Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Separation of *p*-xylene from aromatic compounds through specific inclusion by acyclic host molecule

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General Information

All reagents and solvents were obtained from commercial suppliers and used without further purification. The synthesis of compound **1** was performed according to the previously reported literature.[1] ^{1}H and ^{13}C NMR spectra were performed on a Bruker AV400 spectrometer in $CDCl_3$ using tetramethylsilane as an internal standard at 298 K. X-ray crystal structure data were collected using a Bruker D8 VENTURE diffractometer with CuKα radiation.

(1) M. Tominaga, N. Kunitomi, K. Katagiri and T. Itoh, *Org. Lett.*, 2015, **17**, 786–789.

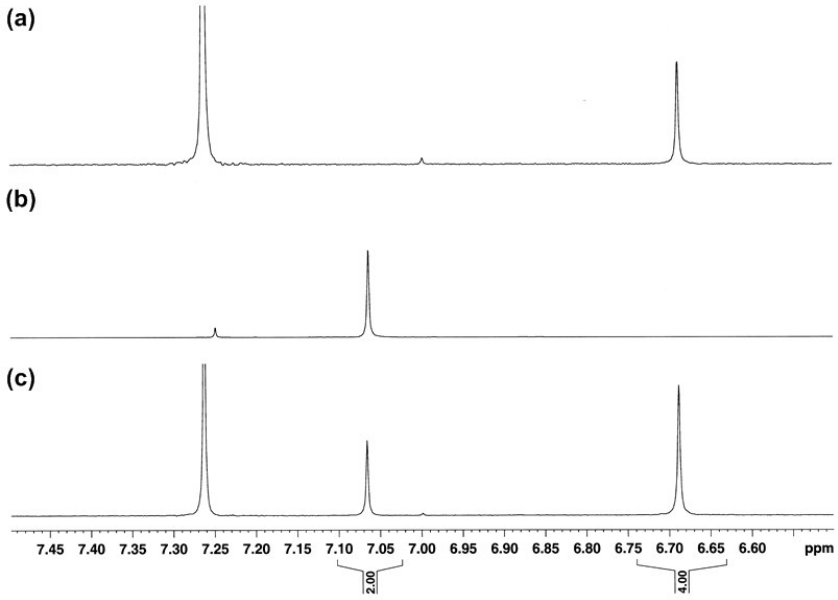

Fig. S1 Partial ^{1}H NMR spectra (400 MHz, $CDCl_3$); (a) crystal **1**, (b) *p*-xylene, and (c) crystal **1**·0.5*p*-xylene.

Single crystal X-ray diffraction experiment for 1·0.5*p*-xylene

The colourless plate crystal (0.200 × 0.120 × 0.050 mm^3), obtained from chloroform/*p*-xylene, was immersed in Paraton-N oil and placed in the N_2 cold stream at 100 K. The diffraction experiment was performed in a Bruker D8VENTURE system (PHOTON-100 CMOS detector, CuKα: λ = 1.54178 Å). Absorption correction was performed by an empirical method implemented in SADABS.[2] Structure solution and refinement were performed by using SHELXT-2014/5[3] and SHELXL-2016/6[4].

$C_{38}H_{39}Cl_2N_4O_6$, *M*r = 718.63; triclinic, space group *P*-1, *Z* = 2, D_{calc} = 1.424 g·cm^{-3}, *a* = 10.7680(5), *b* = 12.2601(6), *c* = 13.3043(6) Å, *α* = 97.054(2)°, *β* = 101.999(2)°, *γ* = 98.839(2)°, *V* = 1675.71(14) $Å^3$, 22483 observed and 5948 independent [$I > 2\sigma(I)$] reflections, 456 parameters, final R_1 = 0.0372, wR_2 = 0.0960, *S* = 1.033 [$I > 2\sigma(I)$]. CCDC 1842175

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 137, 23 and 43) with U_{iso} values constrained to 1.2/1.5 U_{eq} of their parent atoms.

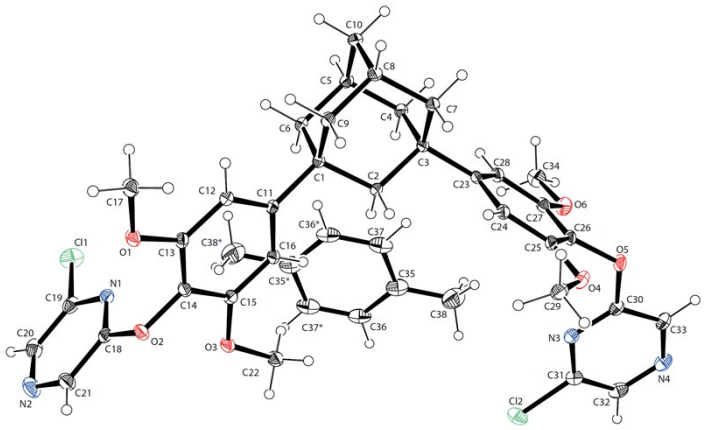

Fig. S2 Ortep drawing of crystal **1**·0.5*p*-xylene (50% probability).

Single crystal X-ray diffraction experiment for 1

The colourless prismatic crystal (0.100 × 0.100 × 0.040 mm^3), obtained from *o*-xylene/chloroform, was immersed in Paraton-N oil and placed in the N_2 cold stream at 100 K. The diffraction experiment was performed in a Bruker D8VENTURE system (PHOTON-100 CMOS detector, CuKα: λ = 1.54178 Å). Absorption correction was performed by an empirical method implemented in SADABS.[2] Structure solution and refinement were performed by using SHELXT-2014/5[3] and SHELXL-2016/6[4].

$C_{34}H_{34}Cl_2N_4O_6$, *M*r = 665.55; monoclinic, space group *C*2/*c*, *Z* = 4, D_{calc} = 1.417 g·cm^{-3}, *a* = 23.5127(11), *b* = 7.1104(3), *c* = 19.6874(9) Å, *β* = 108.636(2)°, *V* = 3118.9(2) Å^3, 20154 observed and 3022 independent [$I > 2\sigma(I)$] reflections, 211 parameters, final R_1 = 0.0307, wR_2 = 0.0867, *S* = 1.092 [$I > 2\sigma(I)$]. CCDC 1842176

All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were refined isotropically on the calculated positions using a riding model (AFIX 13, 137, 23 and 43) with U_{iso} values constrained to 1.2/1.5 U_{eq} of their parent atoms.

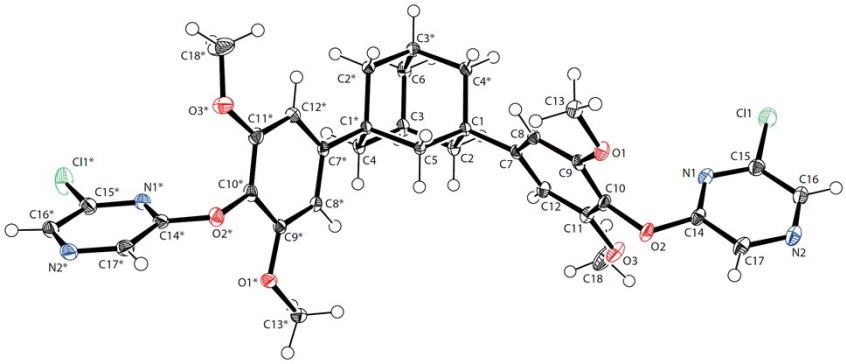

Fig. S3 Ortep drawing of crystal **1** (50% probability).

(2) G. M. Sheldrick, (1996). *SADABS*. University of Göttingen, Germany.

(3) G. M. Sheldrick, *Acta. Cryst.*, 2015, **A71**, 3–8.

(4) G. M. Sheldrick, *Acta. Cryst.*, 2015, **C71**, 3–8.

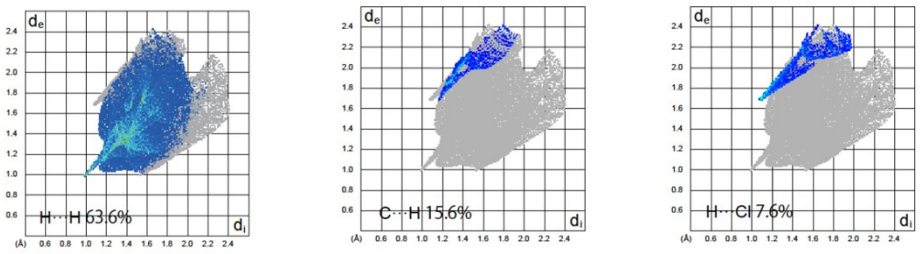

Fig. S4 The 2D fingerprint plots focusing on the specific interactions of *p*-xylene in crystal **1**·0.5*p*-xylene.

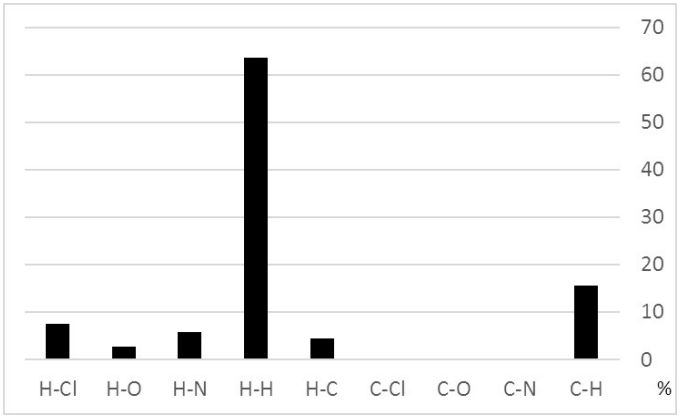

Fig. S5 Distribution of each interactions of *p*-xylene in crystal **1**·0.5*p*-xylene.

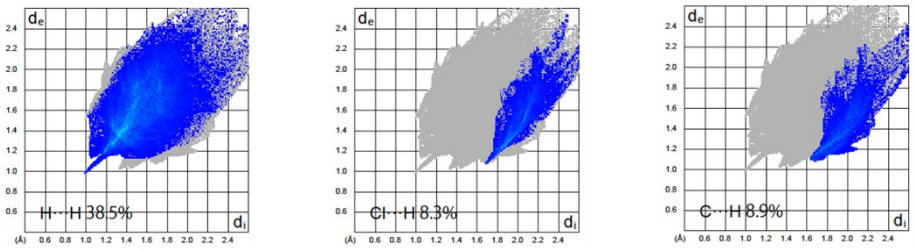

Fig. S6 The 2D fingerprint plots focusing on the specific interactions of **1** in crystal **1**·0.5*p*-xylene.

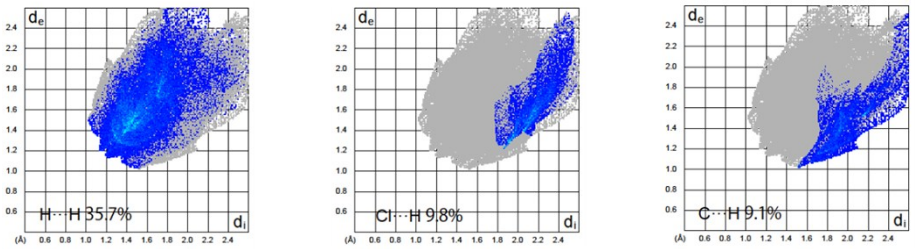

Fig. S7 The 2D fingerprint plots focusing on the specific interactions of **1** in crystal **1**.

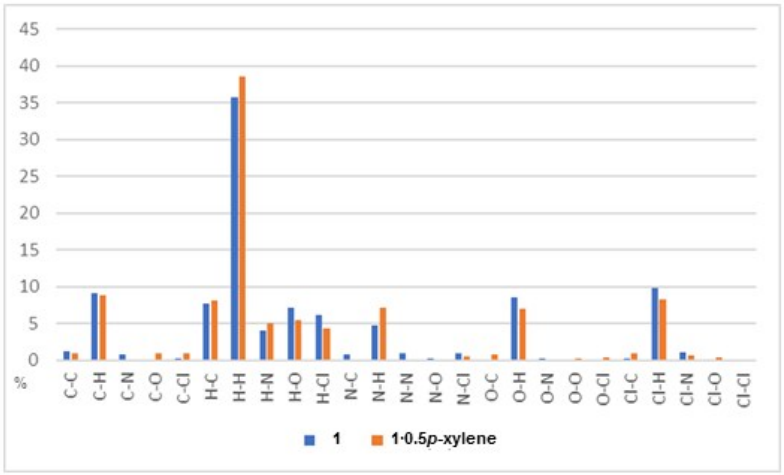

Fig. S8 Distribution of each interactions of **1** in crystal **1**·0.5*p*-xylene and **1** in crystal **1**.