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Supplementary Information

Hydrogen bonding vs halogen bonding: the solvent decides

Craig C. Robertson,[1] James S.Wright,[1] Elliot J. Carrington,[1,†] Robin N. Perutz*,[2] Christopher A. Hunter*,[3] and Lee Brammer*,[1]

[1] Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK
[2] Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK
[3] Department of Chemistry, Lensfield Road, University of Cambridge, Cambridge, CB2 1EW, UK

[†] Current address: Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK.

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1. General Experimental

Chemicals and Spectroscopic Grade Solvents were purchased from Alfa Aeasar, Apollo Scientific Ltd, Fisher Scientific UK Ltd., Fluorochem Ltd, Sigma–Aldrich Company Ltd. or VWR International Ltd and used without further purification.

^{1}H and ^{19}F NMR spectra were recorded on a Bruker Avance II 400 spectrometer at 400.1 MHz and 374.9 Hz respectively, using the deuterated solvent or a capillary insert with D_2O as the lock. In the assignment of ^{1}H NMR spectra, the chemical shift (δH) for each resonance is given in units of parts per million (ppm) relative to trimethylsilane (TMS) where δH TMS = 0.00 ppm.

In the assignment of ^{19}F NMR spectra, the chemical shift (δF) for each resonance is given in units of parts per million (ppm) relative to $CFCl_3$ where δF $CFCl_3$ = 0.00 ppm.

Analyses of NMR spectra were carried out using Topspin version 3.2 or iNMR version 5.2.1.

Measurement of mass of solids was carried out on a Precisa 125A balance.

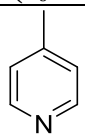
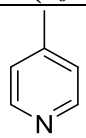
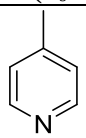
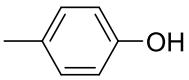
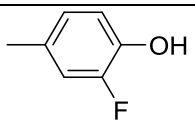
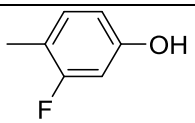
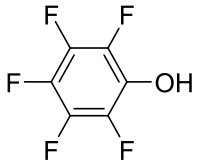
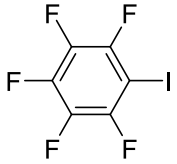
Measurement of volumes of liquids for the preparation of samples for NMR titrations was carried out using Eppendorf Multipette XStream electronic pipettors.

2. Procedure for NMR titrations

10 NMR Norell S-400 tubes, each with different concentrations of host and guest as measured with a programmed Multipette XStream were set up and submitted to BACS automated sample recording. The concentration of guest was chosen to obtain a binding isotherm of >50% saturation in each titration. The specific concentration of guest used in each experiment can be seen in the horizontal axis of the binding isotherm for each titration shown below. Titrations were repeated at least twice for reproducibility and estimation of errors. K_a data were obtained by fitting the experimental results to a binding isotherm using a macro-based Microsoft Excel fitting program written by Christopher A. Hunter (University of Cambridge).

3. Table of Association Constants

Table S1. Association constants (K_a) and errors*

Solvent	Toluene (α_s 1.0; β_s 2.1)	Chloroform (α_s 2.2; β_s 0.8)	Acetonitrile (α_s 1.8; β_s 5.1)
Guest / **Host**			
	**31±1**	**19±2**	**<1**
	**40±1**	**20±1**	**<1**
	**62±5**	**52±2**	**<1**
	**1300±50**	**850±60**	**19±1**
	**1±1**	**<1**	**<1**

*Errors determined by 2 × standard deviation of multiple repeat titrations

4. Spectra and binding isotherms of titrations

Titration of *p*-cresol with 4-picoline in Toluene

Host: *p*-cresol [18.4 mM]

Guest: 4-picoline

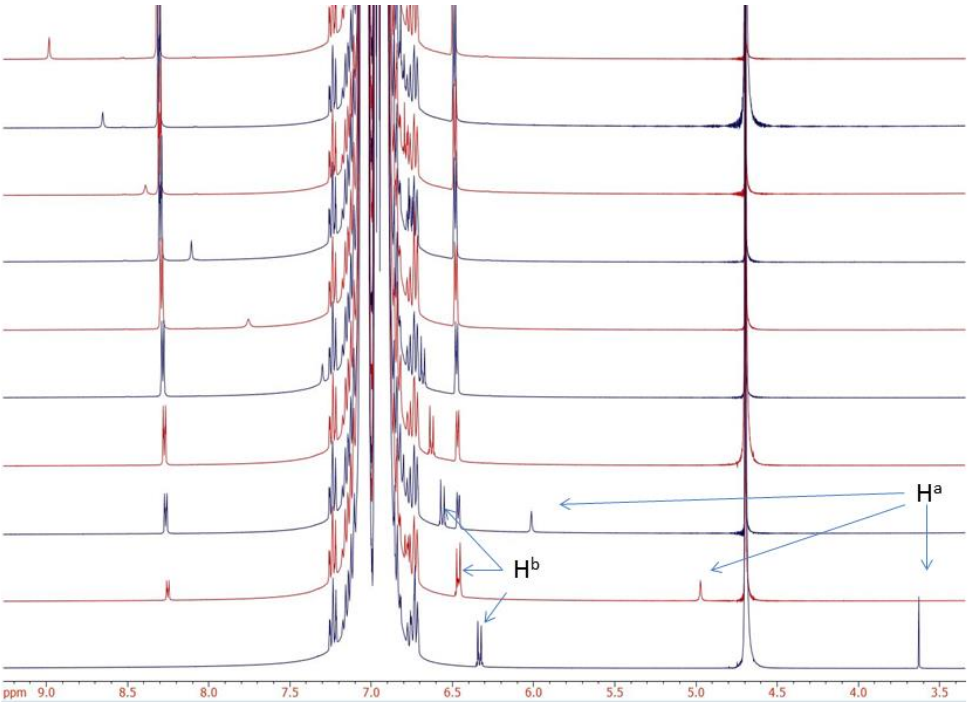


Figure S4.1: partial 400.2 MHz ^{1}H NMR spectra of titration in toluene with monitored signals labelled.

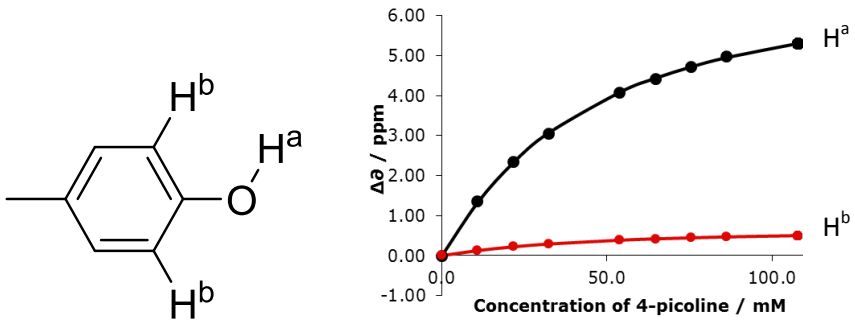


Figure S4.2: Binding isotherms for titration

K_a = 31±1 M^{-1} 74% bound

Titration of *p*-cresol with 4-picoline in chloroform

Host: *p*-cresol [11.5 mM]

Guest: 4-picoline

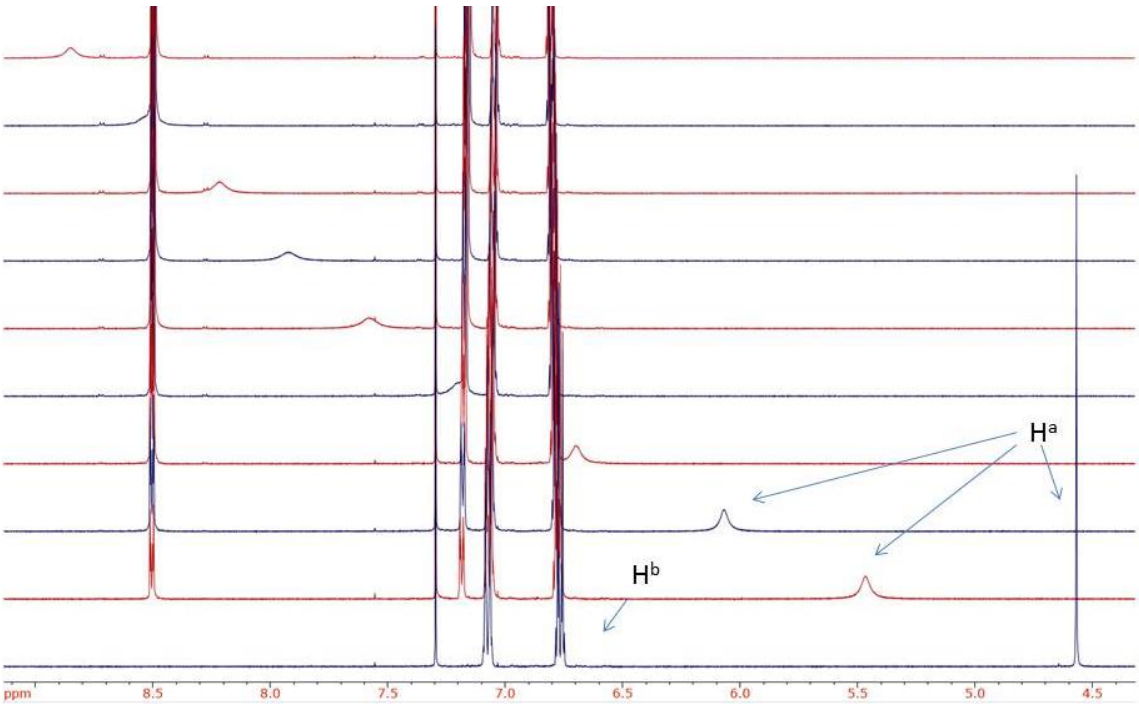


Figure S4.3: partial 400.2 MHz ^{1}H NMR spectra of titration in chloroform with monitored signals labelled.

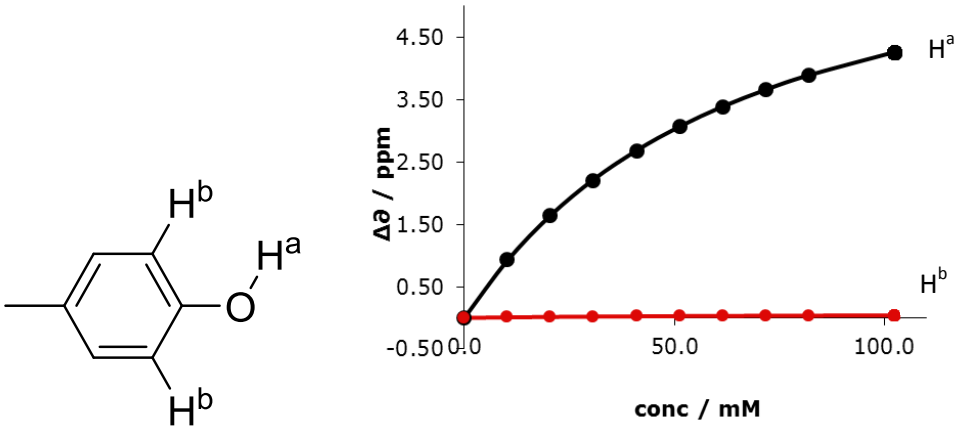


Figure S4.4: Binding isotherm for titration

K_a **= 19±2 M^{-1} 64% bound**

Titration of 2-fluoro-4-methylphenol with 4-picoline in toluene

Host: 2-fluoro-4-methylphenol [8 mM]

Guest: 4-picoline

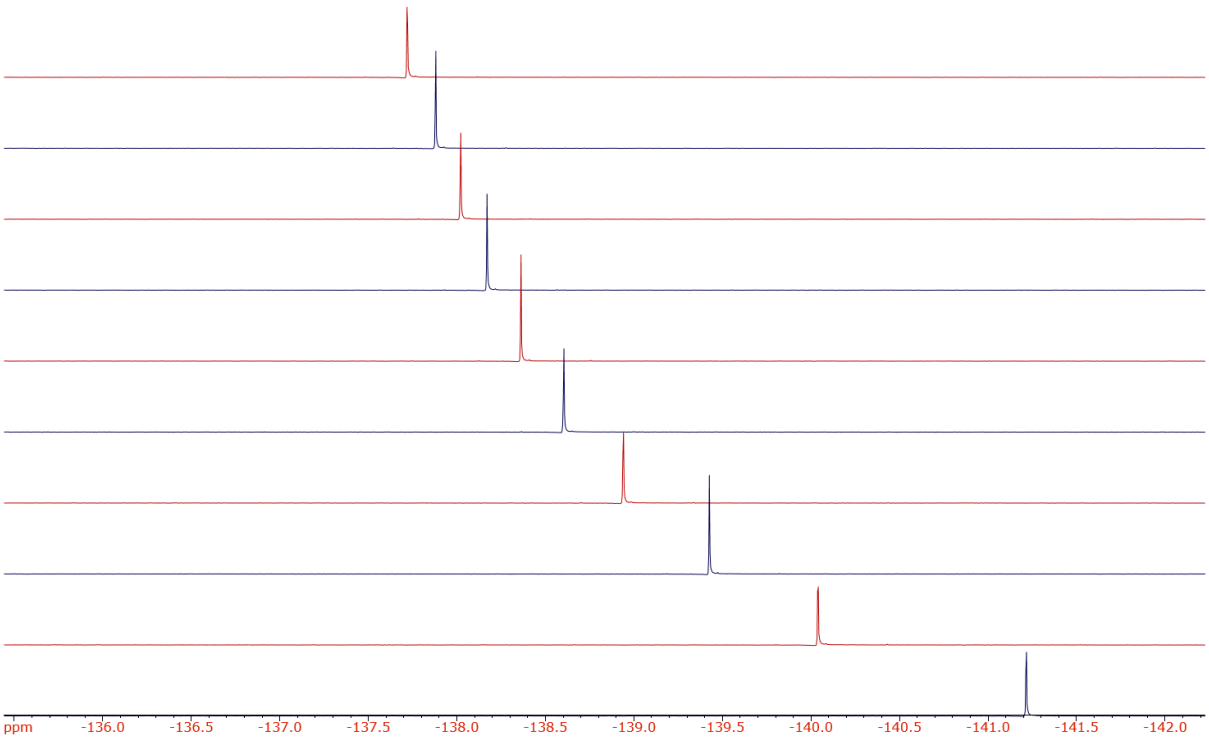


Figure S4.5: partial 376.5 MHz ^{19}F NMR spectra of titration in toluene

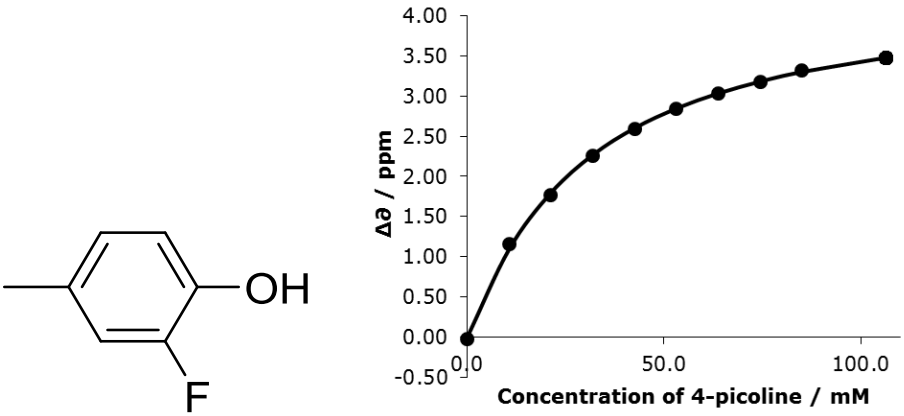


Figure S4.6: Binding isotherm for titration

K_a = 40±1 M^{-1} 80% bound

Titration of 2-fluoro-4-methylphenol with 4-picoline in chloroform

Host: 2-fluoro-4-methylphenol [14.0 mM]

Guest: 4-picoline

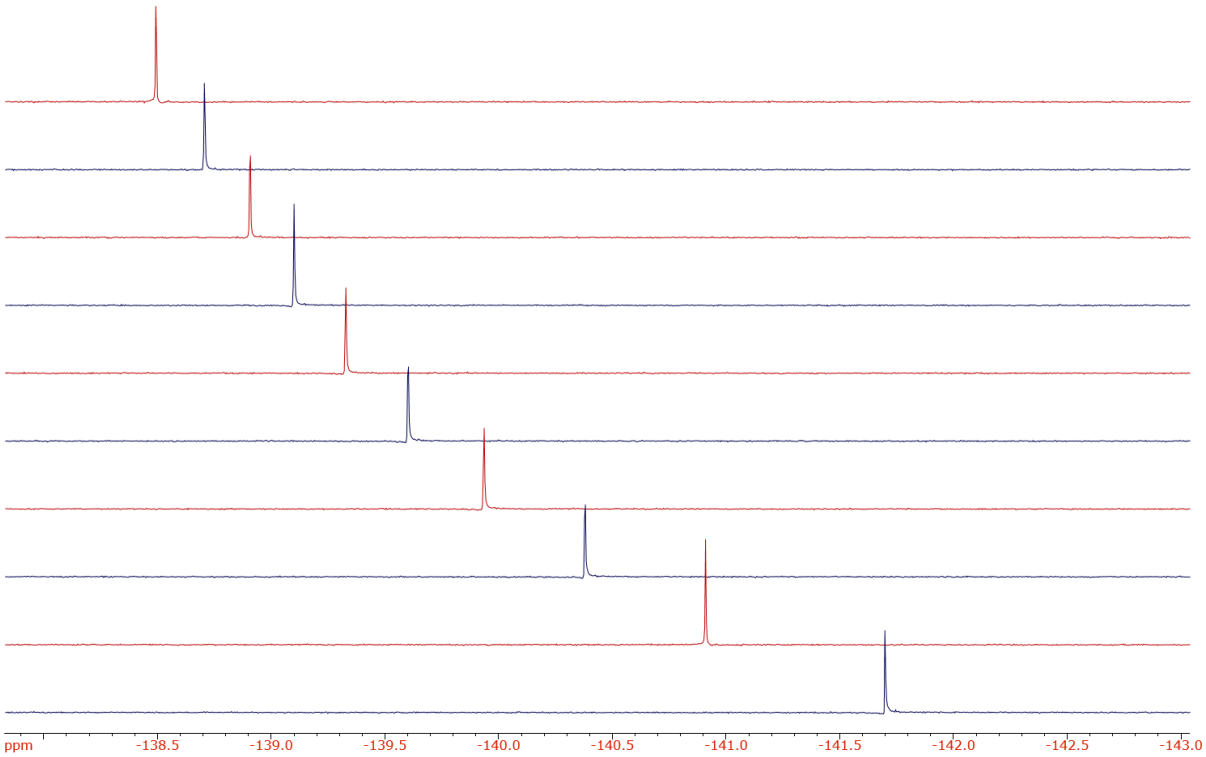


Figure S4.7: partial 376.5 MHz ^{19}F NMR spectra of titration in chloroform

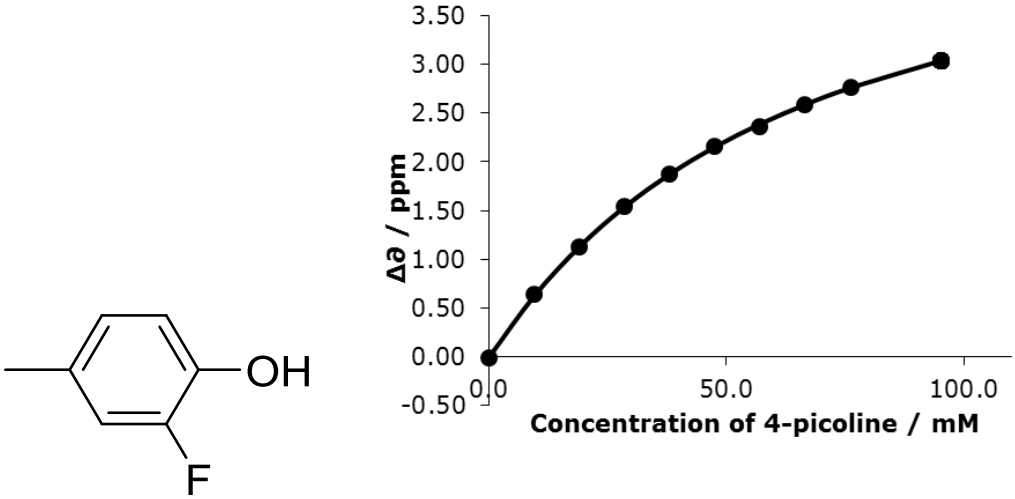


Figure S4.8: Binding isotherm for titration

K_a = 20±1 M^{-1} 62% bound

Titration of 3-fluoro-4-methylphenol with 4-picoline in toluene

Host: 3-fluoro-4-methylphenol [4.44 mM]

Guest:4-picoline

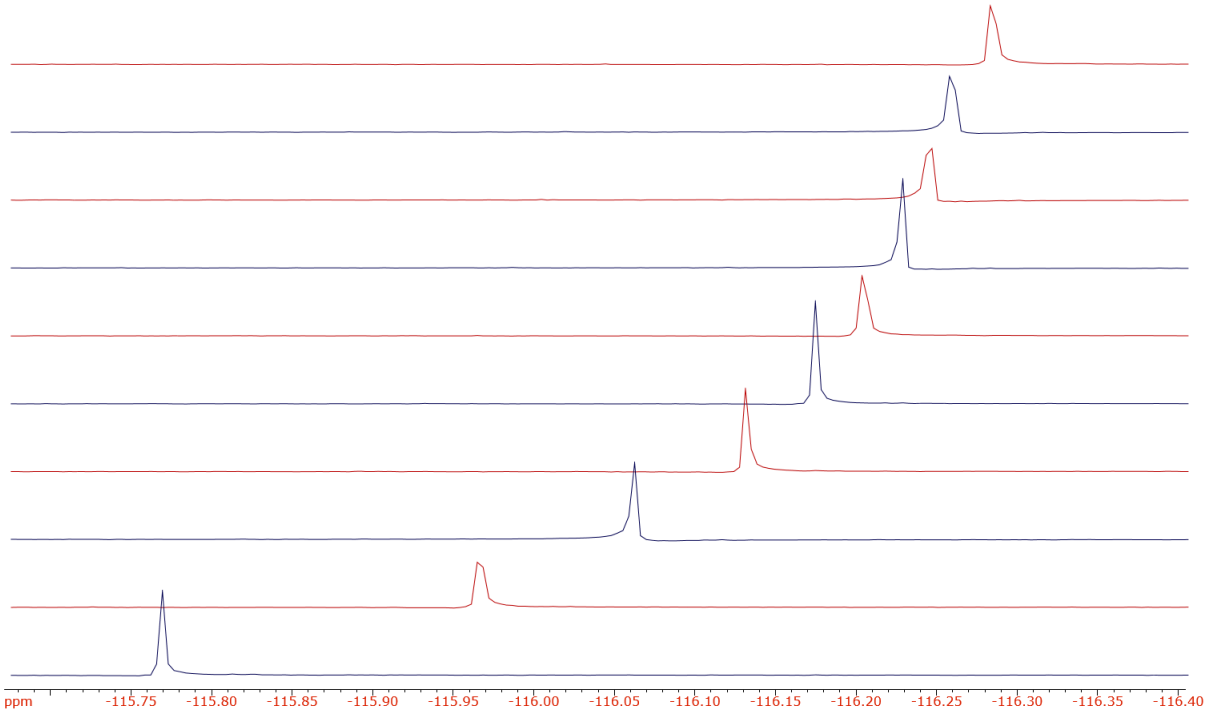


Figure S4.9: partial 376.5 MHz ^{19}F NMR spectra of titration in toluene

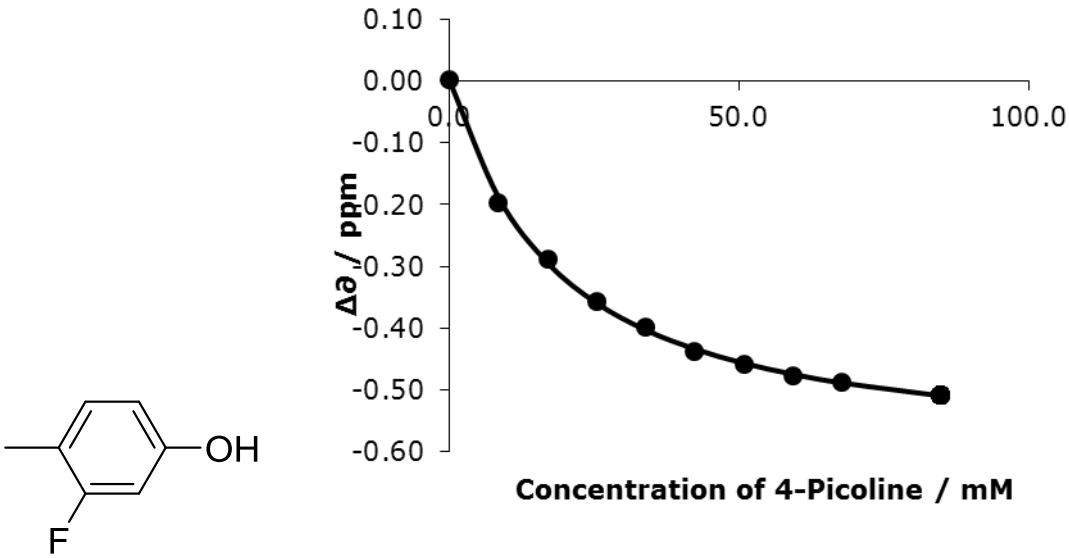


Figure S4.10: Binding isotherm for titration

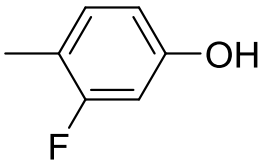
K_a = 62±5 M^{-1} 84% bound

Titration of 3-fluoro-4-methylphenol with 4-picoline in chloroform

Host: 3-fluoro-4-methylphenol [14.2 mM]

Guest: 4-picoline

Figure S4.11: partial 376.5 MHz ^{19}F NMR spectra of titration in chloroform



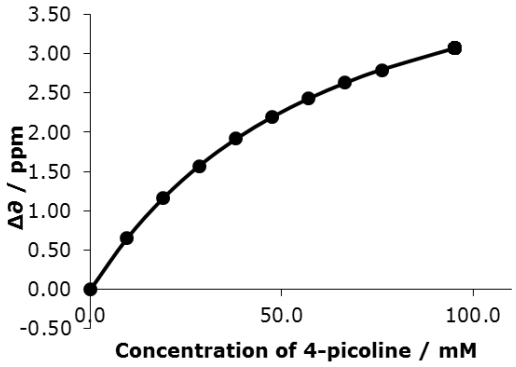


Figure S4.12: Binding isotherm for titration

K_a = 52±1 M^{-1} 78% bound

Titration of pentafluorophenol with 4-picoline in toluene

Host: pentafluorophenol [4 mM]

Guest: 4-picoline

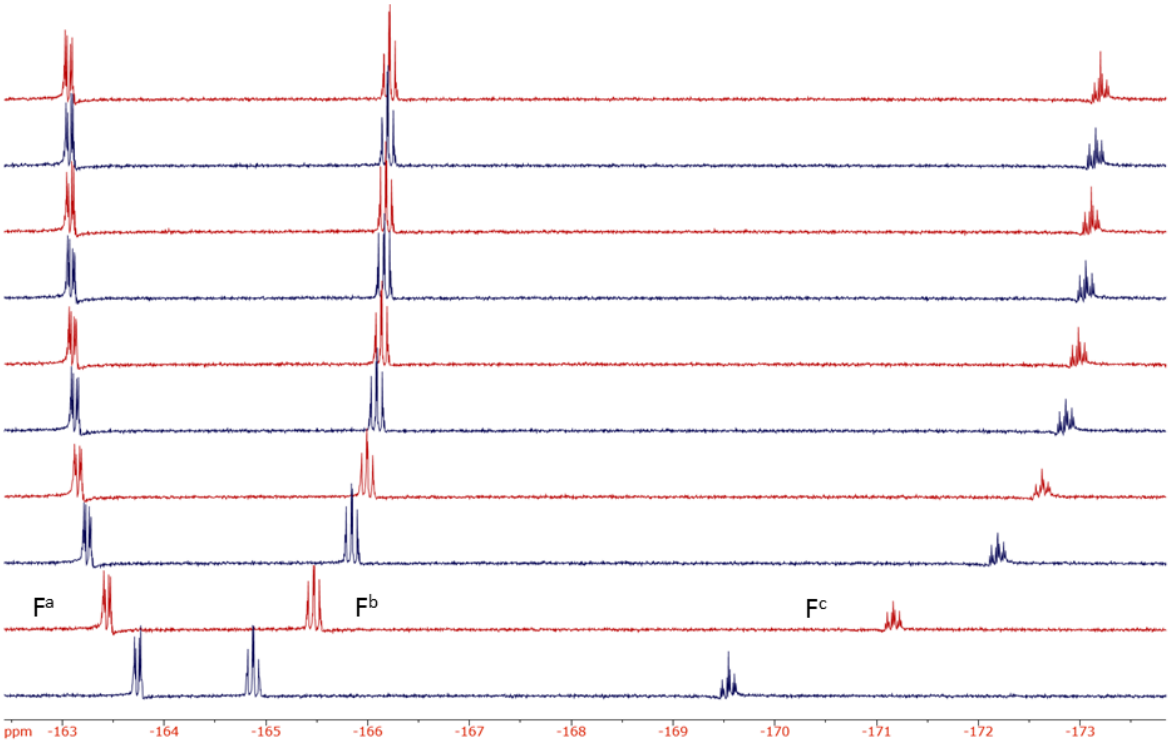


Figure S4.13: partial 376.5 MHz ^{19}F NMR spectra of titration in toluene

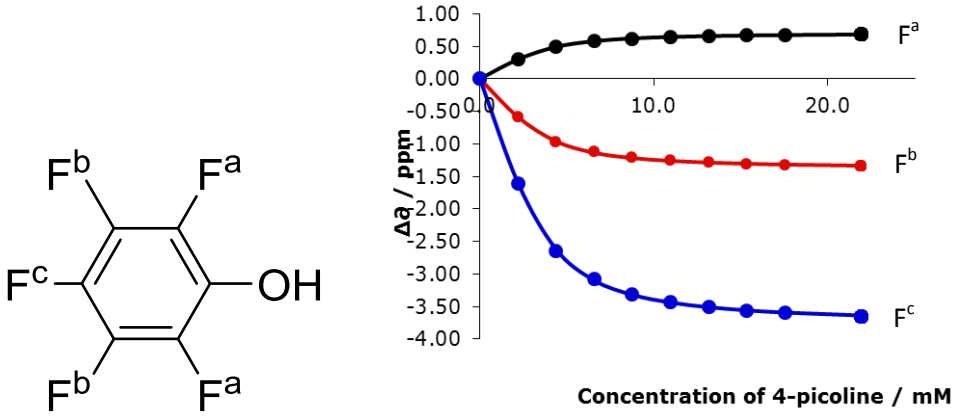


Figure S4.14: Binding isotherms for titration

K_a = 1300±50 M^{-1} 96% bound

Titration of pentafluorophenol with 4-picoline in chloroform

Host: pentafluorophenol [2 mM]

Guest: 4-picoline

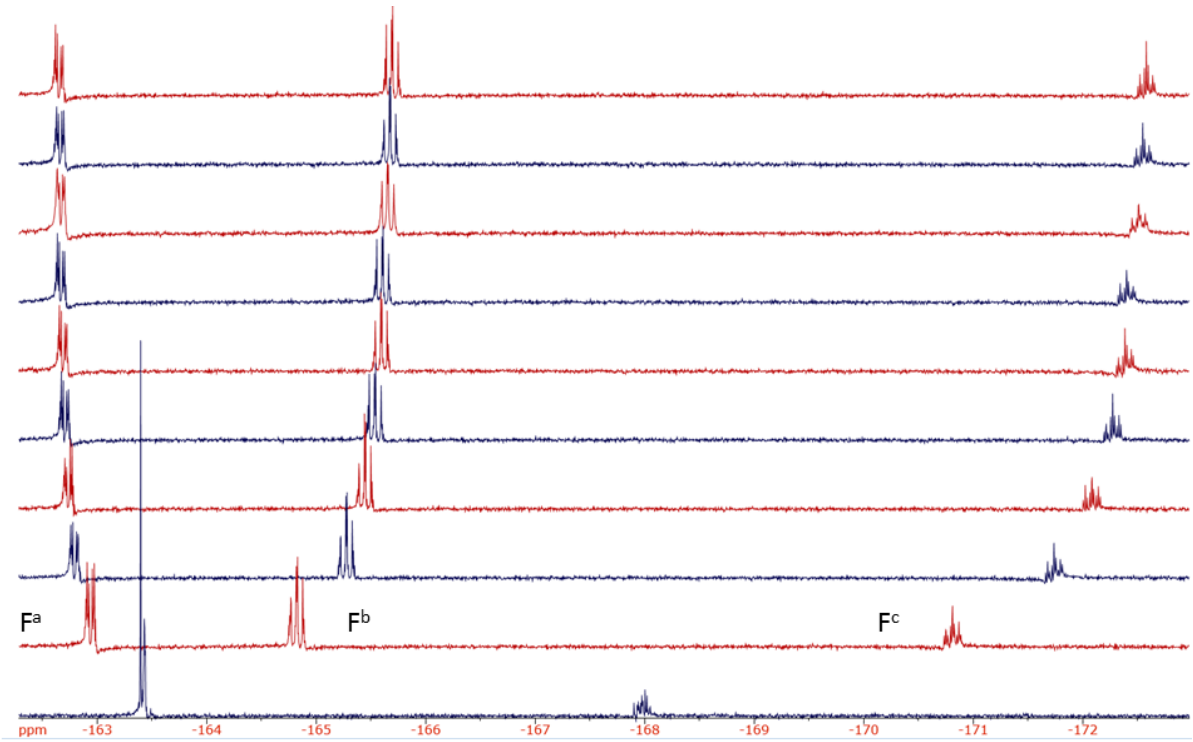


Figure S4.15: partial 376.5 MHz ^{19}F NMR spectra of titration in chloroform

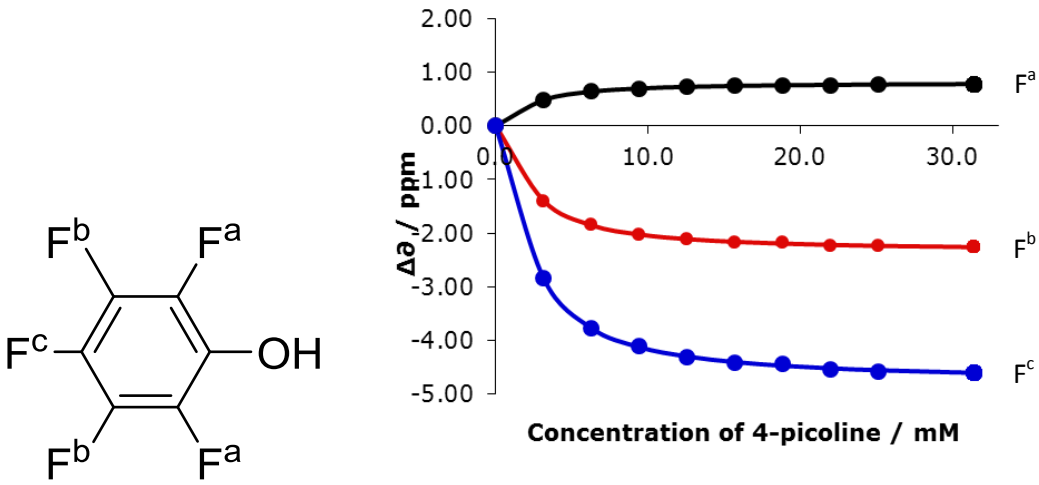


Figure S4.16: Binding isotherms for titration

K_a = **850±60 M^{-1} 96% bound**

Titration of pentafluorophenol with 4-picoline in acetonitrile

Host: pentafluorophenol [12 mM]

Guest: 4-picoline

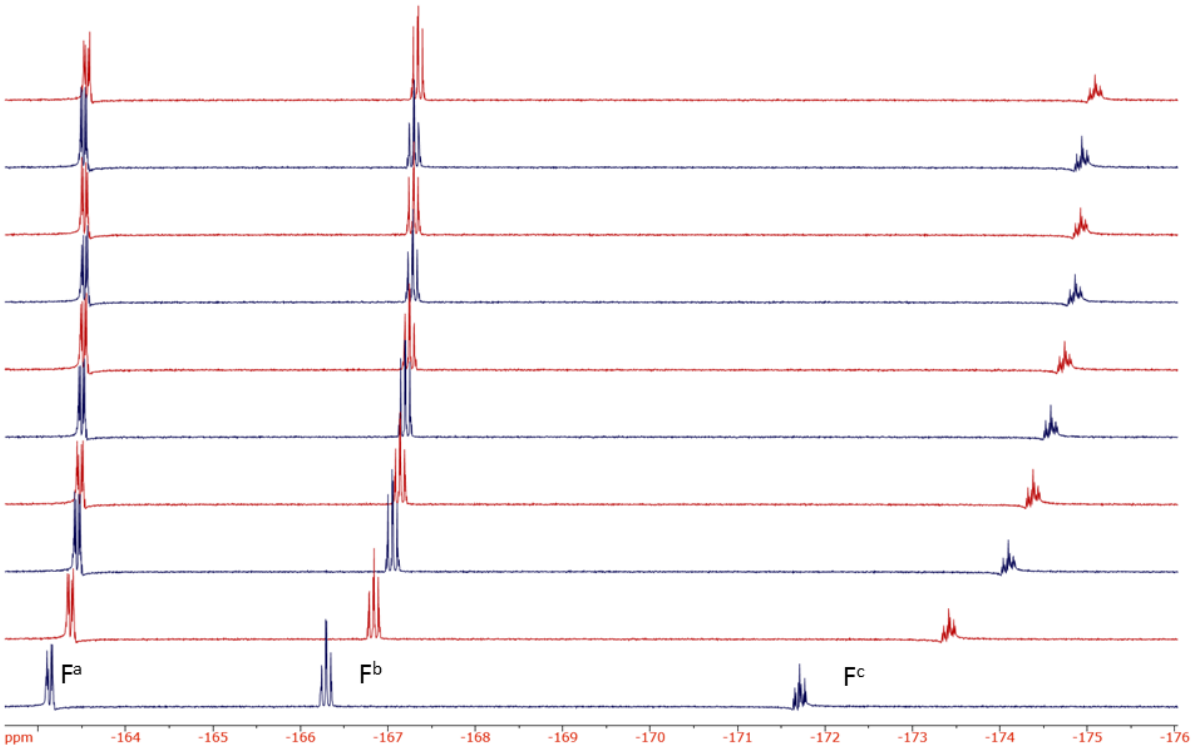


Figure S4.17: partial 376.5 MHz ^{19}F NMR spectra of titration in acetonitrile

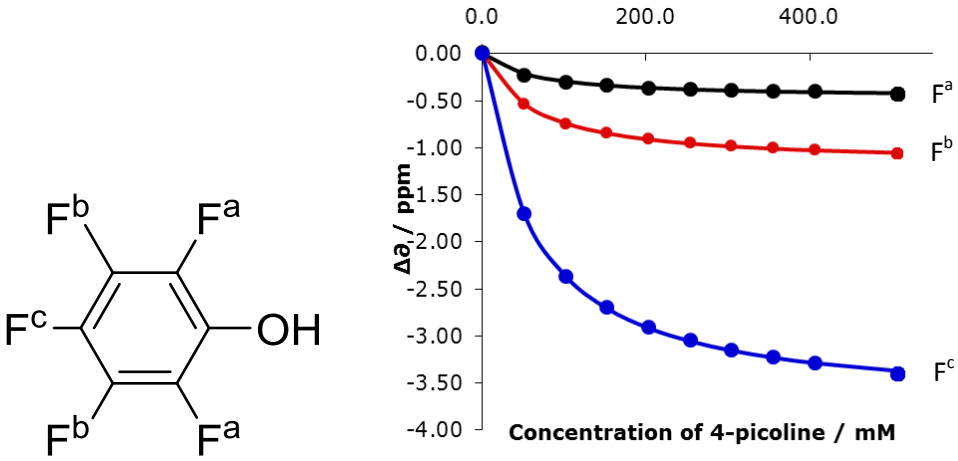


Figure S4.18: Binding isotherms for titration

K_a = 19±1 M^{-1} 90% bound

Titration of pentafluoroiodobenzene with 4-picoline in toluene

Host: pentafluorophenol [100 mM]

Guest: 4-picoline

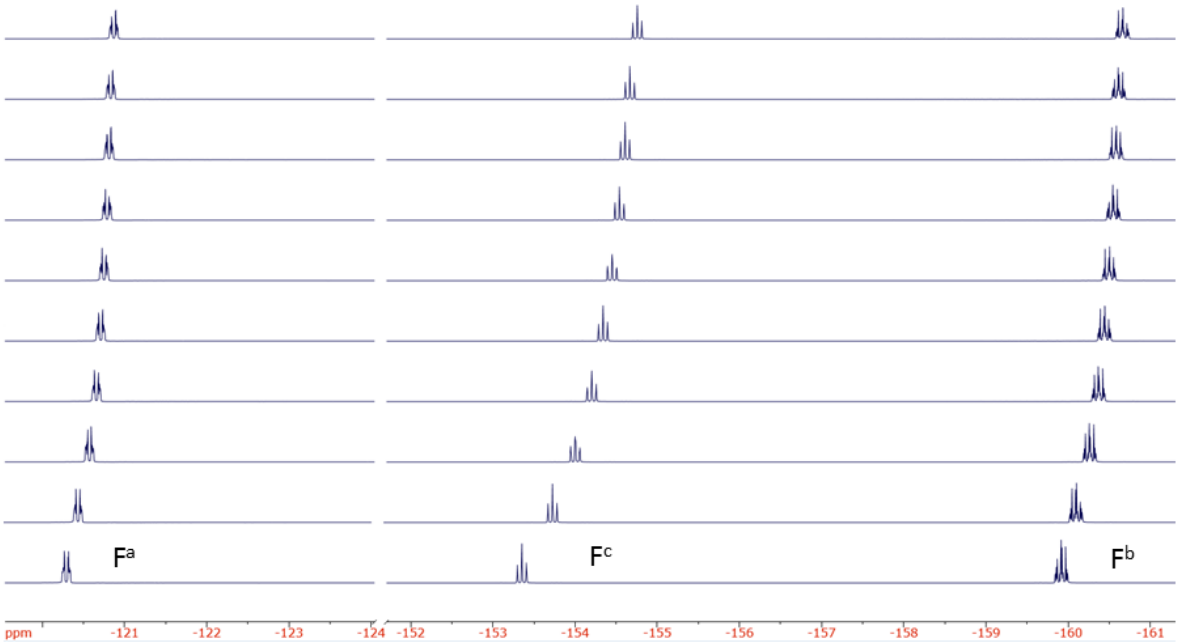


Figure S4.19: partial 376.5 MHz ^{19}F NMR spectra of titration in toluene

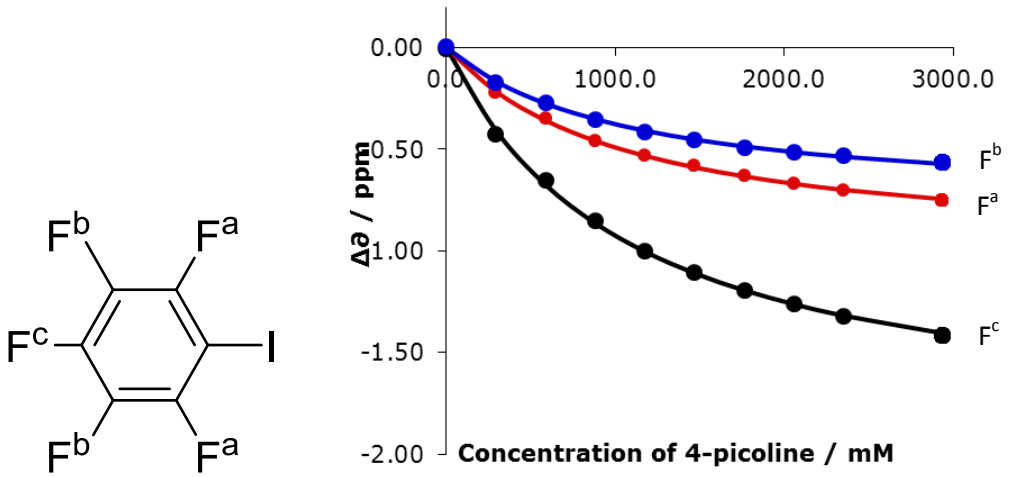
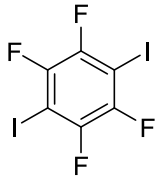


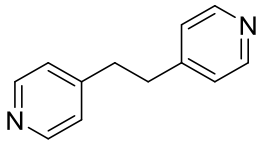
Figure S4.20: Binding isotherm for titration

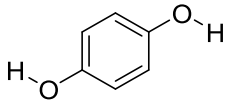
K_a = 1±1 M^{-1} 74% bound

5. Synthesis of Co-Crystals

System A



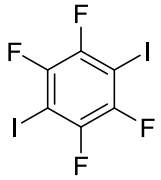


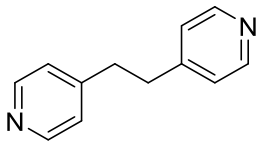


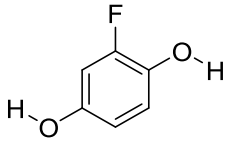
An equimolar quantity of hydroquinone (0.044 g, 0.40 mmol, 1 eq.), 1,4-diiodotetrafluorobenzene (0.16 g, 0.40 mmol, 1 eq.) and 1,2-bis(4-pyridyl)ethane (0.074 g, 0.40 mmol. 1 eq.) were dissolved in the appropriate solvent (100 mL, co-crystallisation concentration 4.0 mM) and the solution placed on a polystyrene box lid to minimise vibrations and the solvent was allowed to slowly evaporate at ambient temperature. The co-crystals which formed after 24 h were isolated by filtration, dried and then investigated by powder X-ray diffraction. The yields of co-crystals, according to their subsequent identity from X-ray powder diffraction, from each solvent were as follows:

Toluene (0.08 g, 68% HB), Chloroform (0.134 g, 20% HB & 47% XB), Dichloromethane (0.086 g, 66% HB & 3% XB), Acetone (0.21 g, 90% XB), Acetonitrile (0.19 g, 81% XB), Nitromethane (0.17 g, 73% XB), Propan-2-ol (0.12 g, 51% XB).

System B



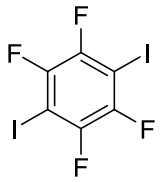


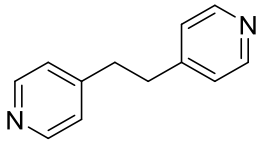


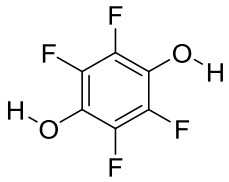
An equimolar quantity of fluorohydroquinone (0.064 g, 0.50 mmol, 1 eq.), 1,4-diiodotetrafluorobenzene (0.20 g, 0.50 mmol, 1 eq.) and 1,2-bis(4-pyridyl)ethane (0.092 g, 0.50 mmol. 1 eq.) were dissolved in the appropriate solvent (125 mL, co-crystallisation concentration 4.0 mM) and the solution placed on a polystyrene box lid to minimise vibrations and the solvent was allowed to slowly evaporate at ambient temperature. The co-crystals which formed after 24 h were isolated by filtration, dried and then investigated by powder X-ray diffraction. The yields of co-crystals from each solvent were as follows:

Toluene (0.115 g, 74% HB), Chloroform (0.105 g, 67% HB), Dichloromethane (0.105 g, 61% HB & 3% XB), Acetone (0.19 g, 65% XB), Acetonitrile (0.135 g, 46% XB), Nitromethane (0.20 g, 68% XB), Propan-2-ol (0.19 g, 65% XB).

System C







An equimolar quantity of tetrafluorohydroquinone (0.1 g, 0.55 mmol, 1 eq.), 1,4-diiodotetrafluorobenzene (0.22 g, 0.55 mmol, 1 eq.) and 1,2-bis(4-pyridyl)ethane (0.1 g, 0.55 mmol. 1 eq.) were dissolved in the appropriate solvent (100 mL, co-crystallisation concentration 5.5 mM) and the solution placed on a polystyrene box lid to minimise vibrations. The solvent was allowed to slowly evaporate at ambient temperature and co-crystals which formed after 24 h were isolated by filtration, dried and then investigated by powder X-ray diffraction. The yields of co-crystals from each solvent were as follows:

Toluene (0.17 g, 85% HB), Chloroform (0.125 g, 62% HB), Dichloromethane (0.105 g, 52% HB), Acetone (0.115 g, 57% HB), Acetonitrile (0.1 g, 50% HB), Nitromethane (0.09 g, 45% HB), Propan-2-ol (0.20 g, 58% HB & 26% XB).

6. Full Table of Powder X-Ray Diffraction Results

Table S2. Table of co-crystal compositions for systems **A**, **B** and **C** obtained from the seven solvents.

	System A	**System B**	**System C**
Toluene	100% HB	100% HB	100% HB
$CHCl_3$	30% HB 70% XB	100% HB	100% HB
CH_2Cl_2	95% HB 5% XB	95% HB 5% XB	100% HB
Acetone	100% XB	100% XB	100% HB
MeCN	100% XB	100% XB	100% HB
NO_2Me	100% XB	100% XB	100% HB
i-Propanol	100% XB	100% XB	69% HB 31% XB

7. Phase Purity Analysis by XRPD: Experimental Description

Microcrystalline powder samples for analysis by XRPD were loaded into 0.7 mm borosilicate capillaries. X-ray diffraction data were collected using either synchrotron radiation at beamline I11 at Diamond Light Source[S1,S2] or at the University of Sheffield using a Bruker D8 ADVANCE X-ray powder diffractometer.

Synchrotron data were collected at different wavelengths (all close to 0.82 Å; specific values reported for each experiment) and the instrument was equipped with a wide angle (90°) PSD detector comprising 18 Mythen-2 modules. A pair of scans was conducted at room temperature, related by a 0.25° detector offset to account for gaps between detector modules. Five such scan pairs were collected at 10 s exposure, preceded and followed by a pair of 1 s scans to compare to check for beam damage. The resulting patterns were summed to give the final pattern for structural analysis (total beam exposure time therefore 104 s).

In house X-ray diffraction data was collected a Cu Kα Bruker D8 ADVANCE X-Ray powder diffractometer. The instrument was fitted with a focusing Göbel mirror optic and a high resolution energy-dispersive Lynxeye XE detector. Scans were collected at room temperature between 5-60° 2θ, using a step size of 0.01532° and step time of 14 s giving a total exposure time of 15 h.

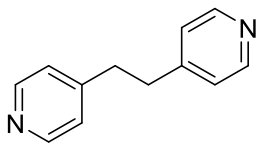
Powder pattern indexing and fitting was carried out using the TOPAS program.[S3]

When fitting powder patterns collected for the starting materials, pure HB or XB networks or from competition experiments in Systems **A**-**C**, the patterns were compared with calculated X-ray powder patterns established from single-crystal X-ray diffraction. The unit cell parameters from the pure HB or XB phases were used as a starting point for the Pawley fitting[S5] of the competition experiment results. Fitting was conducted over a selected 2θ range, based on the visible presence of peaks in each pattern. The fit range is described beneath each figure. For mixed-phase patterns, Rietveld fitting[S10] was employed to establish the relative quantities of each phase.

8. Phase Purity Checks by XRPD: Compounds 1,2a, 2b, 2c and 3

The phase purity of the as-purchased materials used in the crystal syntheses were checked by X-ray powder diffraction before use.

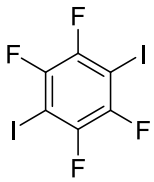
Phase-purity check, 1,2-bis(4-pyridyl)ethane (3)



X-ray diffraction data of the white crystalline powder were collected using synchrotron radiation (λ = 0.82562 (1) Å). The pattern was compared with calculated X-ray powder patterns for **3** already established from single-crystal X-ray diffraction (CSD refcode ZEXKIW).[S4] The unit cell parameters of **3** were used as a starting point for Pawley refinement,[S5] employing 704 parameters (8 background, 1 zero error, 5 profile, 4 cell, 686 reflections). Pawley refinement converged to R_{wp} = 0.0517, R_{wp}' = 0.1304. [*a* = 5.55908 (3) Å, *b* = 8.16704 (3) Å, *c* = 11.36448 (8) Å, β = 100.6657 (6) °, *V* = 507.048 (5) Å^3].

Figure S8.1. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 6.8 - 53 °, d_{min} = 0.92 Å).

Phase-purity check, perfluoro-1,4-diiodobenzene (1)



X-ray diffraction data of the white microcrystalline powder was collected using Cu Kα radiation. The pattern was compared with calculated X-ray powder patterns for **1** already established from single-crystal X-ray diffraction (CSD refcode ZZZAVM).[S6] The unit cell parameters of **1** were used as a starting point for Pawley refinement,[S5] employing 147 parameters (8 background, 1 zero error, 5 profile, 4 cell, 125 reflections). Pawley refinement converged to R_{wp} = 0.0294, R_{wp}' = 0.0942. [a = 6.2529 (1) Å, b = 11.6040 (2) Å, c = 5.9178 (1) Å, β = 92.608 (1) °, V = 428.94 (1) Å^3].

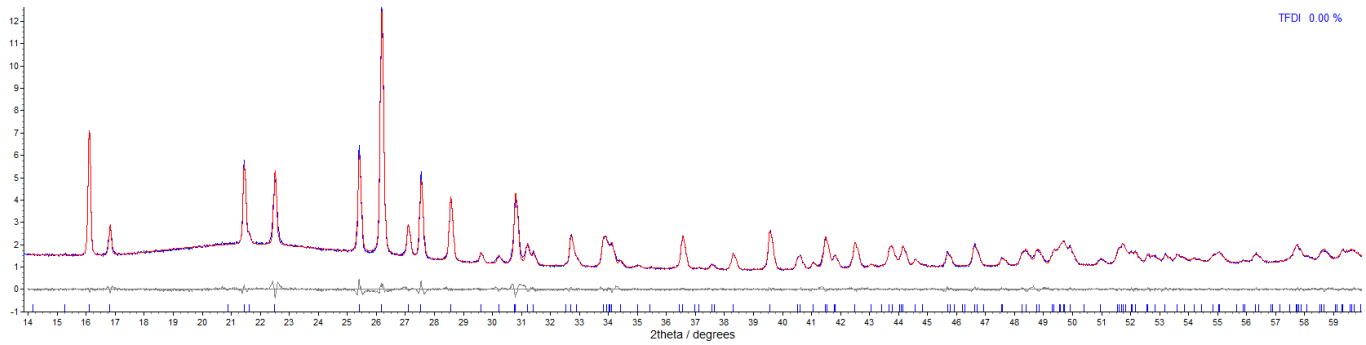
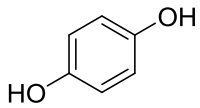


Figure S8.2. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 14 - 60 °, d_{min} = 1.54 Å).

Phase-purity check, hydroquinone (2a)



X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82562 (1) Å). The pattern was compared with calculated X-ray powder patterns for **2a** already established from single-crystal X-ray diffraction (CSD refcode HYQUIN02).[S7] The unit cell parameters of **2a** were used as a starting point for Pawley refinement,[S5] employing 1423 parameters (18 background, 1 zero error, 5 profile, 2 cell, 1397 reflections). Pawley refinement converged to R_{wp} = 0.0142, R_{wp}' = 0.0750 [a = b = 38.5225(2) Å, c = 5.6594 (1) Å, V = 7273.2 (1) Å^3].

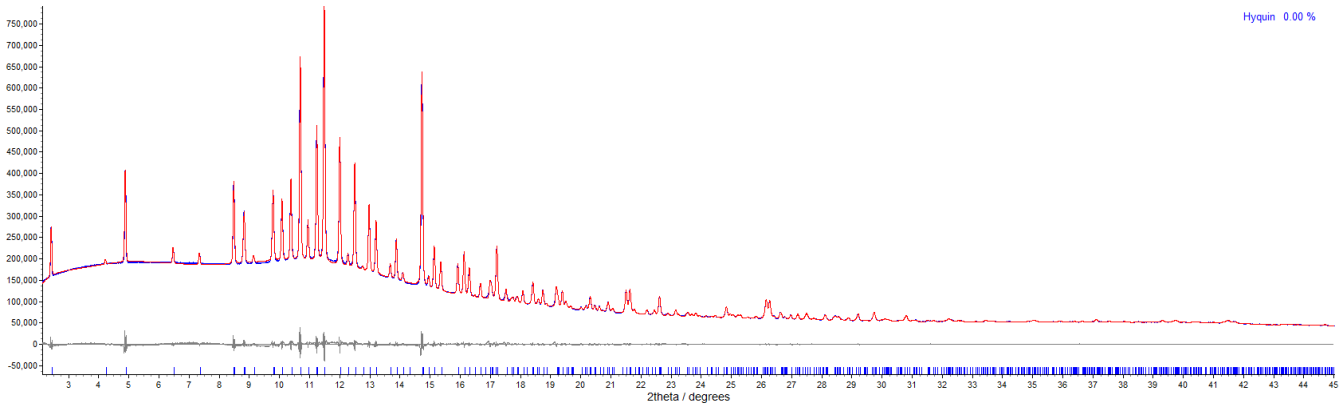
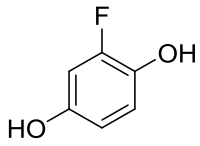


Figure S8.3. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 2.0 - 45 °, d_{min} = 1.08 Å).

Phase-purity check, 2-fluorohydroquinone (2b)



X-ray diffraction data of the off-white microcrystalline powder were collected using synchrotron radiation (λ = 0.82582(1) Å). The pattern was compared with calculated X-ray powder patterns for **2b**, which has established from single-crystal X-ray diffraction.[S8] The unit cell parameters of **2b** were used as a starting point for Pawley refinement,[S4] employing 1675 parameters (16 background, 1 zero error, 5 profile, 6 cell, 1647 reflections). Pawley refinement converged to R_{wp} = 0.0161, R_{wp}' = 0.0781. [a = 5.59470 (4) Å, b = 9.91526 (6) Å, c = 14.15526 (9) Å, α = 109.3048 (3) °, β = 97.5352 (3) °, γ = 100.5002 (2) °, V = 713.008 (8) Å^3].

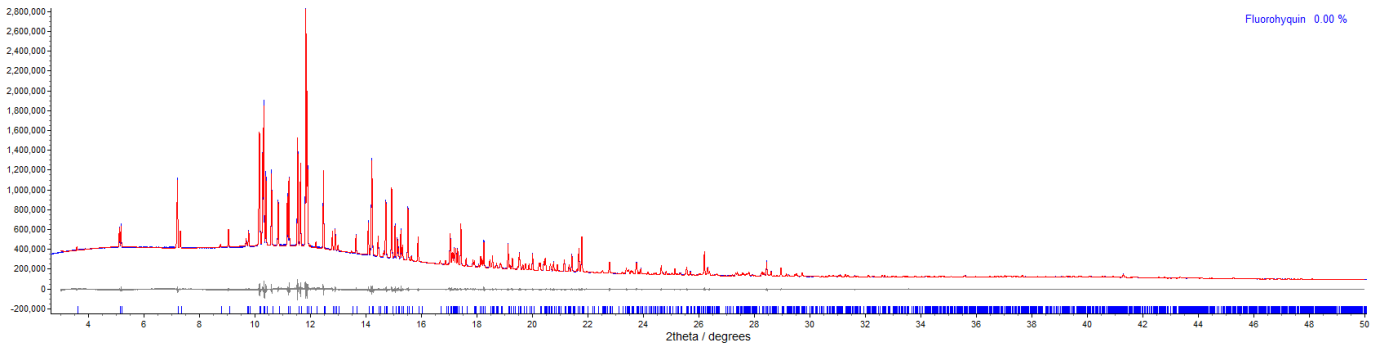
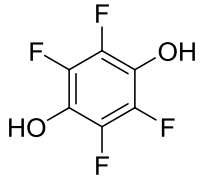


Figure S8.4. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 3 – 50 °, d_{min} = 0.98 Å).

Phase-purity check, perfluorohydroquinone (2c)



X-ray diffraction data of the off-white microcrystalline powder were collected using synchrotron radiation (λ = 0.82582(1) Å). The pattern was compared with calculated X-ray powder patterns for **2c** already established from single-crystal X-ray diffraction (CSD refcode GUFMAV).[S9] The unit cell parameters of **2c** were used as a starting point for Pawley refinement,[S4] employing 599 parameters (6 background, 1 zero error, 5 profile, 4 cell, 583 reflections). Pawley refinement converged to R_{wp} = 0.0613, R_{wp}' = 0.1491. [a = 6.55976 (4) Å, b = 4.88392 (3) Å, c = 10.25333 (6) Å, β = 109.4872 (5) °, V = 309.672 (3) Å^3].

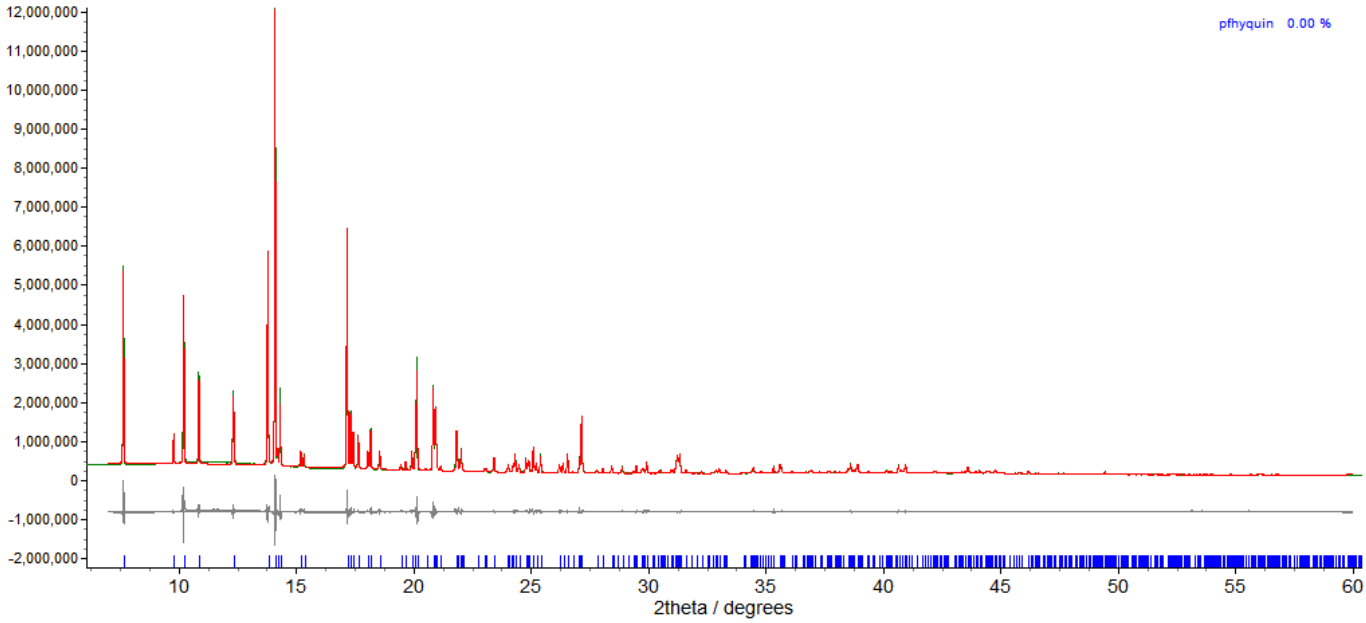
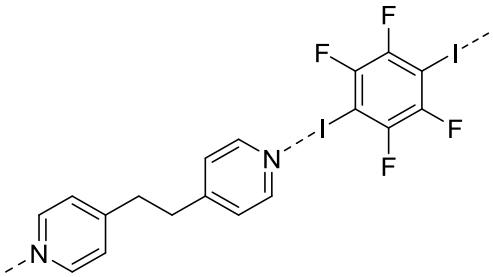


Figure S8.5. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 7.0 – 60 °, d_{min} = 0.83 Å).

9. Phase Purity Check by XRPD: Co-crystals 1•3, 2a•3, 2b•3 and 2c•3

The X-ray powder diffraction patterns of the microcrystalline products resulting from mixing of only two of the components from each set of competition experiments was recorded. This was to investigate and determine experimentally the formation of the hydrogen-bonding only and halogen-bonding only phases, in the absence of a competing reagent.

Two-component co-crystallisation (System A-C, 1 + 3)



X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82652 (1) Å). The pattern was compared with calculated X-ray powder patterns for **1•3** (the halogen-bonded co-crystal phase) already established from single-crystal X-ray diffraction (crystal structure taken from CSD refcode MEKWOO).[S10] The unit cell parameters of **1•3** were used as a starting point for Pawley refinement,[S5] employing 1114 parameters (6 background, 1 zero error, 5 profile, 6 cell, 1096 reflections). Pawley refinement converged to R_{wp} = 0.0587, R_{wp}' = 0.1454. [a = 5.04863 (3) Å, b = 9.92166 (7) Å, c = 10.6267 (1) Å, α = 64.7567 (7) °, β = 82.0664 (7) °, γ = 87.8850 (4) °, V = 476.717 (7) Å^3].

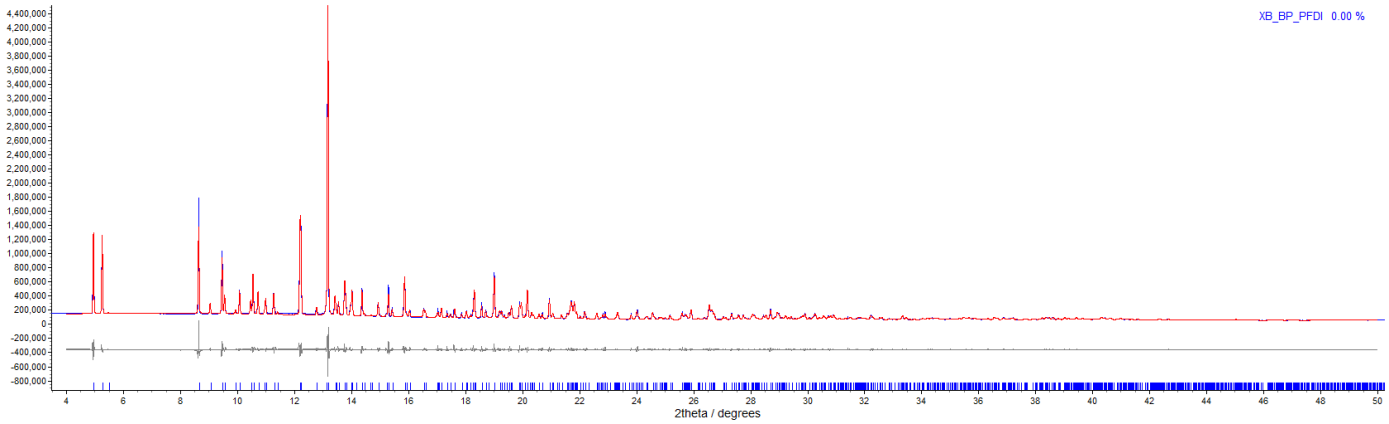
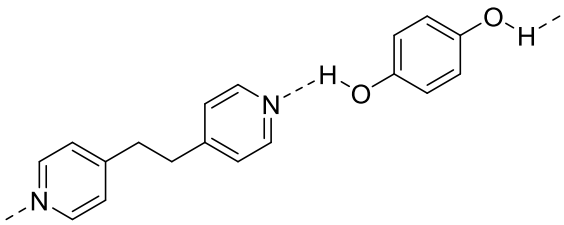


Figure S9.1. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5.0 - 50 °, d_{min} = 0.97 Å).

Two-component co-crystallisation (System A, 2a + 3)



X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82652 (1) Å). The pattern was compared with calculated X-ray powder patterns for **2a•3** (the hydrogen-bonded co-crystal phase) already established from single-crystal X-ray diffraction.[S10] The unit cell parameters of **2a•3** were used as a starting point for Pawley refinement,[S5] employing 1641 parameters (8 background, 1 zero error, 5 profile, 6 cell, 1621 reflections). Pawley refinement converged to R_{wp} = 0.0499, R_{wp}' = 0.0636. [a = 7.43927 (5) Å, b = 9.43980 (5) Å, c = 11.8509 (1) Å, α = 95.2651 (6) °, β = 92.9887 (7) °, γ = 108.1735 (6) °, V = 784.51 (1) Å^3].

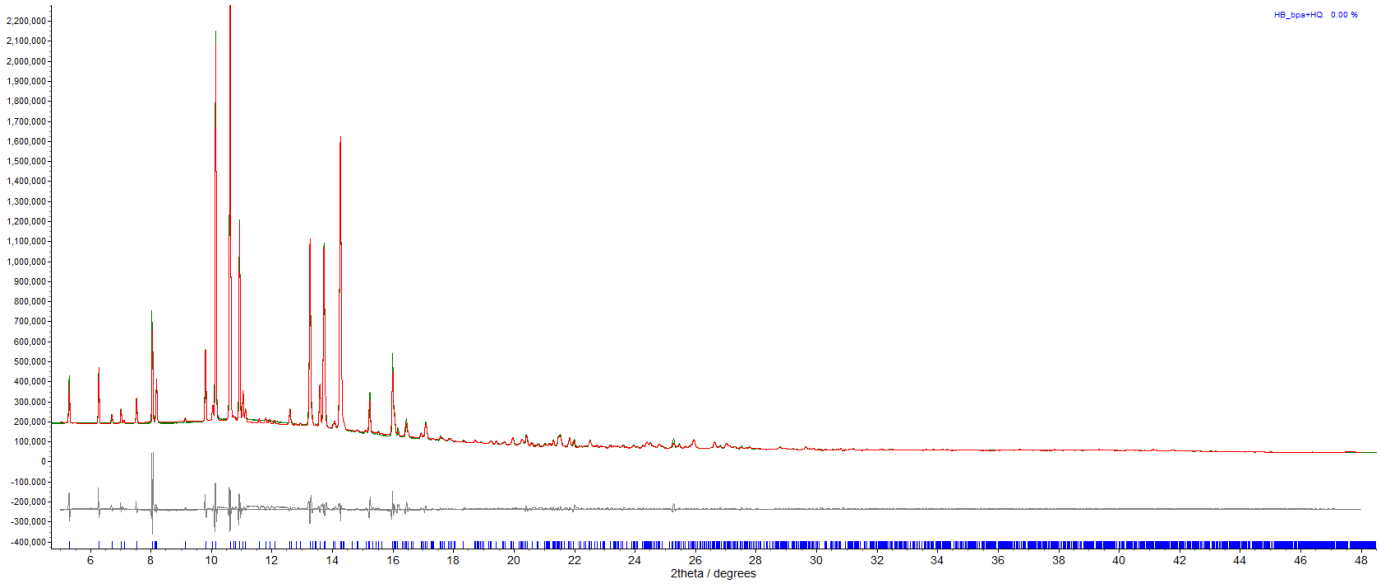
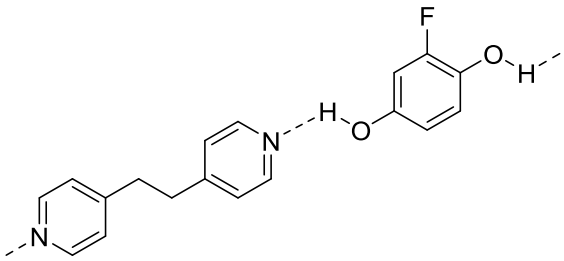


Figure S9.2. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5.0 - 48 °, d_{min} = 1.02 Å).

Two-component co-crystallisation (System B, 2b + 3)



X-ray diffraction data of the white microcrystalline powder was collected in house. The pattern was compared with calculated X-ray powder patterns for **2b•3** (the hydrogen-bonded co-crystal phase), which has been established from single-crystal X-ray diffraction and is reported herein. The unit cell parameters of **2b•3** were used as a starting point for Pawley refinement,[S5] employing 444 parameters (12 background, 1 zero error, 5 profile, 6 cell, 420 reflections). Pawley refinement converged to R_{wp} = 0.0199, R_{wp}' = 0.0498. [a = 7.4266 (1) Å, b = 9.4109 (1) Å, c = 11.9305 (2) Å, α = 96.031 (1) °, β = 92.475 (1) °, γ = 108.2621 (6) °, V = 784.89 (2) Å^3].

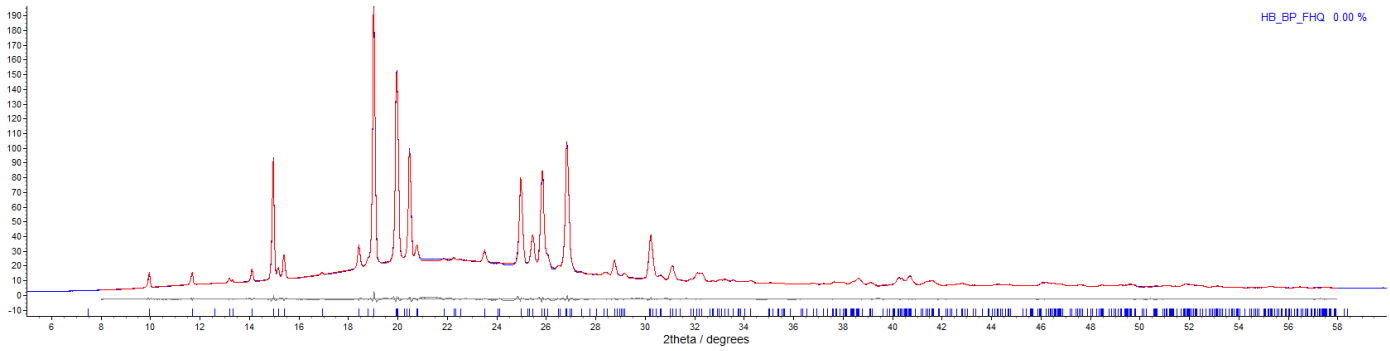
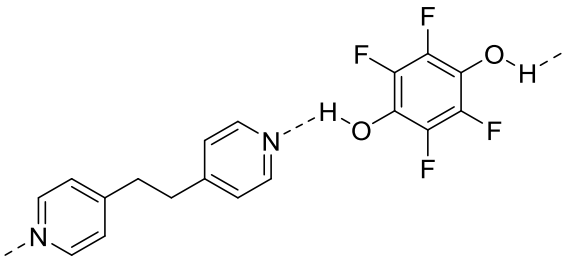


Figure S9.3. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 58 °, d_{min} = 1.59 Å).

Two-component co-crystallisation (System C, 2c + 3)



X-ray diffraction data of the white microcrystalline powder was collected using Cu Kα radiation. The pattern was compared with calculated X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase), which has been established from single-crystal X-ray diffraction and is reported herein. The unit cell parameters of **2c•3** were used as a starting point for Pawley refinement,[S5] employing 249 parameters (14 background, 1 zero error, 5 profile, 6 cell, 223 reflections). Pawley refinement converged to R_{wp} = 0.0268, R_{wp}' = 0.0689. [a = 6.3540 (1) Å, b = 7.4432 (1) Å, c = 9.2267 (2) Å, α = 86.134 (2) °, β = 75.989 (2) °, γ = 71.302 (2) °, V = 401.01 (2) Å^3].

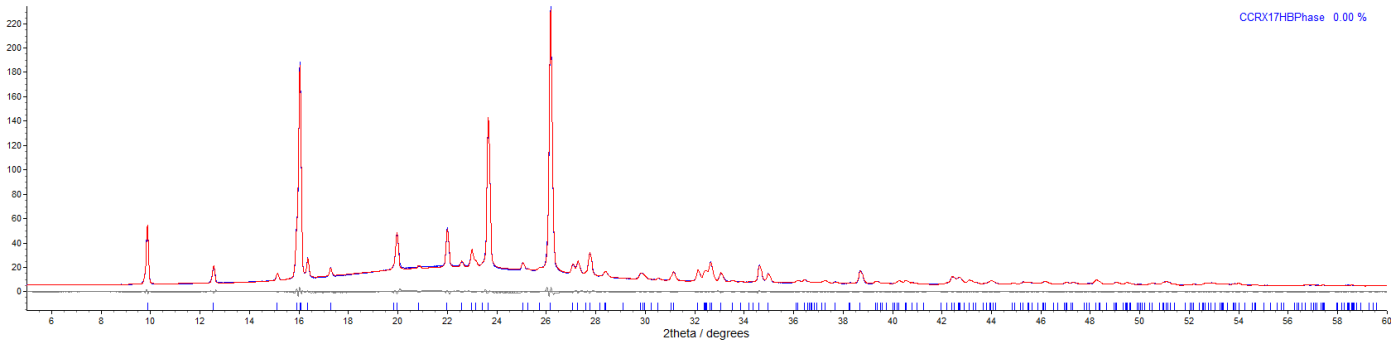
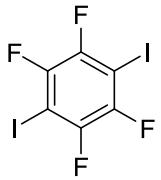
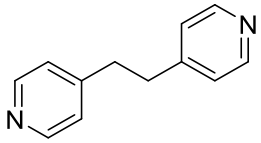
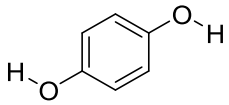


Figure S9.4. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

10. Determination of Product Composition by XRPD: System A [perfluoro-1,4-diiodobenzene (1), hydroquinone (2a) and 1,2-bis(4-pyridyl)ethane (3)]

The X-ray powder diffraction patterns of the microcrystalline products from all competition experiments were recorded. These were compared to the calculated X-ray powder diffraction patterns for the hydrogen-bonded (**2a•3**) and halogen-bonded (**1•3**) co-crystals as well as the individual components (**1**, **2a** and **3**), before conducting quantitative fitting of the data.

System A: Competition experiment in Toluene.

X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82582(1) Å). The pattern was compared with calculated X-ray powder patterns for **2a•3** (the hydrogen-bonded co-crystal phase) for which the crystal structure was already established from single-crystal X-ray diffraction. The unit cell parameters of **2a•3** were used as a starting point for Pawley refinement,[S5] employing 1637 parameters (11 background, 1 zero error, 5 profile, 6 cell, 1614 reflections). Pawley refinement converged to R_{wp} = 0.0277, R_{wp}' = 0.0918. [a = 7.42363 (5) Å, b = 9.42107 (6) Å, c = 11.81438 (9) Å, α = 95.345 (1) °, β = 92.998 (1) °, γ = 108.1405 (6) °, V = 778.91 (1) Å^3].

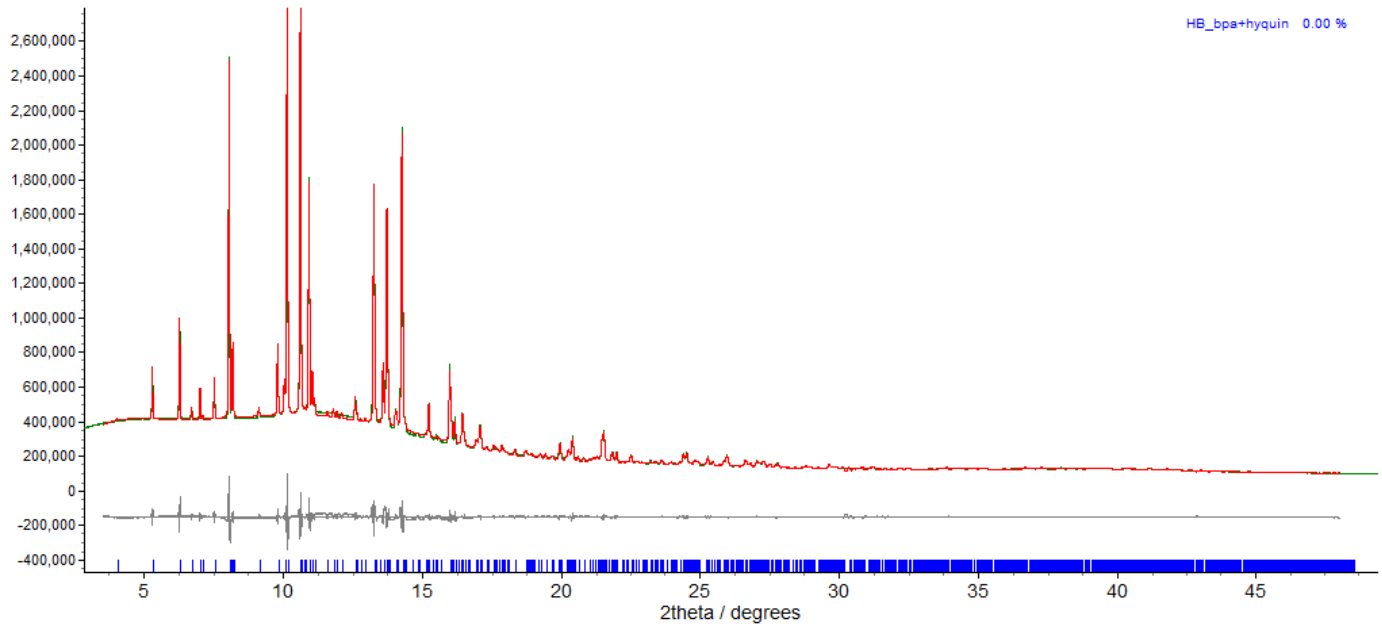


Figure S10.1. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 3.5 - 48 °, d_{min} = 1.01 Å).

System A: Competition experiment in chloroform.

X-ray diffraction data of the white microcrystalline powder were collected using Cu Kα radiation. The pattern was compared with calculated X-ray powder patterns for **2a•3** (the hydrogen-bonded co-crystal phase) and for **1•3** (the halogen-bonded co-crystal phase), for which the crystal structures were already established from single-crystal X-ray diffraction (the halogen-bonded co-crystal phase crystal structure has CSD refcode MEKWOO).[S10] The unit cell parameters of **2a•3**and **1•3** were used as a starting point for a mixed-phase Pawley refinement,[S5] employing 687 parameters (10 background, 1 zero error, 10 profile, 12 cell, 654 reflections), resulting in final indices of fit R_{wp} = 0.0444, R_{wp}' = 0.1088. The starting model used for the mixed-phase Rietveld refinement,[S11] conducted using TOPAS, was derived from the single-crystal structures of **2a•3** and **1•3**. A fourth-order spherical harmonics correction term was applied to account for preferred orientation. Refinement employed 51 parameters (11 background, 1 zero error, 10 profile, 12 cell, 2 scale and 15 spherical harmonic terms). Rietveld refinement converged to R_{wp} = 0.0733, R_{wp}' = 0.2419. The relative phase amounts were found to be 30.1 (9) % of **2a•3** and 69.9 (9) % of **1•3**. [**2a•3**: *a* = 7.419 (3) Å, *b* = 9.424 (4) Å, *c* = 11.807 (5) Å, α = 95.40 (9) °, β = 93.0 (1) °, γ = 108.14 (4) °, *V* = 778.1 (6) Å^3; **1•3**: *a* = 5.0374 (4) Å, *b* = 9.9170 (8) Å, *c* = 10.6145 (7) Å, α = 64.745 (4) °, β = 82.103 (6) °, γ = 87.910 (5) °, *V* = 474.89 (7) Å^3].

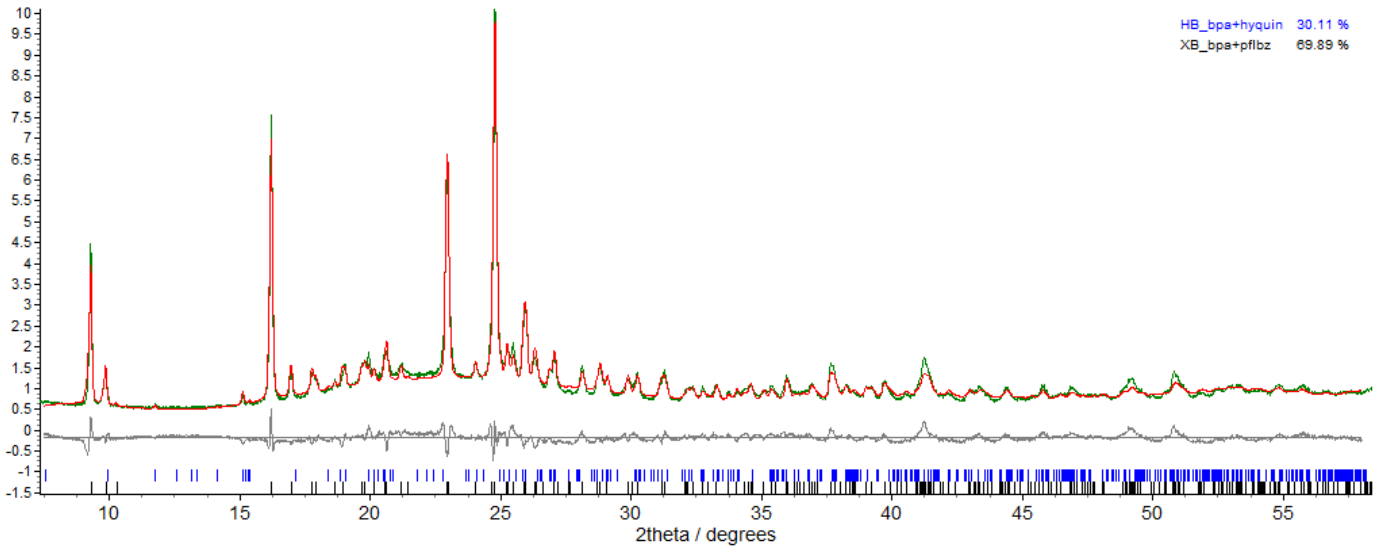


Figure S10.2. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 7.5 - 58 °, d_{min} = 1.59 Å).

System A: Competition experiment in dichloromethane.

X-ray diffraction data of the white microcrystalline powder were collected using Cu Kα radiation. The pattern was compared with calculated X-ray powder patterns for **2a•3** (the hydrogen-bonded co-crystal phase) and for **1•3** (the halogen-bonded co-crystal phase), for which the crystal structures were already established from single-crystal X-ray diffraction (the halogen-bonded co-crystal phase crystal structure has CSD refcode MEKWOO).[S10] The unit cell parameters of **2a•3**and **1•3**were used as a starting point for a mixed-phase Pawley refinement,[S5] employing 697 parameters (8 background, 1 zero error, 10 profile, 12 cell, 666 reflections), resulting in final indices of fit R_{wp} = 0.0496, R_{wp}' = 0.0822. The starting model used for the mixed-phase Rietveld refinement,[S11] conducted using TOPAS, was derived from the single-crystal structures of **2a•3**and **1•3**. Refinement employed 38 parameters (10 background, 1 zero error, 10 profile, 12 cell, 2 scale). Rietveld refinement converged to R_{wp} = 0.0741, R_{wp}' = 0.1407. The relative phase amounts were found to be 95.05(3) % of **2a•3**and 4.95(3) % of **1•3**. [**2a•3**: *a* = 7.4314(2) Å, *b* = 9.4222(2) Å, *c* = 11.8156(4) Å, α = 95.333(5) °, β = 92.993(6) °, γ = 108.176(2) °, *V* = 779.75(4) Å^3; **1•3**: *a* = 5.0402(5) Å, *b* = 9.292(1) Å, *c* = 10.632(9) Å, α = 64.782(6) °, β = 82.081(8) °, γ = 87.849(8) °, *V* = 476.30(8) Å^3].

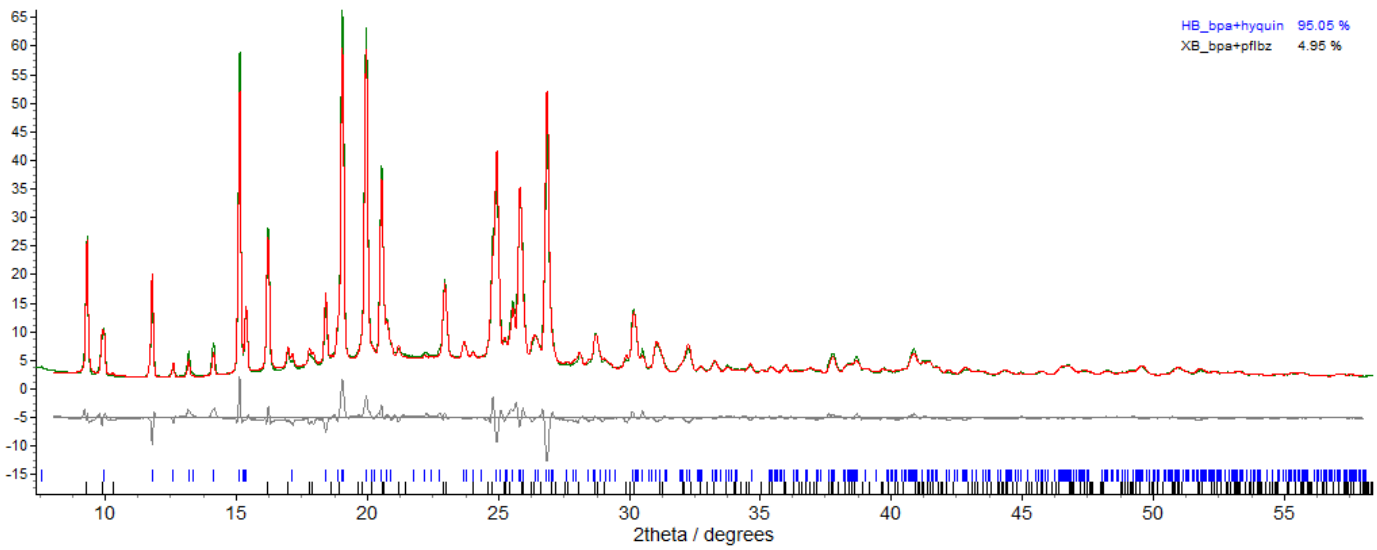


Figure S10.3. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 58 °, d_{min} = 1.59 Å).

System A: Competition experiment in acetone.

X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82665 (1) Å). The pattern was compared with calculated X-ray powder pattern for **1•3** (the halogen-bonded co-crystal phase) for which the crystal structure was already established from single-crystal X-ray diffraction (CSD refcode MEKWOO).[S10] The unit cell parameters of **1•3**were used as a starting point for Pawley refinement,[S5] employing 880 parameters (6 background, 1 zero error, 5 profile, 6 cell, 862 reflections). Pawley refinement converged to R_{wp} = 0.0511, R_{wp}' = 0.1143. [*a* = 5.04384 (7) Å, *b* = 9.9159 (1) Å, *c* = 10.6266 (1) Å, α = 64.7167 (9) °, β = 82.006 (1) °, γ = 87.7912 (9) °, *V* = 475.77 (1) Å^3].

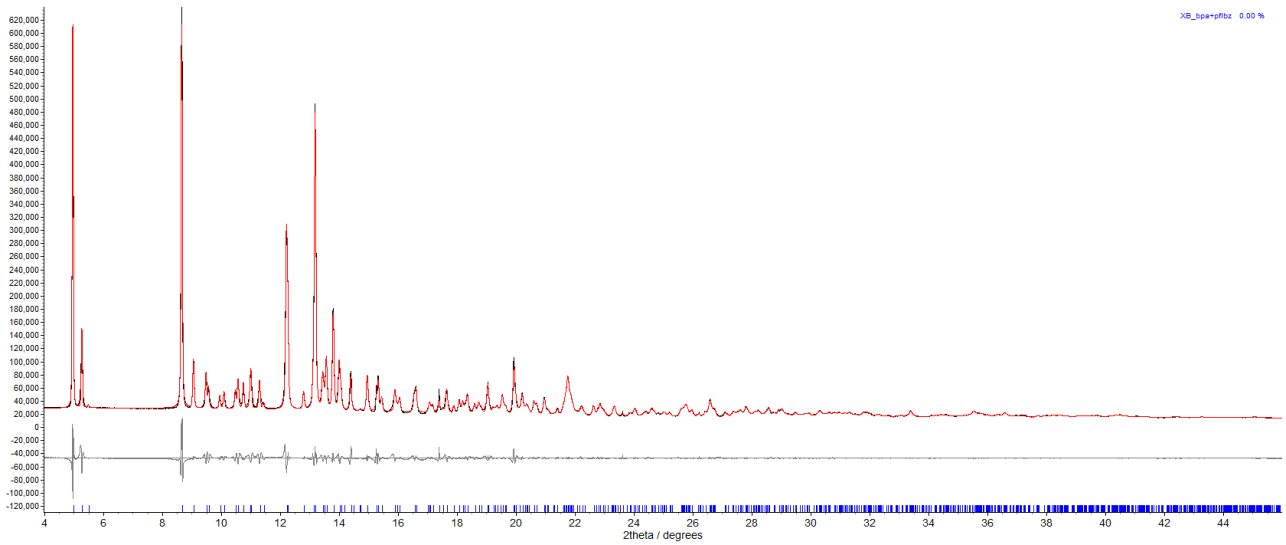


Figure S10.4. Observed (black) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 4.0 - 46 °, d_{min} = 1.06 Å).

System A: Competition experiment in acetonitrile.

X-ray diffraction data of thw white microcrystalline powder were collected using synchrotron radiation (λ = 0.82665 (1) Å). The pattern was compared with calculated X-ray powder pattern for **1•3** (the halogen-bonded co-crystal phase) for which the crystal structures was already established from single-crystal X-ray diffraction (CSD refcode MEKWOO).[S10] The unit cell parameters of **1•3**were used as a starting point for Pawley refinement,[S5] employing 604 parameters (6 background, 1 zero error, 5 profile, 6 cell, 586 reflections). Pawley refinement converged to R_{wp} = 0.0484, R_{wp}' = 0.1128. [*a* = 5.04158 (7) Å, *b* = 9.9050 (2) Å, *c* = 10.6188 (1) Å, α = 64.789 (1) °, β = 82.155 (1) °, γ = 87.890 (1) °, *V* = 475.14 (1) Å^3].

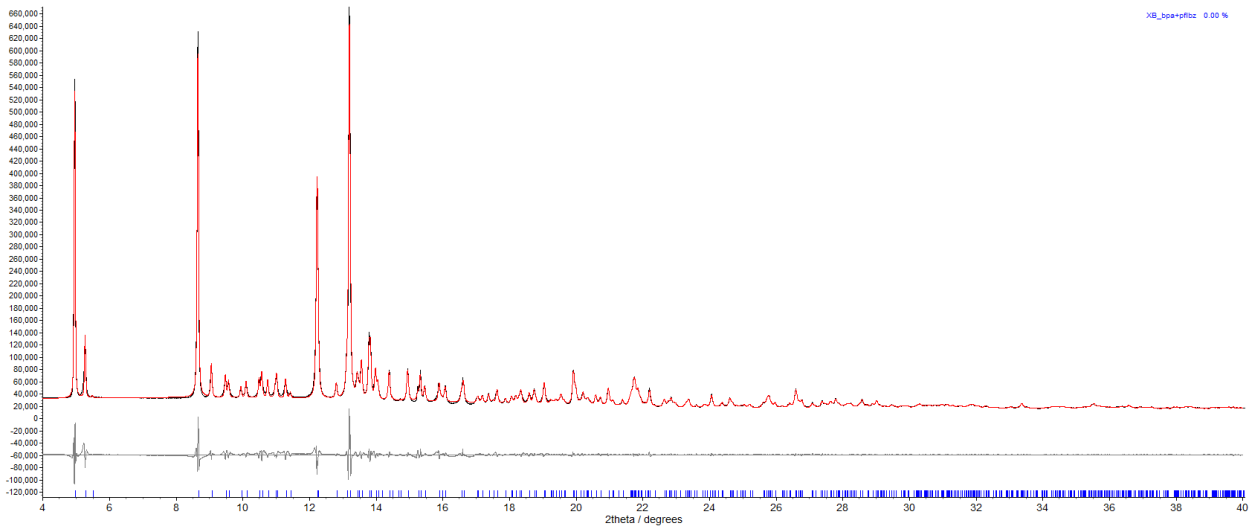


Figure S10.5. Observed (black) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 4.0 - 40 °, d_{min} = 1.21 Å).

System A: Competition experiment in nitromethane.

X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82665 (1) Å). The pattern was compared with calculated X-ray powder patterns for **1•3** (the halogen-bonded co-crystal phase) for which the crystal structure was already established from single-crystal X-ray diffraction (CSD refcode MEKWOO).[S10] The unit cell parameters of **1•3** were used as a starting point for Pawley refinement,[S5] employing 1304 parameters (8 background, 1 zero error, 5 profile, 6 cell, 1284 reflections). Pawley refinement converged to R_{wp} = 0.0417, R_{wp}' = 0.0989. [a = 5.04113 (4) Å, b = 9.90950 (8) Å, c = 10.62338 (8) Å, α = 64.7527 (6) °, β = 82.1148 (7) °, γ = 87.7556 (6) °, V = 475.328 (7) Å^3].

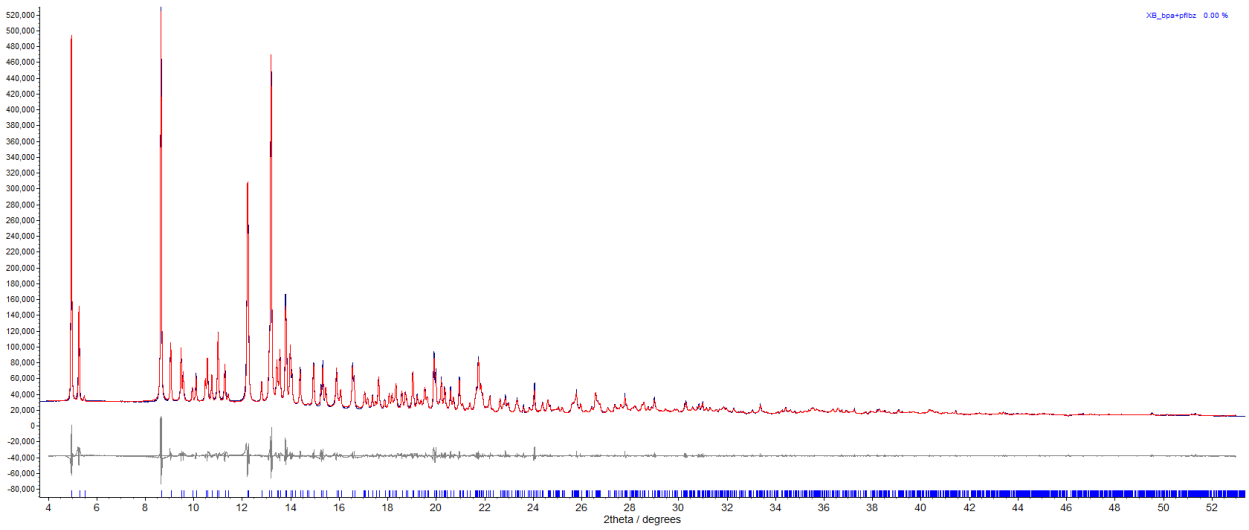


Figure S10.6. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 4.0 - 53 °, d_{min} = 0.93 Å).

System A: Competition experiment in isopropanol

X-ray diffraction data of the white microcrystalline powder were collected using synchrotron radiation (λ = 0.82665 (1) Å). The pattern was compared with calculated X-ray powder patterns for **1•3** (the halogen-bonded co-crystal phase) for which the crystal structure was already established from single-crystal X-ray diffraction (CSD refcode MEKWOO).[S10] The unit cell parameters of **1•3**were used as a starting point for Pawley refinement,[S5] employing 611 parameters (6 background, 1 zero error, 5 profile, 6 cell, 593 reflections). Pawley refinement converged to R_{wp} = 0.0497, R_{wp}' = 0.1097. [*a* = 5.04155 (7) Å, *b* = 9.9110 (2) Å, *c* = 10.6242 (1) Å, α = 64.772 (1) °, β = 82.097 (1) °, γ = 87.834 (1) °, *V* = 475.53 (1) Å^3].

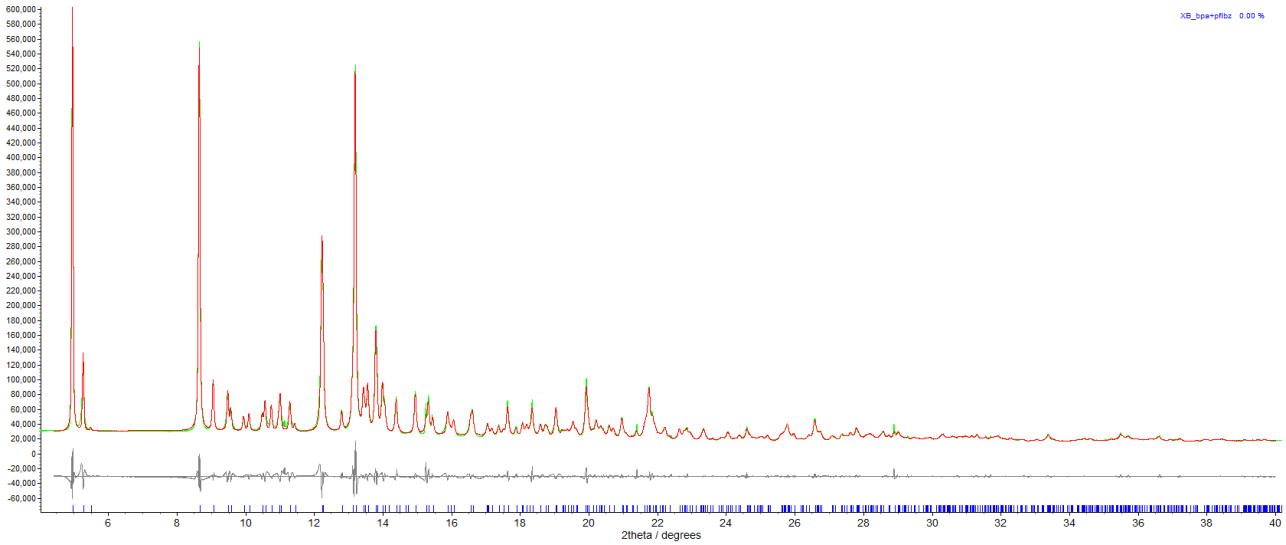
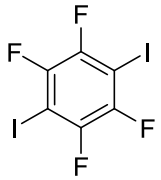
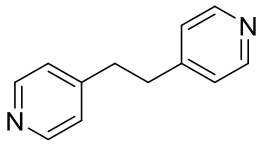
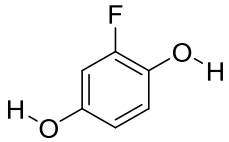


Figure S10.7. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 4.4 - 40 °, d_{min} = 1.21 Å).

11. Determination of Product Composition by XRPD: System B [perfluoro-1,4-diiodobenzene (1), fluorohydroquinone (2b) and 1,2-bis(4-pyridyl)ethane (3)]







The X-ray powder diffraction patterns of the microcrystalline products from all competition experiments were recorded. These were compared to the calculated X-ray powder diffraction patterns for the hydrogen-bonded (**2b•3**) and halogen-bonded (**1•3**) co-crystals as well as the individual components (**1**, **2b** and **3**), before conducting quantitative fitting of the data.

System B: Competition experiment in toluene

X-ray diffraction data of the white microcrystalline powder was collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder pattern for **2b•3** (hydrogen-bonded co-crystal). The unit cell parameters of **2b•3** were used as a starting point for Pawley refinement,[S5] employing 442 parameters (10 background, 1 zero error, 5 profile, 6 cell, 420 reflections). Pawley refinement converged to R_{wp} = 0.0403, $R_{wp'}$ = 0.0751. [a = 7.4247 (5) Å, b = 9.4115 (6) Å, c = 11.9308 (8) Å, α = 96.005 (5) °, β = 92.493 (6) °, γ = 108.253 (4) °, V = 784.83 (9) Å^3].

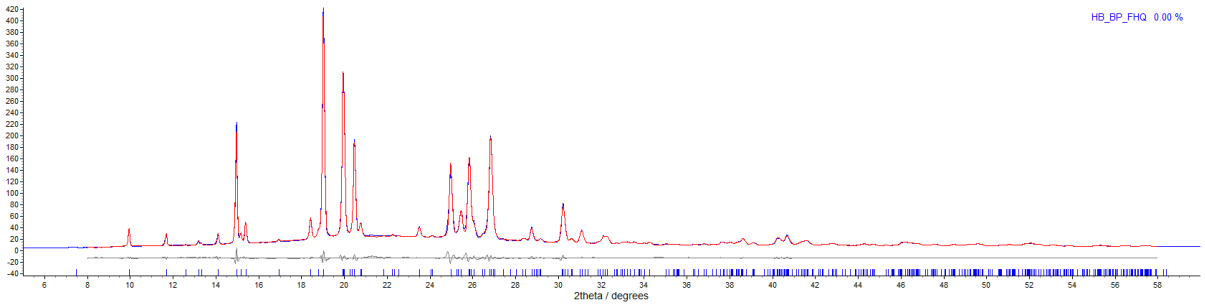


Figure S11.1. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 58 °, d_{min} = 1.59 Å).

System B: Competition experiment in chloroform

X-ray diffraction data of the white microcrystalline powder was collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder pattern for **2b•3** (hydrogen-bonded co-crystal). The unit cell parameters of **2b•3** were used as a starting point for Pawley refinement,[S5] employing 431 parameters (10 background, 1 zero error, 5 profile, 6 cell, 409 reflections). Pawley refinement converged to R_{wp} = 0.0479, $R_{wp'}$ = 0.0768. [a = 7.4250 (1) Å, b = 9.4097 (1) Å, c = 11.9293 (2) Å, α = 96.005 (2) °, β = 92.476 (2) °, γ = 108.248 (1) °, V = 784.66 (2) Å^3].

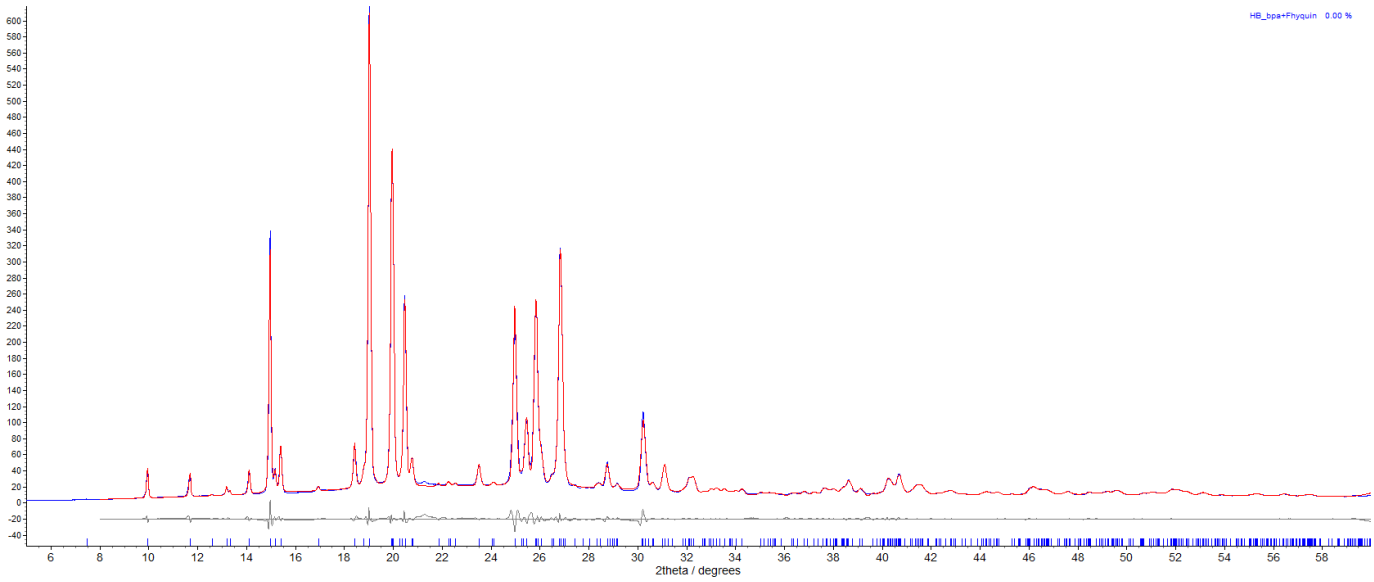


Figure S11.2. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 60 °, d_{min} = 1.54 Å).

System B: Competition experiment in dichloromethane

X-ray diffraction data of the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2b•3** (hydrogen-bonded co-crystal) and for **1•3** (halogen-bonded co-crystal). The unit cell parameters of **1•3** and **2b•3** were used as a starting point for a mixed-phase Pawley refinement,[S5] employing 703 parameters (10 background, 1 zero error, 9 profile, 12 cell, 671 reflections), resulting in final indices of fit R_{wp} = 0.0441, $R_{wp'}$ = 0.0744. The starting model used for the mixed-phase Rietveld refinement,[S11] conducted using TOPAS, used atomic coordinates from the single-crystal structures of **1•3** and **2b•3**. Refinement employed 36 parameters (10 background, 1 zero error, 9 profile, 12 cell, 2 scale, 2 global scale factors for thermal parameters). Rietveld refinement converged to R_{wp} = 0.0751, $R_{wp'}$ = 0.1333. The relative phase amounts were found to be 95.25 (4) % of **2b•3** and 4.75 (4) % of **1•3**. [Unit cell parameters for **2b•3**: *a* = 7.4265 (2) Å, *b* = 9.4132 (2) Å, *c* = 11.9356 (5) Å, α = 96.031 (6) °, β = 92.498 (6) °, γ = 108.290 (3) °, *V* = 785.25 (5) Å^3; unit cell parameters for **1•3**: *a* = 5.0399 (4) Å, *b* = 9.9183 (8) Å, *c* = 10.6230 (7) Å, α = 64.770 (5) °, β = 82.139 (6) °, γ = 87.914 (6) °, *V* = 475.70 (6) Å^3].

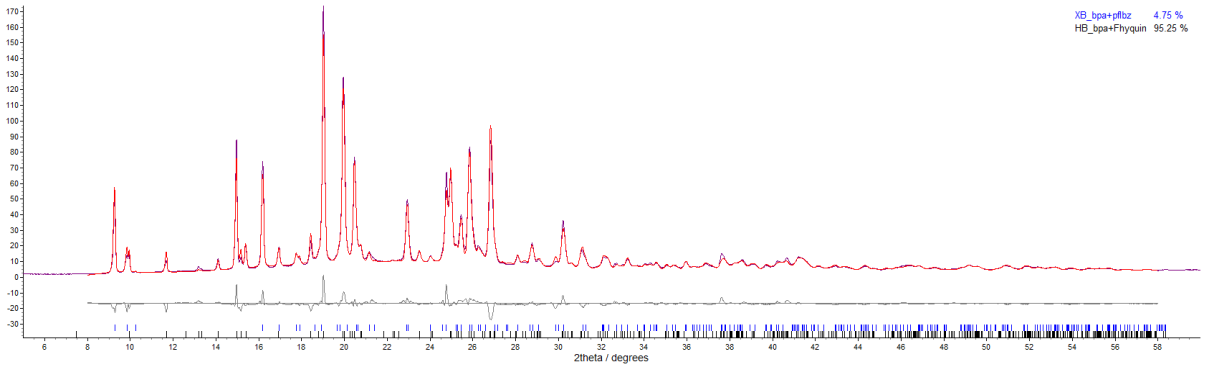


Figure S11.3. Observed (purple) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Rietveld refinement. (2θ range 8.0 - 58 °, d_{min} = 1.59 Å).

System B: Competition experiment in acetone

X-ray diffraction data of the white microcrystalline powder was collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder pattern for **1•3** (halogen-bonded co-crystal). The unit cell parameters of **1•3** were used as a starting point for Pawley refinement,[S5] employing 306 parameters (12 background, 1 zero error, 5 profile, 6 cell, 282 reflections). Pawley refinement converged to R_{wp} = 0.0316, $R_{wp'}$ = 0.1213. [a = 5.0380 (2) Å, b = 9.9020 (4) Å, c = 10.6163 (4) Å, α = 64.783 (2) °, β = 82.105 (3) °, γ = 87.864 (3) °, V = 474.46 (3) Å^3].

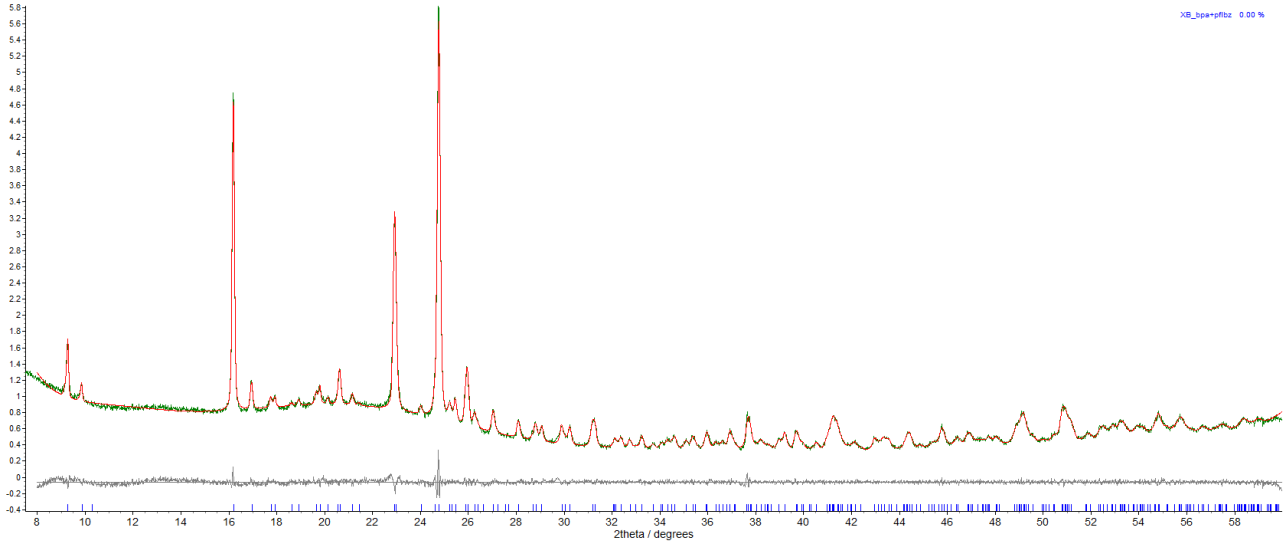


Figure S11.4. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 60 °, d_{min} = 1.54 Å).

System B: Competition experiment acetonitrile

X-ray diffraction data of the white microcrystalline powder was collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder pattern for **1•3** (halogen-bonded co-crystal). The unit cell parameters of **1•3** were used as a starting point for Pawley refinement,[S5] employing 302 parameters (10 background, 1 zero error, 5 profile, 6 cell, 280 reflections). Pawley refinement converged to R_{wp} = 0.0518, $R_{wp'}$ = 0.1442. [a = 5.0392 (2) Å, b = 9.9007 (3) Å, c = 10.6171 (3) Å, α = 64.806 (2) °, β = 82.153 (3) °, γ = 87.881 (3) °, V = 474.70 (3) Å^3].

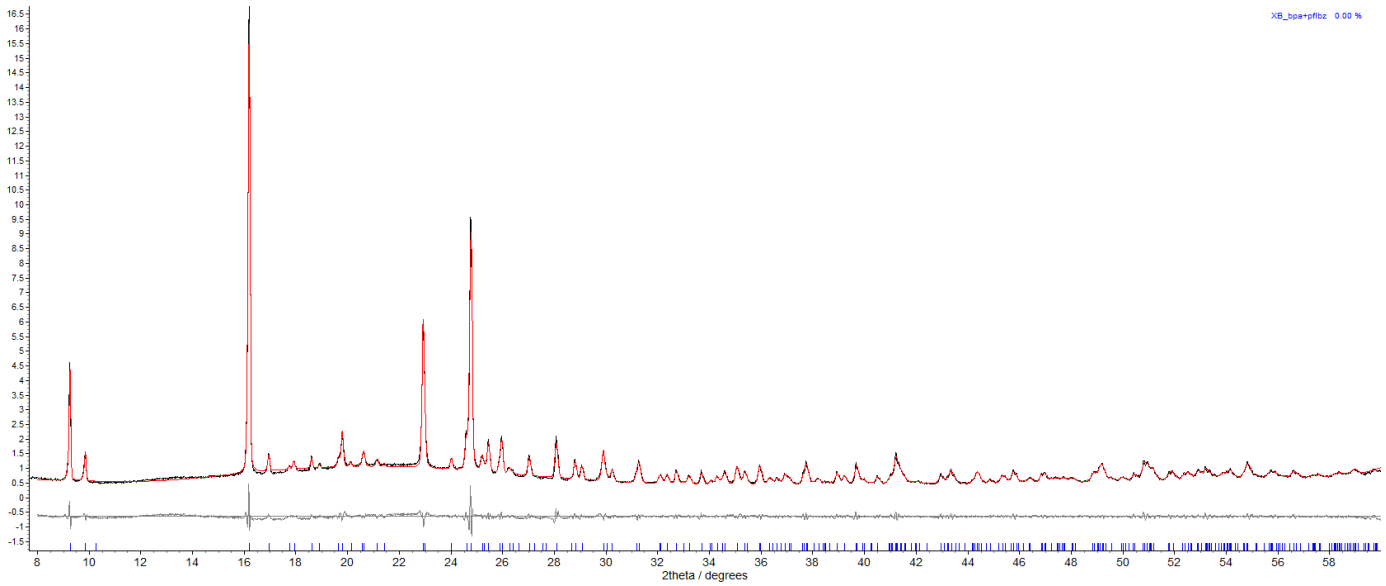


Figure S11.5. Observed (black) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 60 °, d_{min} = 1.54 Å).

System B: Competition experiment in nitromethane

X-ray diffraction data of the white microcrystalline powder were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder pattern for **1•3** (halogen-bonded co-crystal). The unit cell parameters of **1•3** were used as a starting point for Pawley refinement,[S5] employing 302 parameters (10 background, 1 zero error, 5 profile, 6 cell, 280 reflections). Pawley refinement converged to R_{wp} = 0.0372, R_{wp}' = 0.0929. [a = 5.0383 (1) Å, b = 9.9096 (3) Å, c = 10.620 (2) Å, α = 64.785 (2) °, β = 82.142 (2) °, γ = 87.900 (2) °, V = 475.07 (2) Å^3].

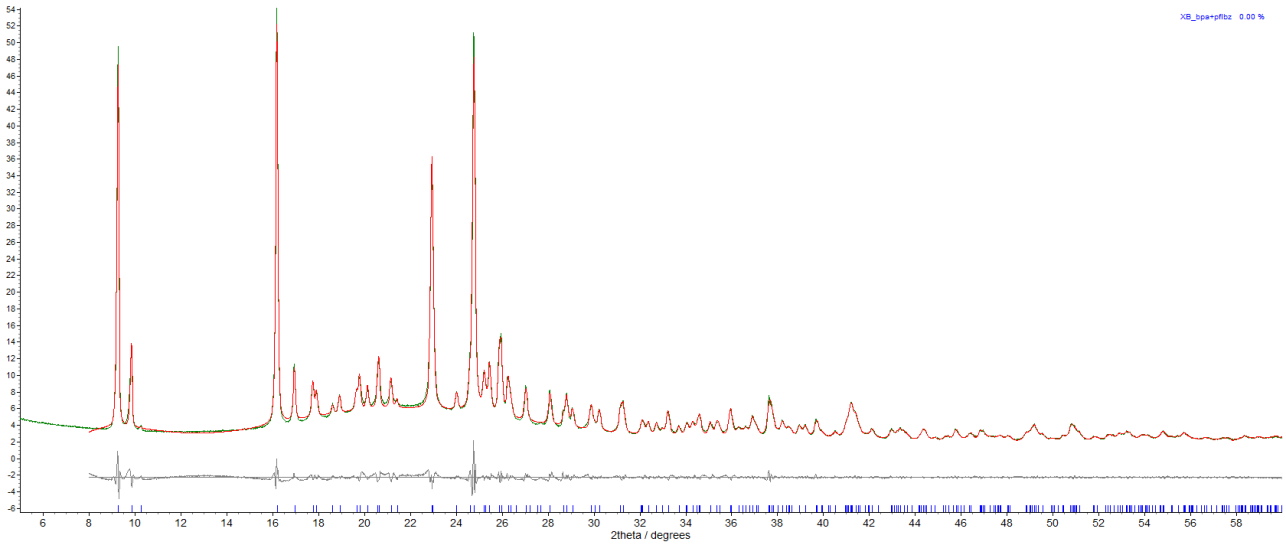


Figure S11.6. Observed (green) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 60 °, d_{min} = 1.54 Å).

System B: Competition experiment in isopropanol

X-ray diffraction data of the white microcrystalline powder were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder pattern for **1•3** (halogen-bonded co-crystal). The unit cell parameters of **1•3** were used as a starting point for Pawley refinement,[S5] employing 301 parameters (10 background, 1 zero error, 5 profile, 6 cell, 279 reflections). Pawley refinement converged to R_{wp} = 0.0387, $R_{wp'}$ = 0.1003. [a = 5.0393 (2) Å, b = 9.9051 (3) Å, c = 10.6223 (3) Å, α = 64.792 (2) °, β = 82.146 (2) °, γ = 87.875 (2) °, V = 475.08 (2) Å^3].

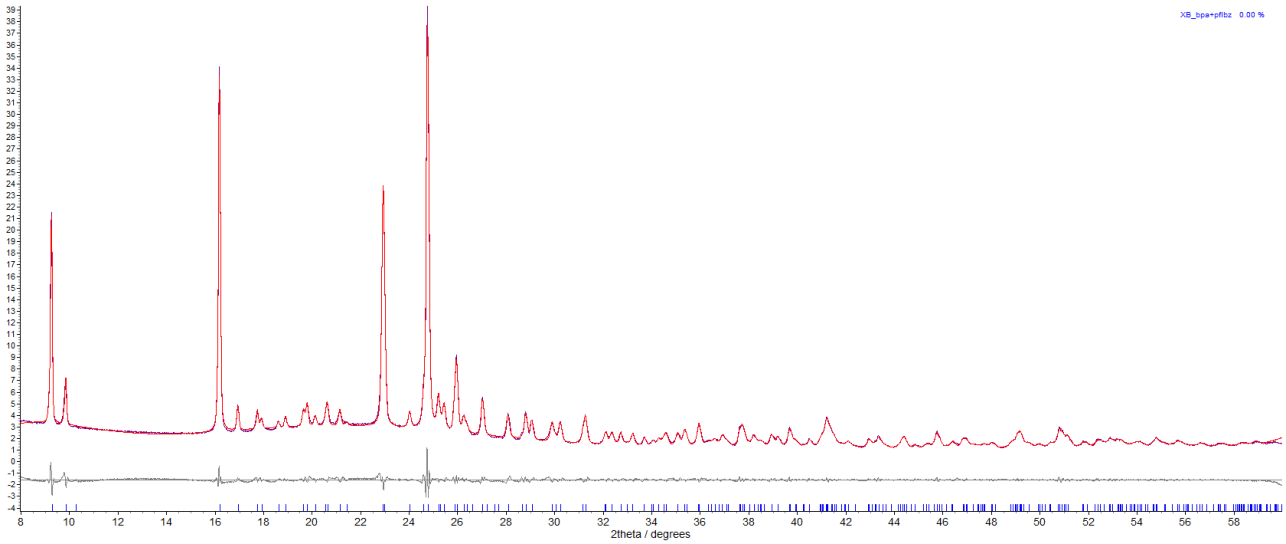
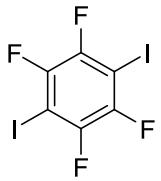
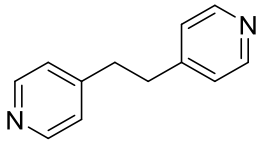


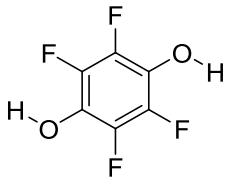
Figure S11.7. Observed (purple) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 8.0 - 60 °, d_{min} = 1.54 Å).

12. Determination of Product Composition by XRPD: System C

[perfluoro-1,4-diiodobenzene (1), perfluorohydroquinone (2c) and 1,2-bis(4-pyridyl)ethane (3)]







The X-ray powder diffraction patterns of the microcrystalline products from all competition experiments were recorded. These were compared to the calculated X-ray powder diffraction patterns for the hydrogen-bonded (**2c•3**) and halogen-bonded (**1•3**) co-crystals as well as the individual components (**1**, **2c** and **3**), before conducting quantitative fitting of the data.

System C: Competition experiment in toluene.

X-ray diffraction data for the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase). The unit cell parameters of **2c•3** were used as a starting point for this Pawley refinement,[S5] employing 257 parameters (14 background, 1 zero error, 5 profile, 6 cell, 277 reflections). Pawley refinement converged to R_{wp} = 0.0364, $R_{wp'}$ = 0.1068. [a = 6.3532 (3) Å, b = 7.4422 (3) Å, c = 9.2290 (4) Å, α = 86.129 (3) °, β = 75.975 (3) °, γ = 71.253 (3) °, V = 400.86 (3) Å^3].

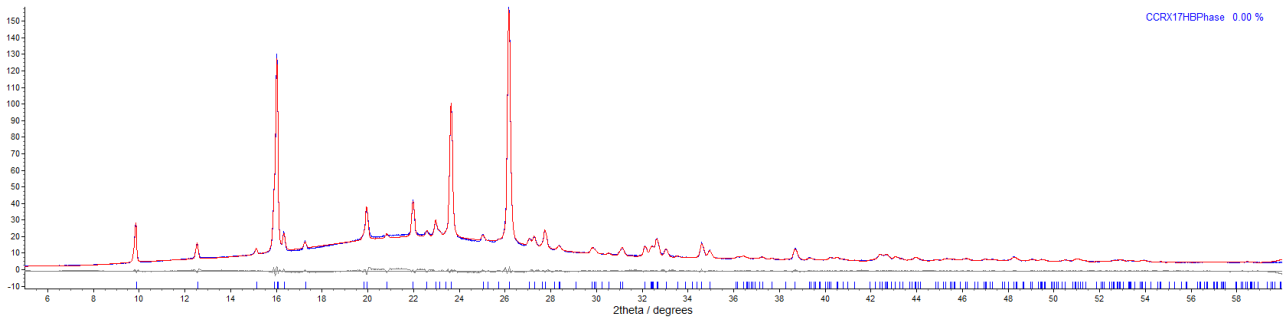


Figure S12.1. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

System C: Competition experiment in Chloroform.

X-ray diffraction data for the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase). The unit cell parameters of **2c•3** were used as a starting point for this Pawley refinement,[S5] employing 256 parameters (13 background, 1 zero error, 5 profile, 6 cell, 277 reflections). Pawley refinement converged to R_{wp} = 0.0344, $R_{wp'}$ = 0.0707. [a = 6.3536 (3) Å, b = 7.4426 (1) Å, c = 9.2272 (2) Å, α = 86.142 (1) °, β = 75.800 (1) °, γ = 71.296 (1) °, V = 400.98 (1) Å^3].

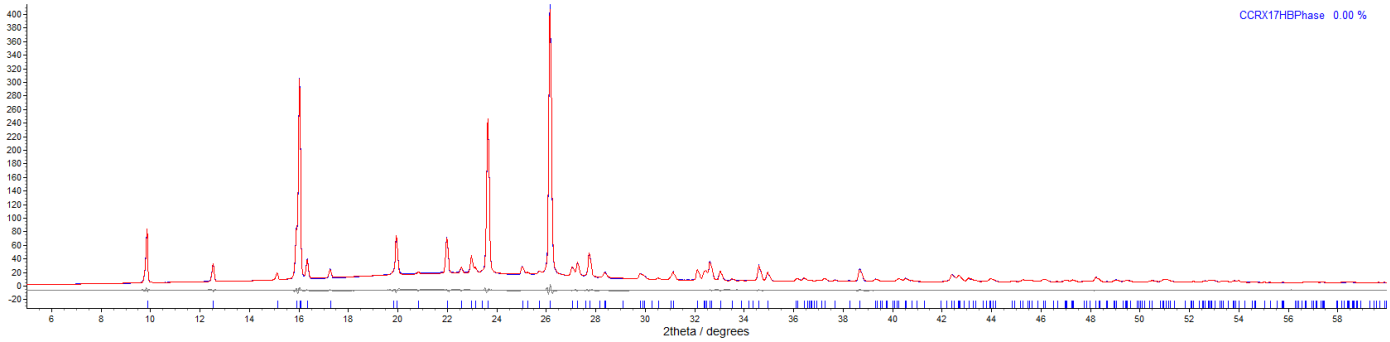


Figure S12.2. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

System C: Competition experiment in dichloromethane.

X-ray diffraction data for the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase). The unit cell parameters of **2c•3** were used as a starting point for this Pawley refinement,[S5] employing 256 parameters (13 background, 1 zero error, 5 profile, 6 cell, 277 reflections). Pawley refinement converged to R_{wp} = 0.0380, $R_{wp'}$ = 0.0756. [a = 6.3552 (2) Å, b = 7.4409 (2) Å, c = 9.2310 (2) Å, α = 86.124 (1) °, β = 75.993 (1) °, γ = 71.238 (2) °, V = 401.00 (2) Å^3].

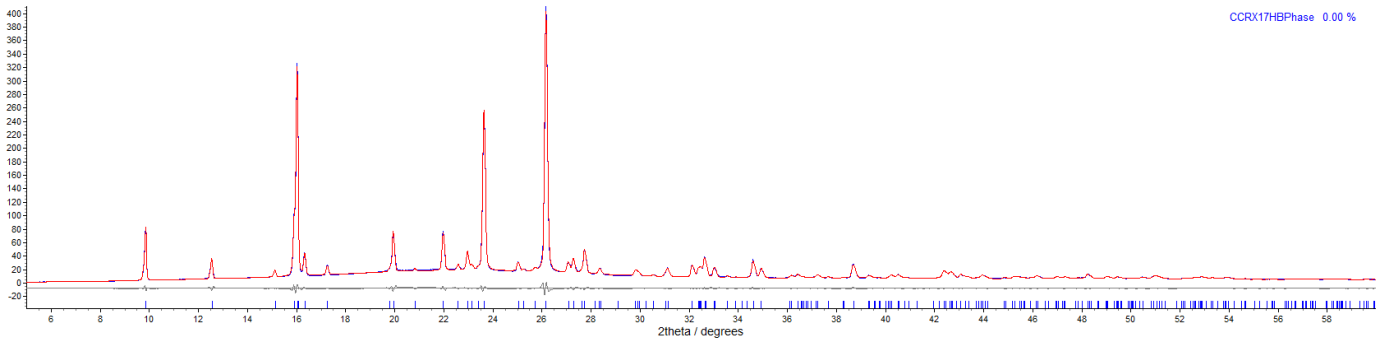


Figure S12.3. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

System C: Competition experiment in acetone

X-ray diffraction data for the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase). The unit cell parameters of **2c•3** were used as a starting point for this Pawley refinement,[S5] employing 256 parameters (12 background, 1 zero error, 5 profile, 6 cell, 232 reflections). Pawley refinement converged to R_{wp} = 0.0477, $R_{wp'}$ = 0.0990. [a = 6.3571 (3) Å, b = 7.4374 (3) Å, c = 9.2277 (4) Å, α = 86.167 (3) °, β = 76.087 (4) °, γ = 71.354 (3) °, V = 401.23 (3) Å^3].

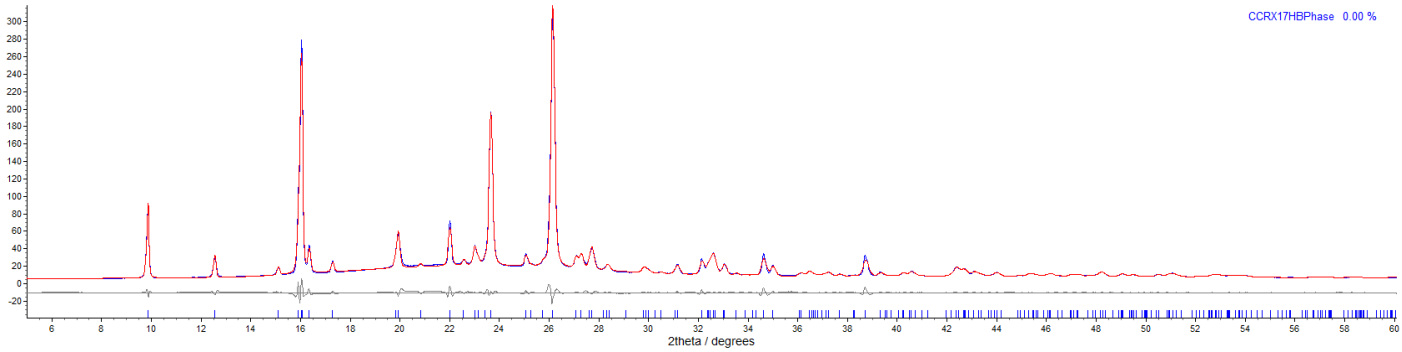


Figure S12.4. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

System C: Competition in acetonitrile

X-ray diffraction data for the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase). The unit cell parameters of **2c•3** were used as a starting point for this Pawley refinement,[S5] employing 256 parameters (12 background, 1 zero error, 5 profile, 6 cell, 232 reflections). Pawley refinement converged to R_{wp} = 0.0369, R_{wp}' = 0.1622. [a = 6.3603 (2) Å, b = 7.4371 (2) Å, c = 9.2348 (2) Å, α = 86.109 (2) °, β = 76.028 (2) °, γ = 71.216 (2) °, V = 401.30 (2) Å^3].

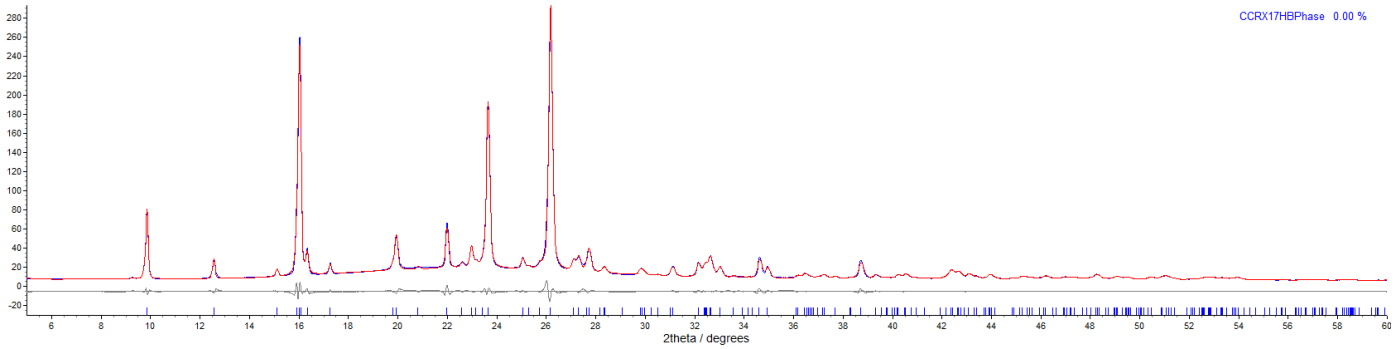


Figure S12.5. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

System C: Competition experiment in nitromethane

X-ray diffraction data for the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (the hydrogen-bonded co-crystal phase). The unit cell parameters of **2c•3** were used as a starting point for this Pawley refinement,[S5] employing 255 parameters (12 background, 1 zero error, 5 profile, 6 cell, 277 reflections). Pawley refinement converged to R_{wp} = 0.0343, $R_{wp'}$ = 0.0754. [a = 6.3561 (1) Å, b = 7.4401 (1) Å, c = 9.2312 (2) Å, α = 86.121 (1) °, β = 75.994 (1) °, γ = 71.228 (1) °, V = 401.001(1) Å^3].

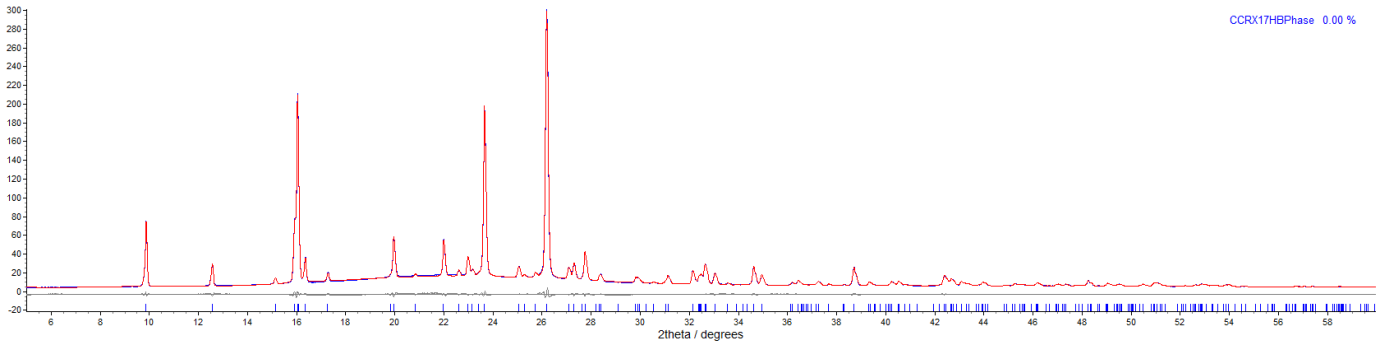


Figure S12.6. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

System C: Competition experiment in isopropanol

X-ray diffraction data of the white microcrystalline product were collected using Cu Kα radiation. The pattern was compared with experimental X-ray powder patterns for **2c•3** (hydrogen-bonded co-crystal) and for **1•3** (halogen-bonded co-crystal). The unit cell parameters of **1•3** and **2c•3** were used as a starting point for a mixed-phase Pawley refinement,[S5] employing 546 parameters (12 background, 1 zero error, 9 profile, 12 cell, 512 reflections), resulting in final indices of fit R_{wp} = 0.0297, $R_{wp'}$ = 0.0615. The starting model used for the mixed-phase Rietveld refinement,[S11] conducted using TOPAS, used atomic coordinates from the single-crystal structures of **1•3** and **2c•3**. Refinement employed 38 parameters (12 background, 1 zero error, 9 profile, 12 cell, 2 scale, 2 global thermal displacement scale factors). Rietveld refinement converged to R_{wp} = 0.0845, $R_{wp'}$ = 0.1550. The relative phase amounts were found to be 69.3 (5) % of **2c•3** and 30.7 (5) % of **1•3**. [Unit cell parameters for **2c•3**: *a* = 6.358 (1) Å, *b* = 7.431 (2) Å, *c* = 9.227 (2) Å, α = 85.87 (2) °, β = 76.04 (1) °, γ = 71.20 (2) °, *V* = 400.5 (2) Å^3; unit cell parameters for **1•3**: *a* = 5.0301 (5) Å, *b* = 9.9476 (9) Å, *c* = 10.622 (1) Å, α = 64.749 (6) °, β = 82.020 (7) °, γ = 87.947 (7) °, *V* = 475.89 (8) Å^3].

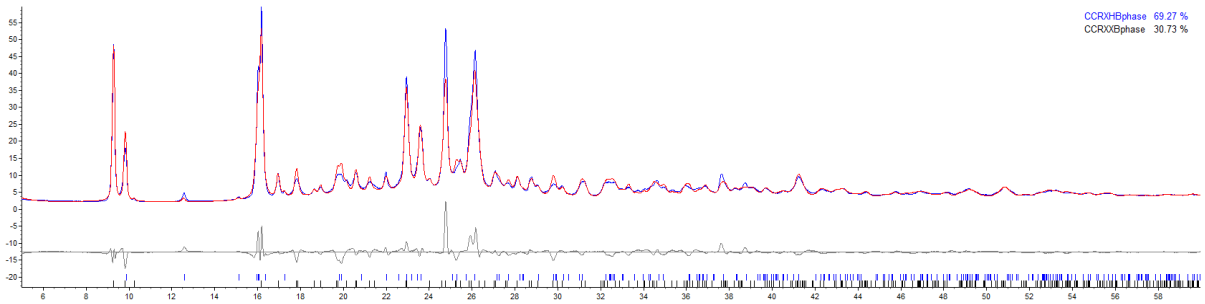


Figure S12.7. Observed (blue) and calculated (red) profiles and difference plot [I_{obs}-I_{calc}] (grey) of the Pawley refinement. (2θ range 5 - 60 °, d_{min} = 1.54 Å).

13. Single Crystal Diffraction Studies

Crystals were mounted on a mylar loop using a viscous hydrocarbon oil and transferred directly to the cold nitrogen stream at 100 K for data collection on a either a Bruker SMART APEX-II CCD diffractometer operating with a Mo-K_α sealed tube X-ray source or Bruker D8 VENTURE diffractometer equipped with the PHOTON 100 CMOS detector, using Cu-K_α micro-focus X-ray source. For Bruker D8 VENTURE collections, intensity data were collected in shutterless mode, with a frame width of 0.5°, and a total exposure of 60 s per degree. A final fast scan was collected at lower incident beam intensity to enable correction for any detector saturation for low-angle data.

A summary of data collection and structure refinement information is provided in Table S3. Intensity data were corrected for absorption using empirical methods (SADABS) based upon symmetry equivalent reflections combined with measurements at different azimuthal angles.[S12] The crystal structure was solved and refined against all F^2 values using the SHELXL[S13] accessed via the Olex2 program.[S14] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions with idealized geometries and then refined by employing a riding model and isotropic displacement parameters. Disordered fluorine and hydrogen atoms in **2b·3** were modelled by refinement of site occupancies.

Table S3. Data collection, structure solution and refinement parameters for crystal structures of 2b•3 and 2c•3

	(2b•3) $C_6H_3F(OH)_2$•$C_{12}H_{12}N_2$	**(2c•3)** $C_6F_4(OH)_2$•$C_{12}H_{12}N_2$
Crystal habitat	Block	Plate
Crystal colour	Colourless	Colourless
Crystal size (mm)	0.14 x 0.12 x 0.02	0.20 x 0.20 x 0.050
Crystal system	Triclinic	Triclinic
Space group, *Z*	*P*-1, 2	*P*-1, 1
a (Å)	7.1389(13)	6.1939(4)
b (Å)	9.2830(15)	7.4692(5)
c (Å)	11.8655(16)	9.0672(6)
α (˚)	95.669(10)	86.863(5)
β (˚)	91.769(11)	75.722(5)
γ (˚)	107.117(13)	71.755(4)
V (Å^3)	749.5(2)	385.97(5)
Wavelength (Å)	1.54178	0.71073
Density (Mg m^{-3})	1.384	1.576
Temperature (K)	100	100
μ (mm^{-1})	0.822	0.136
θ range (˚)	3.751 to 66.961	2.318 to 27.562
Reflns. collected	7125	6725
Independent reflns. (R_{int})	2511 (0.0690)	1778 (0.0313)
Reflns. used in refinement, *n*	2511	1778
LS parameters, *p*	219	119
Restraints, *r*	0	0
*R*1 (*F*)^a *I>2.0s(I)*	0.0700	0.0388
*wR*2 (F^2)^a, all data	0.2097	0.0955
S(F^2)^a, all data	1.018	1.022

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