Supplementary Information

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

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Table of Contents

General Information S2

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

Fig. S2 Additional crystal data for crystal 1·0.5p-xylene. S3

Fig. S3 Additional crystal data for crystal 1. S4

Fig. S4 The 2D fingerprint plots of specified interactions of p-xylene in 1·0.5p-xylene.

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

Fig. S6 The 2D fingerprint plots of specified interactions of 1 in crystal 1·0.5p-xylene.

Fig. S7 The 2D fingerprint plots of specified interactions of 1 in crystal 1.

Fig. S8 Distribution of each interactions of 1 in crystals 1·0.5p-xylene and 1. S6
**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 CuK\(\alpha\) radiation.


![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.](image-url)
Single crystal X-ray diffraction experiment for 1\(\cdot\)0.5\(p\)-xylene

The colourless plate crystal (0.200 \(\times\) 0.120 \(\times\) 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, CuK\(\alpha\): \(\lambda = 1.54178\) 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\(^4\).

\(\text{C}_{38}\text{H}_{39}\text{Cl}_2\text{N}_4\text{O}_6\), \(M_r = 718.63\); triclinic, space group \(P-1\), \(Z = 2\), \(D_{\text{calc}} = 1.424\) g\(\cdot\)cm\(^{-3}\), \(a = 10.7680(5)\) Å, \(b = 12.2601(6)\) Å, \(c = 13.3043(6)\) Å, \(\alpha = 97.054(2)^\circ\), \(\beta = 101.999(2)^\circ\), \(\gamma = 98.839(2)^\circ\), \(V = 1675.71(14)\) 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 \(U_{\text{iso}}\) values constrained to 1.2/1.5 \(U_{eq}\) of their parent atoms.

**Fig. S2** Ortep drawing of crystal 1\(\cdot\)0.5\(p\)-xylene (50% probability).
Single crystal X-ray diffraction experiment for 1

The colourless prismatic crystal (0.100 × 0.100 × 0.040 mm³), obtained from o-xylene/chloroform, was immersed in Paraton-N oil and placed in the N² 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. Structure solution and refinement were performed by using SHELXT-2014/5 and SHELXL-2016/6.

C₃₄H₃₄Cl₂N₄O₆, Mr = 665.55; monoclinic, space group C2/c, Z = 4, Dcalc = 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) Å³, 20154 observed and 3022 independent [I > 2σ(I)] reflections, 211 parameters, final R₁ = 0.0307, wR₂ = 0.0867, S = 1.092 [I > 2σ(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 Uiso values constrained to 1.2/1.5 Ueq of their parent atoms.

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

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

Fig. S5 Distribution of each interactions of $p$-xylene in crystal 1-$0.5p$-xylene.
Fig. S6 The 2D fingerprint plots focusing on the specific interactions of 1 in crystal 1·0.5p-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 1·0.5p-xylene and 1 in crystal 1.