64 II = 0.61	I = 0.36 II = 0.39	I = 0.60 II = *NA*	I = 0.40 II = *NA*	(i) I is similar to H1·2(2,3-LUT/3,4-LUT) and II is similar to H2·2(2,3-LUT/3,4-LUT) (ii) *NA* = tiny crystals, could not be charectarized by X-ray.
H1/H3. (2,3-LUT/ 3,4-LUT)	0.5	0.5	III = 0.65 IV = *NA*	III = 0.35 IV = *NA*	III = *Cell check IV = *Cell check	III = *cell check IV = *Cell check	(i) III is similar to H1·2(2,3-LUT/3,4-LUT) and IV is similar to H3·2,3-LUT (ii) *Cell parameters were confirmed by X-ray. (iii) *NA* = could not be characterized due to less quantity.
H2/H3. (2,3-LUT/ 3,4-LUT)	0.5	0.5	V= 0.60 VI = 0.07	V = 0.40 VI = 0.93	NIL*	NIL*	(i) V = Similar to H2·2(2,3-LUT/3,4-LUT) and VI = Similar to H3·3,4-LUT (ii) *No X-ray experiment was done in both the cases due to poor quality of the crystals and the NMR spectra were identical to H2·2(2,3-LUT/3,4-LUT) and H3·3,4-LUT, respectively.

Table S3 Details of Hydrogen bonds

Compound name	D-H···A	D···H/Å	H···A/Å	D···A/Å	∠D-H···A/°
H1.2,3-LUT	O14-H14...N24	0.96	1.77	2.811(1)	169(1)
H1.3,4-L UT	O14-H14...N24	0.97(2)	1.84(2)	2.791(2)	165(1)
H1.2,3-LUT/3,4-LUT	O13-H13...N23	0.952(1)	1.638(9)	2.568(6)	165 (2)
	O13-H13...N31	0.952(1)	2.048(1)	2.968(6)	161.9(17)
H2.2,3-LUT	O13-H13...N40	0.97	1.84	2.796(3)	169.3
	O13-H13...N32	0.97	1.84	2.769(5)	159.4
H2.3,4 -LUT	O14-H14...N62	0.95	1.78	2.721(2)	171.7
	O41-H41...O14	0.88	1.89	2.752(2)	163.6
H2.2,3-LUT/3,4-LUT	O14-H14...N32	1.04	1.71	2.718(4)	161.7
	O14-H14...N41	1.04	1.92	2.861(6)	148.7
H3.2,3-LUT	O14-H14...N20	0.97	1.85	2.788(1)	161.6
H3.3,4 -LUT	O14-H14...N20	0.97	1.82	2.792(1)	176.9

Figure S2 ^{1}H NMR results of additional Dutch resolution attempts carried out by the different combination of hosts (H1/H3 and H2/H3) with equimolar mixture of 2,3-LUT/3,4-LUT.