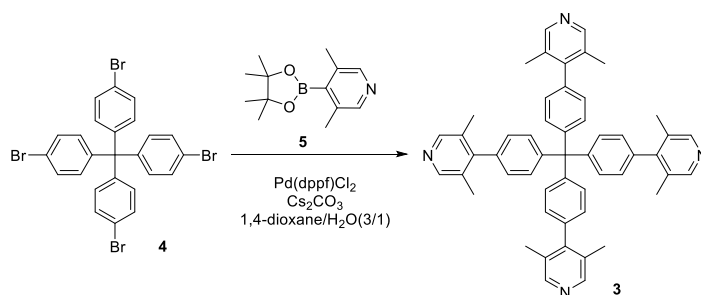


General methods. All reagents were obtained from commercial suppliers and used without further purification unless otherwise noted. ^1H and ^{13}C NMR spectra were recorded with a 400 MHz or 100 MHz spectrometer in the indicated solvents at 25 °C. Chemical shifts are expressed in parts per million (δ) using residual proton resonances of the deuterated solvents as the internal standards. Crystals were measured using Bruker D8 Venture-Metaljet diffractometer equipped with an PHOTON II area detector and HELIOS multilayer optics monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$). Crystal structures were solved by direct method and refined by full-matrix least-squares methods based on F2 using SHELXL-2014 software. X-ray diffraction (XRD) patterns were obtained on a Bruker D8 Advance diffractometer with a Cu K α radiation operated at 40 kV and 40 mA. Hirshfeld surfaces and fingerprint plots were calculated by CrystalExplorer-21.5 software. CCDC (Nos. 2261133, 2261139, 2261140) contains the related crystallographic data, which can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Compound 3. To a solution of compound **4** (365 mg, 0.57 mmol), compound **5** (670 mg, 2.87 mmol), Pd(dppf)Cl₂ (42 mg, 0.057 mmol) and Cs₂CO₃ (819 mg, 1.72 mmol) in 1,4-dioxane/H₂O (20 mL). The reaction mixture was stirred at 85°C for overnight under N₂. The reaction was monitored by TLC. After reaction finished, the mixture was concentrated and purified by flash column chromatography on silica gel eluted with (DCM/MeOH=10/1) to give compound **3** (184 mg, 44 %) as an off-white solid. ^1H NMR (400 MHz, CDCl₃): δ 8.36 (s, 8H), 7.42 (d, $J = 8.4 \text{ Hz}$, 8H), 7.11 (d, $J = 8.8 \text{ Hz}$, 8H), 2.08 (s, 24H). ^{13}C NMR (100 MHz, CDCl₃) δ (ppm): 148.85, 148.47, 145.73, 136.22, 131.39, 130.76, 127.56, 29.72, 17.34. HR-MS (ESI): Calcd for C₅₃H₄₉N₄ [M+H]⁺: 741.3957. Found: 741.3963.

Co-crystal of 1·2. Compound **2** (10.8 mg, 0.027 mmol) and Compound **1** (10 mg, 0.013 mmol) were dissolved in dichloromethane (5.0 mL), and then dimethyl sulfoxide (0.05 mL) was added to the mixture. The co-crystal suitable for X-ray diffraction of compound **1** and **2** was obtained by slowly evaporation crystallization of the mixed solvent.

Co-crystal of solvate 1·2·CHCl₃. Compound **2** (10.8 mg, 0.027 mmol) and Compound **1** (10 mg, 0.013 mmol) were dissolved in chloroform (5.0 mL), and then dimethyl sulfoxide (0.05 mL) was added to the mixture. The co-crystal suitable for X-ray diffraction of compound **1**, **2** and CHCl₃ was obtained by slowly evaporation crystallization of the mixed solvent.

Co-crystal of solvate 1·CHCl₃. Compound **1** (10 mg, 0.013 mmol) were dissolved in

chloroform (5.0 mL). The co-crystal suitable for X-ray diffraction of **solvate 1**·CHCl₃ was obtained by slowly evaporation crystallization of the mixed solvent.

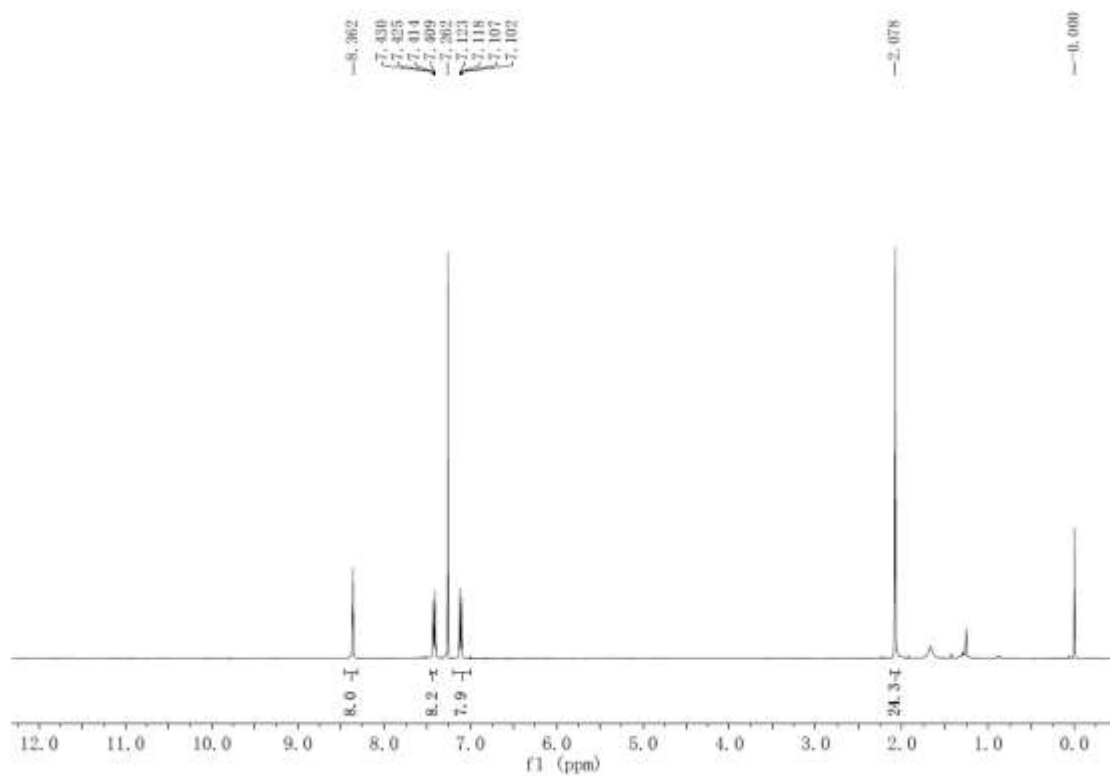


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **3** at 25 °C.

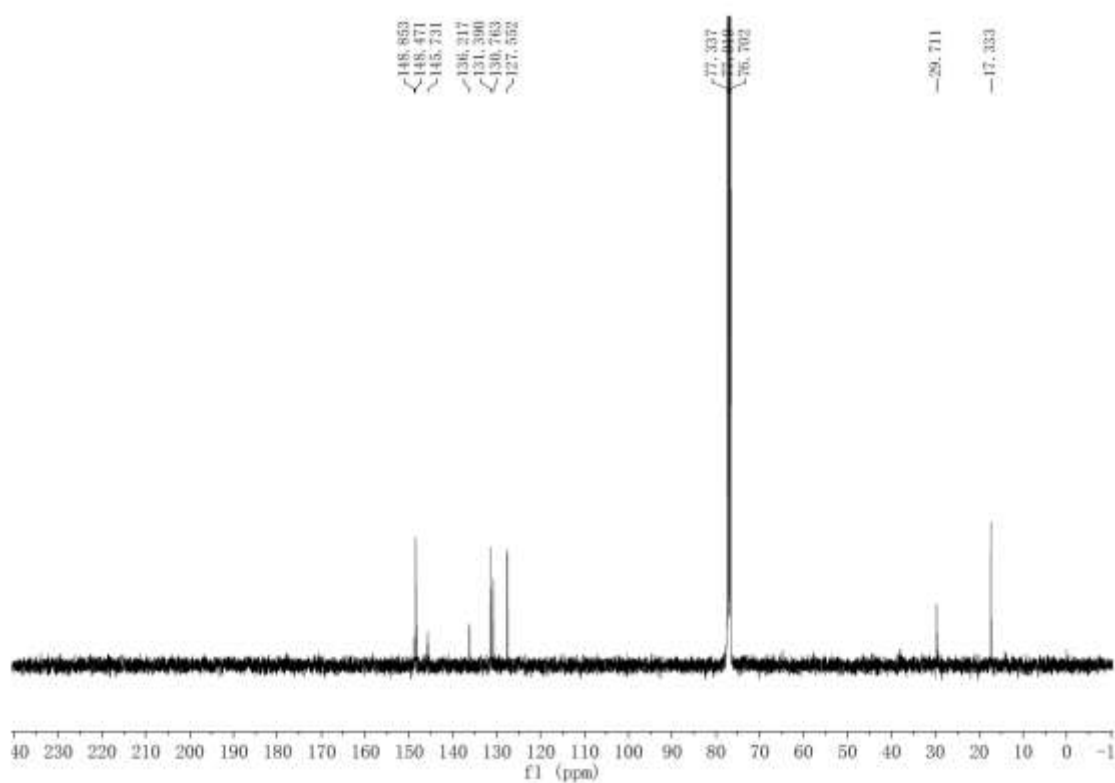


Figure S2. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **3** at 25 °C.

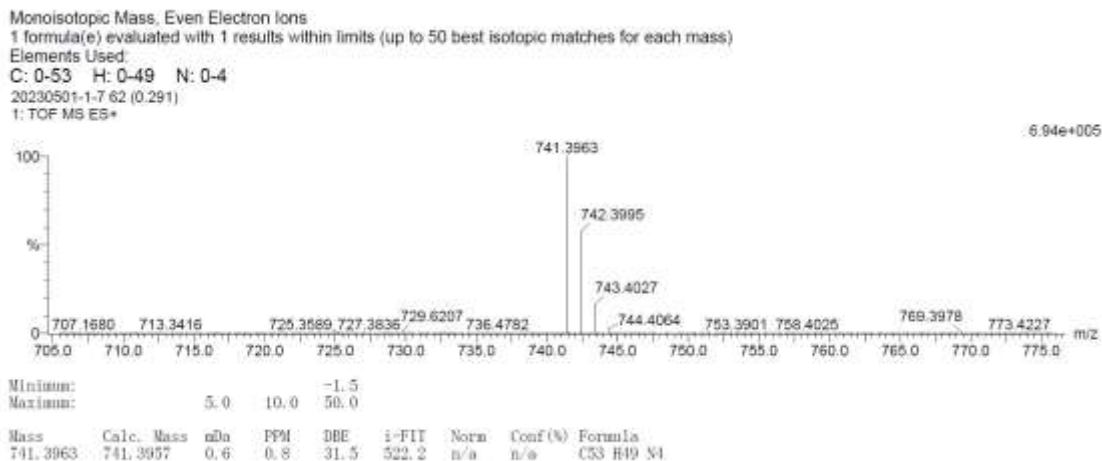


Figure S3. HR-MS (ESI) of compound **3**.

The preparation of powder samples were similar to that of co-crystal samples, but the difference was that the solvent was evaporated quickly, dried under vacuum at room temperature, and then ground with a mortar to obtain samples suitable for powder X-ray diffraction (PXRD).

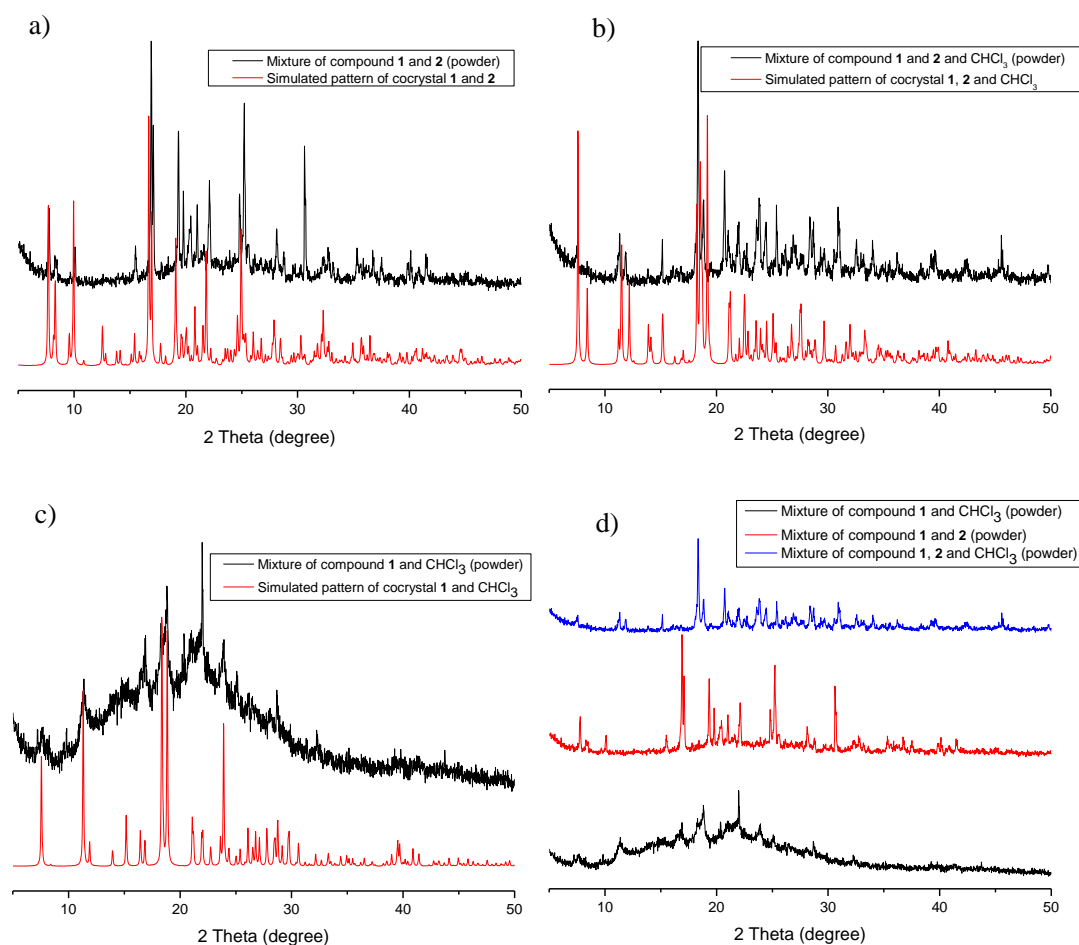


Figure S4. PXRD patterns of powder samples and simulated PXRD pattern of the cocrystal samples. (a) Comparison of the mixture of compound **1** and **2** (powder, red line) and simulated pattern of the co-crystal of **1**·**2** (black line). (b) Comparison of the

mixture of compound **1**, compound **2** and CHCl_3 (powder, red line) and simulated pattern of the co-crystal of **solvate 1·2·CHCl₃** (black line). (c) Comparison of the mixture of compound **1** and CHCl_3 (powder, red line) and simulated pattern of the co-crystal of **solvate 1·CHCl₃** (black line). (d) Comparison of the mixture of compound **1** and CHCl_3 (powder, black line), mixture of compound **1** and compound **2** (powder, red line), mixture of compound **1**, compound **2** and CHCl_3 (powder, blue line). (The equivalence ratio of compound **2** to **1** is 2:1.)

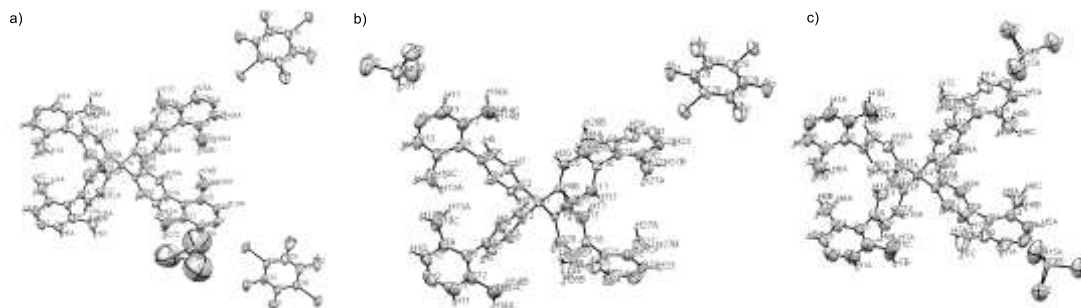


Figure S5. The co-crystal structure of a) **1·2**; b) **solvate 1·2·CHCl₃**; c) **solvate 1·CHCl₃** (all atoms were labeled).

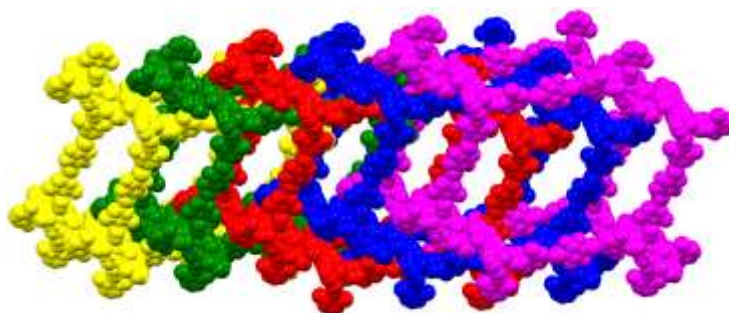


Figure S6. The five-interpenetrated networks of co-crystal **solvate 1·2·CHCl₃** (For clarity, hydrogen atoms and molecules of chloroform were omitted from the interpenetrating structure).

The 3D network structure of co-crystal **solvate 1·2·CHCl₃** exhibited five-interpenetrated networks (Figure S5). From the crystal structure, it can be seen that the red grid unit in the middle was associated with four other grid units on the left and right sides, resulting in a five-interpenetrated structure.

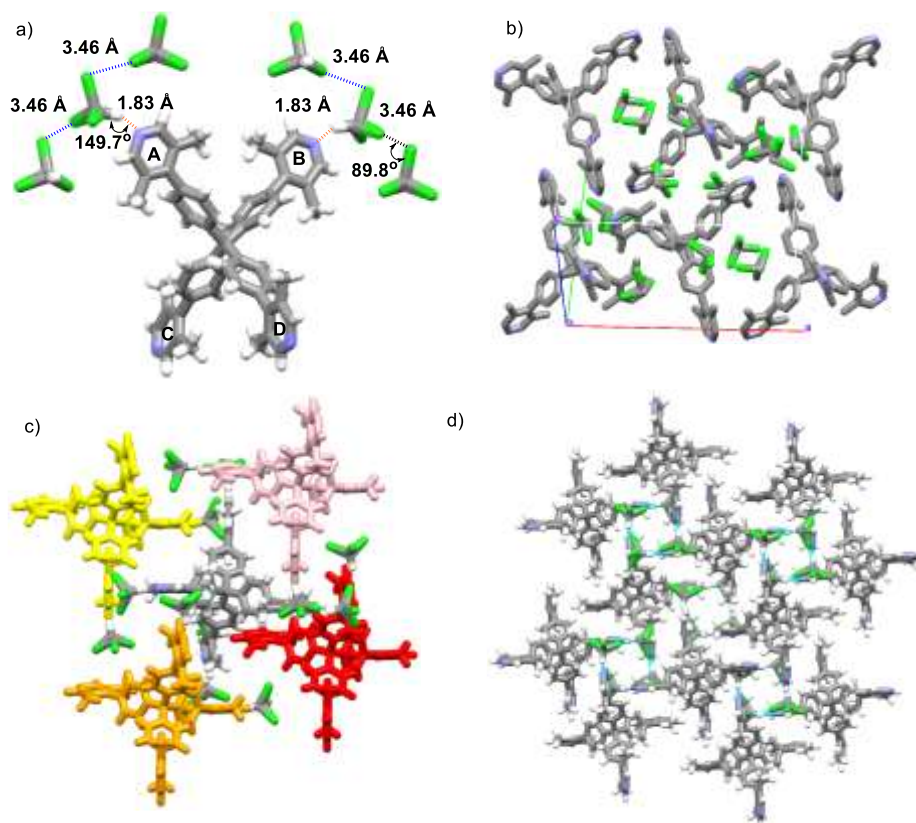


Figure S7. a) The co-crystal structure of **solvate 1·CHCl₃**. (For clarity, molecules of chloroform associated with pyridine rings C and D were not shown). b) The intermolecular packing mode of compound **1** (For clarity, the hydrogen atoms in compound **1** were omitted). c) The five-monomer array. d) The 3D supramolecular XBOF.

When compound **1** was crystal cultured in chloroform without compound **2**, as expected, the co-crystal suitable for X-ray diffraction of compounds **solvate 1·CHCl₃** was obtained. The asymmetric unit has one quarter of compound **1** with C14 centre and one molecule of CHCl₃ in a general position and linked to compound **1** by a well-defined C15-H15···N1 hydrogen bond. And the co-crystal structure revealed that The N atoms in the four terminal pyridine groups of compound **1** were respectively hydrogen-bonded (H···N distance: 1.83 Å, C-H···N bond angle: 149.7°) to a chloroform molecules. Each molecule of chloroform further bonded two other molecules of chloroform through Cl···Cl (Cl···Cl distance: 3.459(5) Å, C-Cl···Cl bond angle: 89.8(5)°) halogen bonding (Figure S7a, 7b). Detailed halogen and hydrogen bond lengths and angles for co-crystal of solvate **1·CHCl₃** were given in Table S4-S5. The three nearest molecules of chloroform were hydrogen-bonded with pyridine terminals, which belong to three independent monomers, to form a five-monomer array shown in Figure S7c. In this five-monomer array, one tetraphenylmethane tetrapyridine molecule associated with other four molecules simultaneously through H···N hydrogen bonding and Cl···Cl halogen bonding, and the other four molecules further binded to other molecules. Finally, a 3D supramolecular XBOF was obtained (Figure S7d).

Table S1 Halogen bonds for co-crystal of **1·2** [Å and °]

D-I...A	d(D-I)	d(I...A)	d(D...A)	<(DIA)
C(30)-I(1)...N(1)	2.100(8)	2.849(6)	4.95(1)	178.4(2)
C(33)-I(2)...N(2)	2.092(7)	2.859(7)	4.93(1)	170.5(2)

Table S2 Hydrogen bonds for co-crystal of **solvate 1·2·CHCl₃** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(31)-H(31)...N(2)	0.98	2.33	3.24(3)	153

Table S3 Halogen bonds for co-crystal of **solvate 1·2·CHCl₃** [Å and °]

D-I...A	d(D-I)	d(I...A)	d(D...A)	<(DIA)
C(29)-I(1)...N(1)	2.09(1)	2.83(1)	4.92(2)	176.5(5)

Table S4 Hydrogen bonds for co-crystal of **solvate 1·CHCl₃** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(15)-H(15A)...N(1)	0.979	1.829	2.72(1)	149.7

Table S5 Halogen bonds for co-crystal of **solvate 1·CHCl₃** [Å and °]

D-Cl...A	d(D-Cl)	d(Cl...A)	d(D...A)	<(DCIA)
C(15')-Cl(3)...Cl(1)	1.85(1)	3.459(5)	3.91(1)	89.8(5)

Table S6 Crystal data and structure refinement of co-crystal of **1·2**, co-crystal of **solvate 1·2·CHCl₃** and co-crystal of **solvate 1·CHCl₃**.

	co-crystal of 1·2	co-crystal of solvate 1·2·CHCl₃	co-crystal of solvate 1·CHCl₃
Formula	C ₆₆ H ₄₈ Cl ₃ F ₈ I ₄ N ₄	C ₆₁ H ₅₀ Cl ₆ F ₄ I ₂ N ₄	C ₅₇ H ₅₂ Cl ₁₂ N ₄
Mr.	1663.03	1381.55	1218.43
Cryst. system	Monoclinic	Monoclinic	Tetragonal
<i>T</i> (K)	296	297	296
Space group	C2/c	C2/c	I4(1)/a
<i>a</i> /Å	13.123(4)	29.043(3)	21.037(5)
<i>b</i> /Å	43.843(14)	14.0514(12)	21.037(5)
<i>c</i> /Å	13.393(4)	20.8239(17)	14.026(4)
<i>α</i> /Å	90	90	90
<i>β</i> /Å	114.914(5)	133.661(2)	90
<i>γ</i> /Å	90	90	90
<i>V</i> (Å ³)	6989(4)	6147.9(10)	6207(3)
<i>Z</i>	4	4	4
<i>D_x</i> (g/cm ³)	1.581	1.493	1.304
<i>μ</i> (mm ⁻¹)	1.959	1.337	0.574
<i>F</i> (000)	3228.0	2752.0	2504.0
R (reflections)	0.0442 (4773)	0.1065 (3854)	0.1350 (1707)
wR2 (reflections)	0.1422 (6077)	0.2587 (5405)	0.2750 (2658)

Co-crystal of 1.2

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: a

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	Calculated	Reported	
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Hall group	-C 2yc	?	
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Sum formula	C66 H48 Cl3 F8 I4 N4	C66 H48 Cl3 F8 I4 N4	
Mr	1663.03	1663.03	
Dx, g cm-3	1.581	1.581	
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Mu (mm-1)	1.959	1.959	
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F000'	3223.55		
h, k, lmax	15, 52, 15	15, 52, 15	
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S =	1.058	Npar=	393

Co-crystal of 1.2

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C1	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C9	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C17	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C15	Check
PLAT250_ALERT_2_C	Large	U3/U1	Ratio for Average U(i,j) Tensor	3.8	Note
PLAT260_ALERT_2_C	Large	Average	Ueq of Residue Including	C11	0.295	Check
PLAT342_ALERT_3_C	Low	Bond	Precision on C-C Bonds	0.00871	Ang.
PLAT601_ALERT_2_C	Unit	Cell	Contains Solvent Accessible VOIDS of	.	89	Ang**3

Alert level G

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PLAT005_ALERT_3_G	No Embedded	Refinement Details	Found in the CIF		Please	Do !
PLAT083_ALERT_2_G	SHELXL	Second	Parameter in Wght	Unusually	Large	15.90 Why ?
PLAT300_ALERT_4_G	Atom Site	Occupancy of C11	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site	Occupancy of C34	Constrained at		0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue	Disorder (Read 3 1			50%	Note
PLAT380_ALERT_4_G	Incorrectly?	Oriented X(sp2)-Methyl	Molety	C7	Check
PLAT380_ALERT_4_G	Incorrectly?	Oriented X(sp2)-Methyl	Molety	C6	Check
PLAT431_ALERT_2_G	Short	Inter HL..A	Contact I1	..N1	2.85	Ang.
				1+x,-1+y,z =	1.645	Check
PLAT431_ALERT_2_G	Short	Inter HL..A	Contact I2	..N2	2.86	Ang.
				3/2-x,-1/2+y,3/2-z =	4.646	Check
PLAT764_ALERT_4_G	Overcomplete	CIF	Bond List	Detected (Rep/Expd)	.	1.16 Ratio
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PLAT899_ALERT_4_G	SHELXL97	is	Deprecated and Succeeded by	SHELXL/	2018	Note

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
10 ALERT level C = Check, Ensure it is not caused by an omission or oversight
19 ALERT level G = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

Co-crystal of 1.2

```
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

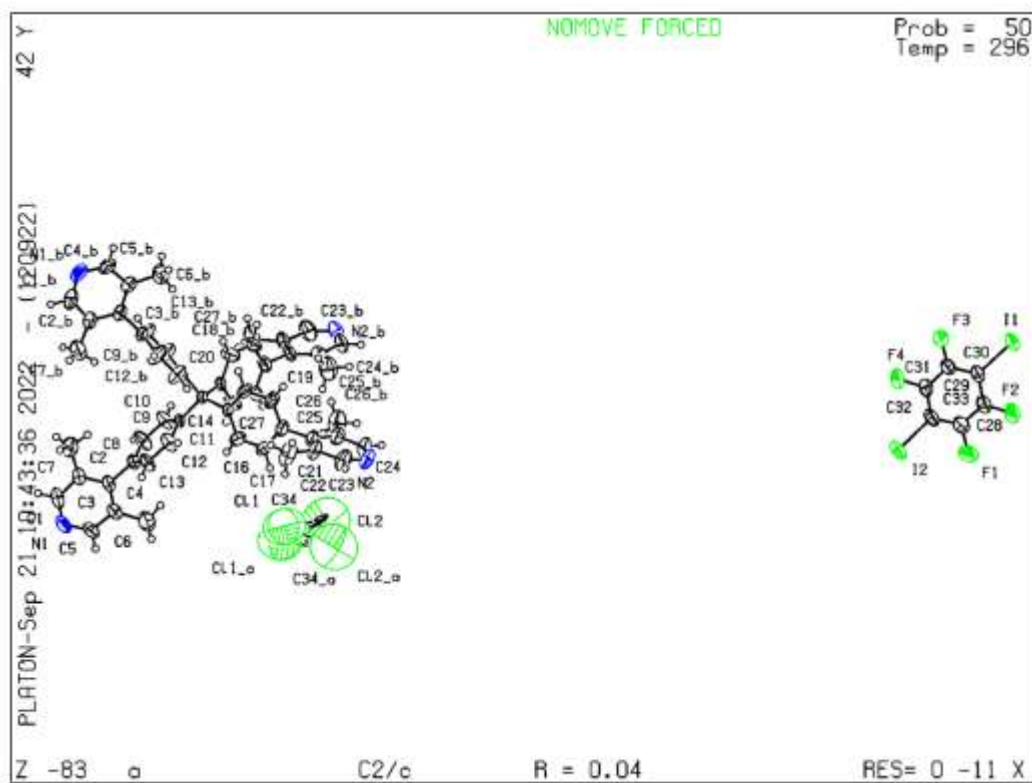
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Co-crystal of 1·2



Co-crystal solvate 1·2·CHCl₃

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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No syntax errors found. CIF dictionary Interpreting this report

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	Calculated	Reported	
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Hall group	-C 2yc	-C 2yc	
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Dx, g cm ⁻³	1.493	1.493	
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Mu (mm ⁻¹)	1.337	1.337	
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F000'	2752.73		
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S =	1.110	Npar=	352

Co-crystal solvate 1·2·CHCl₃

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.187
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.187 Report

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoletyFormula Strings Differ Please Check
PLAT082_ALERT_2_C High R1 Value 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.26 Report
PLAT220_ALERT_2_C NonSolvent Resd I C Ueq(max)/Ueq(min) Range 6.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd I H Uiso(max)/Uiso(min) Range 4.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C23 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C9 --C13 0.20 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C31 Check
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PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11 0.126 Check
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PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C15 -C20 1.36 Ang.
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PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 40 Ang**3
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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.722 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.606 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.482 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 10 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 5 Note

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 121.61 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/4 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Molety C27 Check
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1-x,y,3/2-z = 2_656 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact I1 ..C24 3.46 Ang.
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PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 54% Note
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PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

Co-crystal solvate 1·2·CHCl₃

```
0 ALERT level A - Most likely a serious problem - resolve or explain
2 ALERT level B - A potentially serious problem, consider carefully
25 ALERT level C - Check, Ensure it is not caused by an omission or oversight
11 ALERT level G - General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
13 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

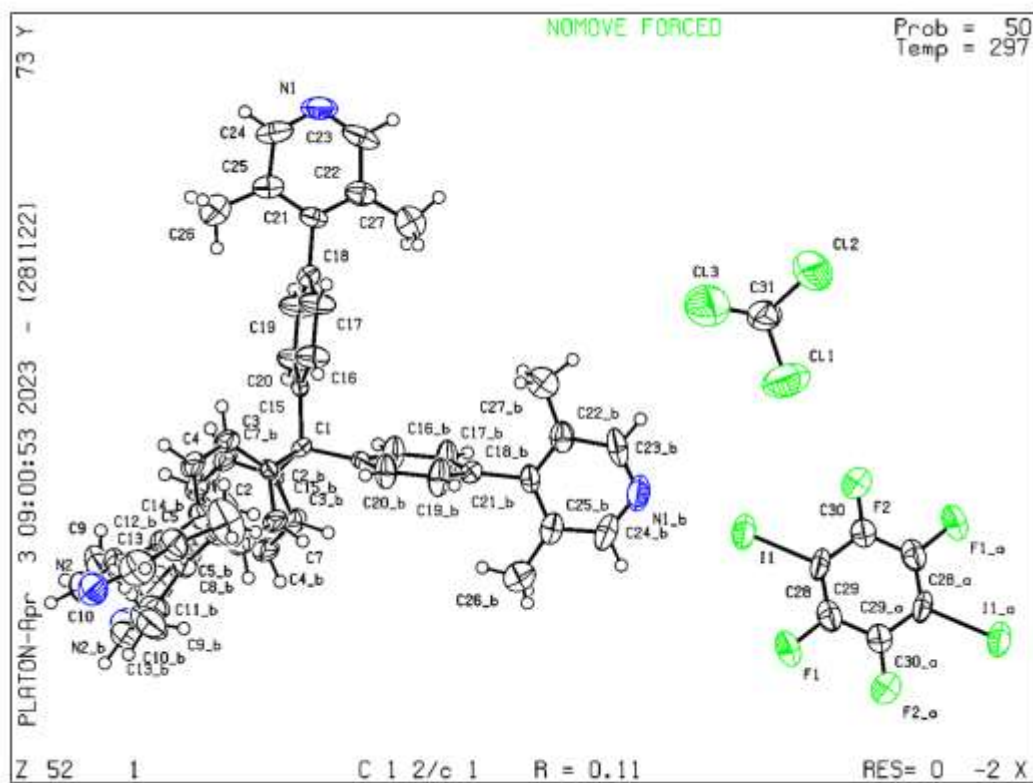
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT212_ALERT_2_B ADP of Atom C15 is N.P.D. or (nearly) 2D . Please Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01057 Ang.

Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.970 Why?
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ... 2.875 Sigma
PLAT082_ALERT_2_C High R1 Value 0.14 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report
PLAT220_ALERT_2_C NonSolvent Resd I C Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C11 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C12 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11 0.113 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C8 -C13 . 1.37 Ang.
PLAT336_ALERT_2_C Long Bond Distance for C15 -C11 1.881 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C53 H48 N4

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 72.00 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of C15 Constrained at 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15' Constrained at 0.4 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 25% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C7 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact N1 ..C15 . 2.72 Ang.
-1/2+x,y,3/2-z = 10_557 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.19 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 12.20 Deg.
C15' -C11 -C15 1_555 1_555 1_555 # 2 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 13.20 Deg.
C15' -C12 -C15 1_555 1_555 1_555 # 3 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 7.70 Deg.
C15' -C13 -C15 1_555 1_555 1_555 # 4 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 6 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note

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