Supporting Information

Dissecting the Conformational and Interaction Topological Landscape of *N*-ethynylphenylbenzamide by the Device of Polymorphic Diversity

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CSD search of all reported *N*-phenylbenzamides yielded 1500 hits:

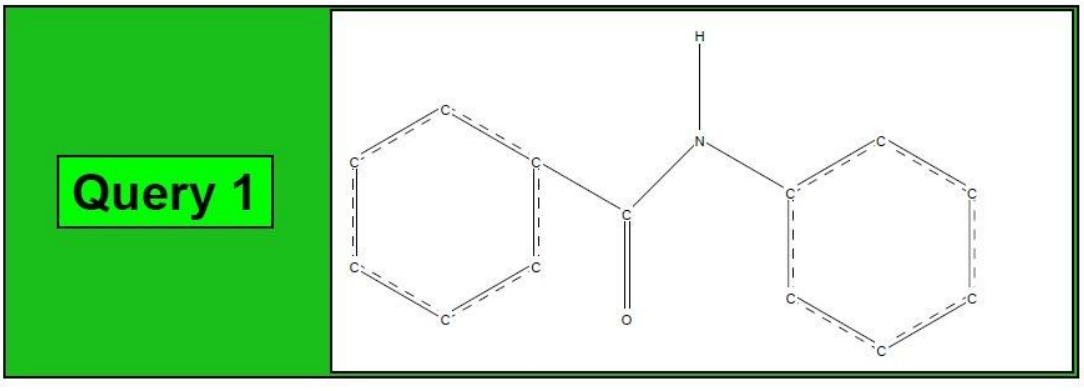
Search Overview

Search:	search8
Date/Time done:	Fri Mar 30 20:11:51 2018
Database(s):	CSD version 5.39 updates (Nov 2017) CSD version 5.39 (November 2017) CSD version 5.39 (November 2017) CSD version 5.39 updates (Feb 2018)
Restriction Info:	No refcode restrictions applied
Filters:	3D coordinates determined Only Single crystal structures Only Organics
Percentage Completed:	100%
Number of Hits:	1500

Single query used. Search found structures that:

match

Query 1



Reported Polymorphs of the *N*-phenylbenzamide moiety with the text search '*Polymorph*' (120 hits):

Search Overview

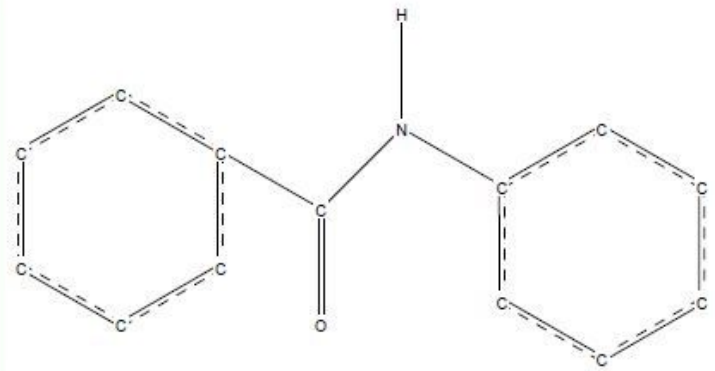
Search:	search9	
Date/Time done:	Fri Mar 30 20:14:52 2018	
Database(s):	CSD version 5.39 updates (Nov 2017) CSD version 5.39 (November 2017) CSD version 5.39 (November 2017) CSD version 5.39 updates (Feb 2018)	
Restriction Info:	No refcode restrictions applied	
Filters:	3D coordinates determined Only Single crystal structures	Not polymeric Only Organics
Percentage Completed:	100%	
Number of Hits:	102	

Summary of queries used. Search found structures that:

match

Query 1 **Query 2**

Query 1



Query 2

Text Search **polymorph**

Crystallization of Polymorphs

All the newly synthesized (scheme described in the reference 28) bulk compounds were put for crystallization (2-3 mg of each) in a large number of single component and different mixture of organic solvents in various conditions by slow to fast evaporation methods. At least 60-80 different crystallization combinations for each compounds were taken for screening of polymorphic forms. In addition, melt crystallization technique was also used by varying different heating/ cooling rates in DSC for crystallization. All positive crystallization outcomes are shown in Table S1.

Table S1. Screening of polymorphic forms (only positive crystallization attempts are shown) obtained from various techniques

Method	Solvent medium	Conditions	Polymorphic phase*
		***p*-TF**	
Slow evaporation	Ethanol	RT (25-28 °C)	Form I
Fast evaporation	Ethanol	40-42 °C (at programmable oven)	Form I
Melt crystallization (oven)	-	-	Form I
Slow evaporation	Toluene	RT (25-28 °C)	Form II
Slow evaporation	Benzene	RT (25-28 °C)	Form II
Slow evaporation	Isopropanol	RT (25-28 °C)	Form I
		23-F	
Slow evaporation	DCM+Hex.	LT (4-6 °C)	Form I and III (concomitance; The **Form III** was not observed further)
Slow evaporation	Hexaflurobenzene	RT (25-28 °C)	Form II
Slow evaporation	Deuterated chloroform	LT (4-6 °C)	Form I
Slow evaporation	Acetonitrile	RT (25-28 °C)	Form I
		24-F	
Slow evaporation	DCM+Hex.	LT (4-6 °C)	Form I
Slow evaporation	Hexafluorobenzene	RT (25-28 °C)	Form II
Slow evaporation	Toluene	RT (25-28 °C)	Form I
Slow evaporation	Benzene	RT (25-28 °C)	Form I
		25-F	
Slow evaporation	Methanol	RT (25-28 °C)	Form I

Melt crystallization (DSC)	-	Heating/ Cooling at 1°C min^{-1}	Form I
Slow evaporation	DCM+Hex.	LT (4-6 °C)	Form II
Slow evaporation	Hexafluorobenzene	RT (25-28 °C)	Form II
Slow evaporation	Trifluorotoluene	RT (25-28 °C)	Form II
Slow evaporation	Deuterated chloroform	LT (4-6 °C)	Form III
26-F			
Slow evaporation	DCM+Hex.	LT (4-6 °C)	Form I
Slow evaporation	Toluene	RT (25-28 °C)	Form I
Slow evaporation	Benzene	RT (25-28 °C)	Form I
Melt crystallization (DSC)	-	Heating/ Cooling at 3 and 10 °C min^{-1}	Form II
***p*-Cl**			
Slow evaporation	DCM+Hex.	LT (4-6 °C)	Form I
Slow evaporation	Acetonitrile	RT (25-28 °C)	Form I
Slow evaporation	Toluene	RT (25-28 °C)	Form I
Slow evaporation	Benzene	RT (25-28 °C)	Form I
Slow evaporation	Methanol	RT (25-28 °C)	Form II
Slow evaporation	Ethanol	RT (25-28 °C)	Form II
Slow evaporation	Isopropanol	RT (25-28 °C)	Form III
***o*-Br**			
Slow evaporation	Toluene	RT (25-28 °C)	Form I
Slow evaporation	Acetonitrile	RT (25-28 °C)	Form I
Slow evaporation	Hexafluorobenzene	RT (25-28 °C)	Form II

***** Confirmed by the SCXRD for various randomly picked single crystals in each crystallization container. See below for the crystal images.

Single Crystal X-ray Diffraction (SCXRD), Structure Solution and Refinement

Single crystal data of all polymorphic phases have been collected either on the Bruker D8 VENTURE diffractometer equipped with CMOS type PHOTON 100 detector or on the Bruker Smart Apex II CCD instrument (as mentioned in the individual cif) using monochromated Mo Kα radiation (λ = 0.71073 Å). Unit cell measurement, data collection, integration, scaling and absorption corrections for the crystal were done using Bruker Apex II software.[1] Data reduction was performed by Bruker SAINT Suite.[2] The crystal structures were solved by direct methods using by SHELXS-2013 [3]/ SIR 2014 [4] program. All structures were refined by the full matrix least squares method using SHELXL-2016 [5] present in the program suite WinGX (version 2014.1) [6]. Absorption correction (multi-scan)

was applied using SADABS [7]. All non-hydrogen atoms were refined anisotropically and all hydrogen atoms were positioned geometrically [HFIX 43 for C(sp^2), N and HFIX 163 for C(*sp*)] and refined using a riding model. The diflurophenyl ring of the second symmetry independent molecule for **24-FII** structure was refined as two components positional disorder the final occupancy refining in the ratio of 83:17. Similarly, the bromophenyl ring of ***O*-BrI** structure was also refined as two-component positional disorder (90:10). All ORTEPs were generated using Mercury 3.8 (CCDC) program.[8] Geometrical calculations were carried out using PARST [9] and PLATON.[10]

Crystal morphologies of all polymorphs in all molecules-

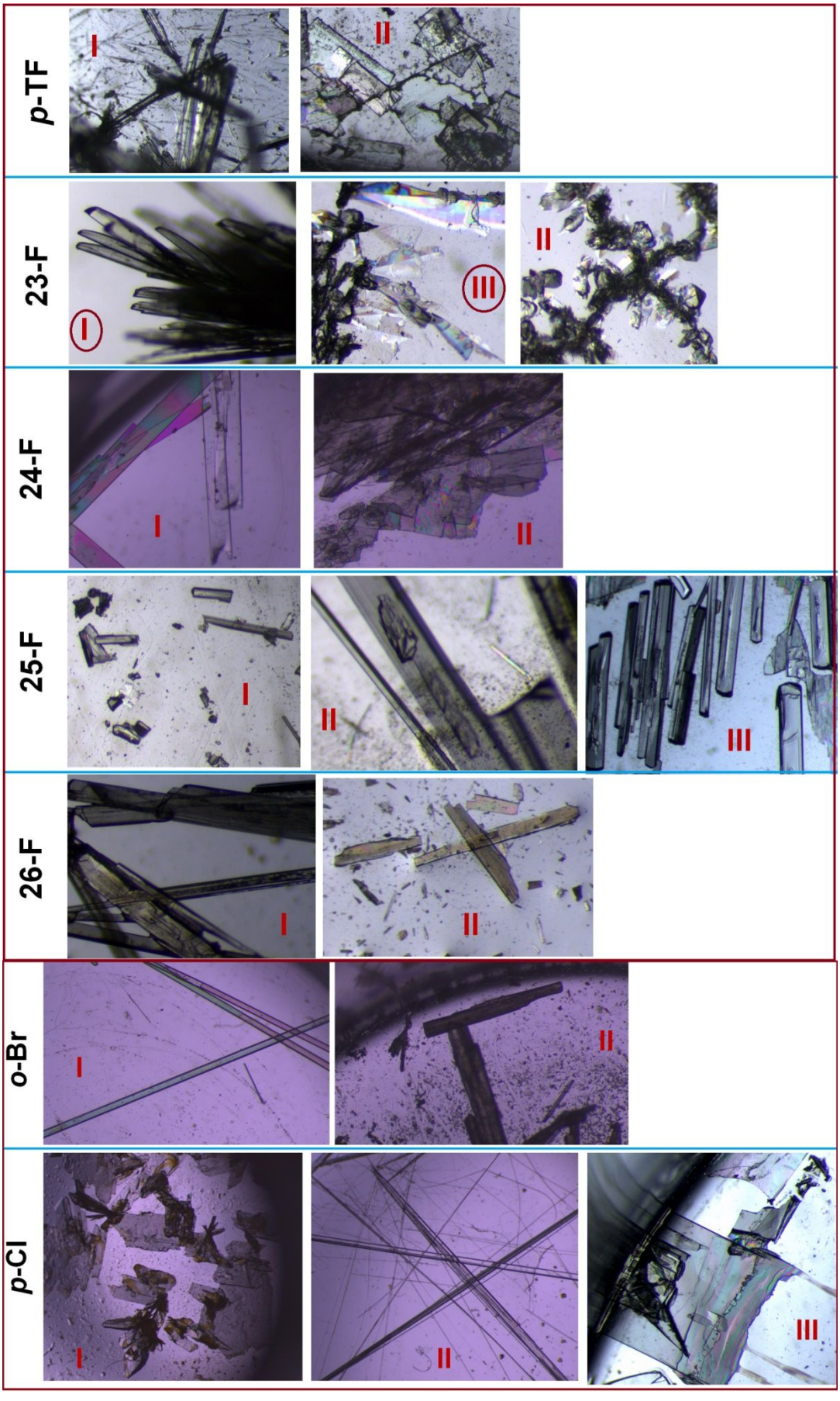


Table S2. Single crystal X-ray diffraction data and refinement parameters for all new crystal structures

	p-TF		23-F		
	I	**II**	**I**	**II**	**III**
Formula	$C_{16}H_{10}F_3NO$	$C_{16}H_{10}F_3NO$	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$
Formula weight	289.25	289.25	257.23	257.23	257.23
CCDC number	1870729	1870732	1870720	1870717	1870716
Temperature/K	100(2)	100(2)	110(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	$P2_1/c$	Pn	P-1	$P1$
***a* (Å)**	5.1535(3)	27.759(2)	8.4570(2)	5.1329(7)	4.5110(3)
***b* (Å)**	14.3809(10)	5.0104(4)	13.3235(3)	8.8511(14)	5.0837(3)
***c* (Å)**	17.7643(12)	19.5535(18)	10.5043(3)	12.867(2)	12.7338(9)
$\alpha/\beta/\gamma$ (°)	90/ 97.165(2)/ 90	90/107.800(3) / 90	90/ 90.222(2) /90	91.063(6)/92.926(5)/ 90.026(5)	93.872(3)/92.090(3) / 90.106(3)
V(Å^3)	1306.27(15)	2589.4(4)	1183.58(5)	583.72(15)	291.16(3)
Z	4	8	4	2	1
Density (g cm^{-3})	1.471	1.484	1.444	1.464	1.467
F (000)/ μ (mm^{-1})	592/ 0.122	1184/ 0.123	528/ 0.113	264/ 0.114	132/ 0.114
θ (min, max)	2.711, 30.108	2.188, 27.876	1.528, 28.694	2.301, 29.566	3.209, 30.102
$h_{min, max}$, $k_{min, max}$, $l_{min, max}$	-7 5, -20 20, -24 25	-36 36, -6 6, -25 25	-11 11, -18 18, -14 14	-7 7, -12 12, -17 17	-6 6, -7 7, -17 17
No. of ref.	18640	38251	18327	22217	12058
No. of unique ref./ obs. Ref.	3843/ 2532	6182/ 4612	5557/ 4292	3270/ 2378	3416/ 2676
No. parameters	190	379	344	172	172
R_{all}, R_{obs}	0.0972, 0.0516	0.0637, 0.0419	0.0642, 0.0463	0.0807, 0.0489	0.0814, 0.0519
$wR2_{all}$, $wR2_{obs}$	0.1191, 0.1028	0.1091, 0.0993	0.1120, 0.1017	0.1155, 0.1015	0.1092, 0.0975
$\Delta\rho_{min, max}$ (eÅ^{-3})	-0.372, 0.348	-0.249, 0.341	-0.274, 0.206	-0.327, 0.338	-0.359, 0.269
G. O. F.	1.006	1.031	1.062	1.047	1.041

	24-F		25-F		
	I	**II**	**I**	**II**	**III**
Formula	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$
Formula weight	257.23	257.23	257.23	257.23	257.23
CCDC number	1870718	1870723	1870719	1870722	1870724
Temperature/K	100(2)	100(2)	110(2)	110(2)	110(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/c$	$P2_1$	$C2/c$	$P2_1/n$	$Pna2_1$
***a* (Å)**	13.9185(10)	6.7906(2)	25.8507(6)	6.7728(2)	15.0658(4)
***b* (Å)**	4.9937(4)	25.1321(7)	6.62700(10)	11.1204(3)	6.6213(2)
***c* (Å)**	17.0918(12)	6.9320(2)	13.8577(3)	15.5379(3)	23.1760(6)
$\alpha/\beta/\gamma$ (°)	90/ 97.502(6) / 90	90/ 92.416(2) / 90	90/101.888(2) / 90	90/93.9210(10)/ 90	90/ 90/ 90
V(Å^3)	1177.79(15)	1181.98(6)	2323.08(8)	1167.52(5)	2311.93(11)
Z	4	4	8	4	8
Density (g cm^{-3})	1.451	1.446	1.471	1.463	1.478
F (000)/ μ (mm^{-1})	528/ 0.113	528/ 0.113	1056/ 0.115	528/ 0.114	1056/ 0.115
θ (min, max)	1.476, 27.483	2.941, 30.167	1.610, 24.998	2.254, 29.128	1.757, 29.130
$h_{min, max}$, $k_{min, max}$, $l_{min, max}$	-15 18, -6 6, -22 21	-9 9, -35 35, -9 9	-30 30, -7 7, -16 16	-9 9, -15 15, -21 21	-20 20, -9 9, -31 31
No. of ref.	10224	16144	16422	13187	22301
No. of unique ref./ obs. Ref.	2658/ 1381	16144/ 12863	2044/ 1624	3135/ 2472	6161/ 4351
No. parameters	173	315	172	172	343
R_{all}, R_{obs}	0.1408, 0.0608	0.0664, 0.0514	0.0539, 0.0388	0.0562, 0.0427	0.0807, 0.0505
$wR2_{all}$, $wR2_{obs}$	0.1484, 0.1211	0.1108, 0.1029	0.1004, 0.0935	0.1064, 0.1002	0.1242, 0.1085
$\Delta\rho_{min, max}$ (eÅ^{-3})	-0.268, 0.272	-0.306, 0.485	-0.232, 0.161	-0.230, 0.316	-0.249, 0.208

G. O. F.	0.973	1.060	1.037	1.077	1.005

	26-F		***p*-Cl**		
	I	**II**	**I**	**II**	**III**
Formula	$C_{15}H_9F_2NO$	$C_{15}H_9F_2NO$	$C_{15}H_{10}ClNO$	$C_{15}H_{10}ClNO$	$C_{15}H_{10}ClNO$
Formula weight	257.23	257.23	255.69	255.69	255.69
CCDC number	1870721	1870725	1870728	1870727	1870730
Temperature/K	100(2)	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	triclinic	monoclinic	orthorhombic
Space group	*Cc*	$P2_1/n$	*P*-1	$P2_1/c$	$Pca2_1$
***a* (Å)**	10.7966(2)	4.7576(3)	6.3360(6)	5.1739(4)	8.9704(2)
***b* (Å)**	12.9518(2)	20.4429(16)	7.4193(8)	14.1904(10)	5.76550(10)
***c* (Å)**	8.41980(10)	12.5360(10)	26.349(3)	16.6037(12)	47.7280(10)
***α*/ *β*/ *γ* (°)**	90 /90.4850(10)/ 90	90/ 92.433(6)/ 90	88.304(3)/ 86.219(3)/86.311(3)	90/ 95.744(4)/ 90	90/ 90/ 90
V(Å^3)	1177.34(3)	1218.14(16)	1233.0(2)	1212.92(15)	2468.44(9)
Z	4	4	4	4	8
Density (g cm^{-3})	1.451	1.403	1.377	1.400	1.376
F (000)/ *μ* (mm^{-1})	528/ 0.113	528/ 0.109	528/ 0.295	528/ 0.300	1056/ 0.295
θ (min, max)	2.456, 30.069	1.992, 27.876	2.325, 25.000	2.466, 30.096	1.707, 30.113
$h_{min, max}$, $k_{min, max}$, $l_{min, max}$	-15 15, -18 18, -11 11	-6 6, -26 22, -16 13	-7 7, -8 8, -31 31	-7 7, -19 19, -23 23	-12 12, -8 6, -67 55
No. of ref.	9984	10890	16539	25473	20222
No. of unique ref./ obs. Ref.	3399/ 3260	2765/ 1401	4339/ 3373	3561/ 2850	5994/ 4601
No. parameters	172	172	325	163	326
R_{all}, R_{obs}	0.0319, 0.0305	0.1570, 0.0648	0.0588, 0.0415	0.0661, 0.0469	0.0682, 0.0483
$wR2_{all}$, $wR2_{obs}$	0.0834, 0.0820	0.1540, 0.1242	0.1081, 0.0997	0.1053, 0.0983	0.1063, 0.0975
$\Delta\rho_{min, max}$ (eÅ^{-3})	-0.218, 0.297	-0.274, 0.229	-0.301, 0.146	-0.371, 0.364	-0.377, 0.311
G. O. F.	1.065	1.019	1.039	1.096	1.051

	***o*-Br**		**30**
	I	**II**	
Formula	$C_{15}H_{10}BrNO$	$C_{15}H_{10}BrNO$	$C_{15}H_{11}NO$
Formula weight	300.15	300.15	221.25
CCDC number	1870731	1870726	1870733
Temperature/K	100(2)	100(2)	110(2)
Crystal system	orthorhombic	orthorhombic	orthorhombic
Space group	*Pbca*	$Pna2_1$	$Pca2_1$
***a* (Å)**	12.0680(7)	8.8324(3)	8.6256(2)
***b* (Å)**	8.9418(5)	12.8240(5)	8.3342(2)
***c* (Å)**	23.7883(14)	11.4691(5)	16.0889(4)
***α*/ *β*/ *γ* (°)**	90/ 90/ 90	90/ 90/ 90	90/ 90/ 90
V(Å^3)	2567.0(3)	1299.07(9)	1156.59(5)
Z	8	4	4
Density (g cm^{-3})	1.553	1.535	1.271
F (000)/ *μ* (mm^{-1})	1200/ 3.188	600/ 3.150	464/ 0.080
θ (min, max)	2.404, 30.144	2.382, 30.102	2.444, 27.870
$h_{min, max}$, $k_{min, max}$, $l_{min, max}$	-17 16, -12 12, -33 33	-12 12, -18 18, -16 16	-11 11, -10 10, -21 21
No. of ref.	58524	14680	8750
No. of unique ref./ obs. Ref.	3782/ 3082	14680/ 13091	3248/ 2946
No. parameters	185	164	155
R_{all}, R_{obs}	0.0617, 0.0463	0.0343, 0.0282	0.0449, 0.0397
$wR2_{all}$, $wR2_{obs}$	0.0980, 0.0937	0.0584, 0.0562	0.0961, 0.0924
$\Delta\rho_{min, max}$ (eÅ^{-3})	-0.727, 0.815	-0.398, 0.701	-0.295, 0.225
G. O. F.	1.114	1.037	1.089

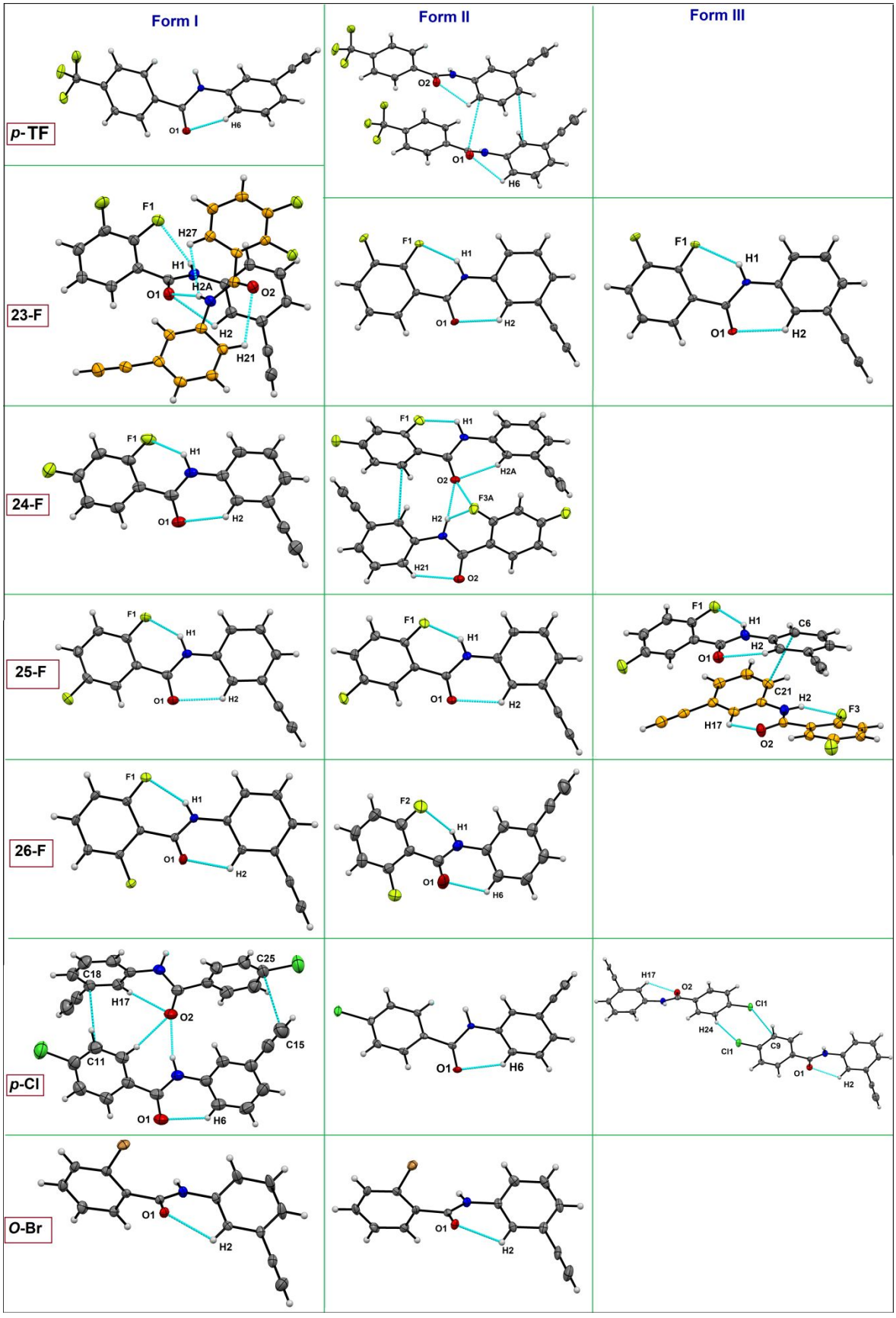


Figure S1. *ORTEP*s (50% ellipsoidal probability) of all seven new polymorphic families. Dotted lines show all non-covalent interactions in the asymmetric unit of each.

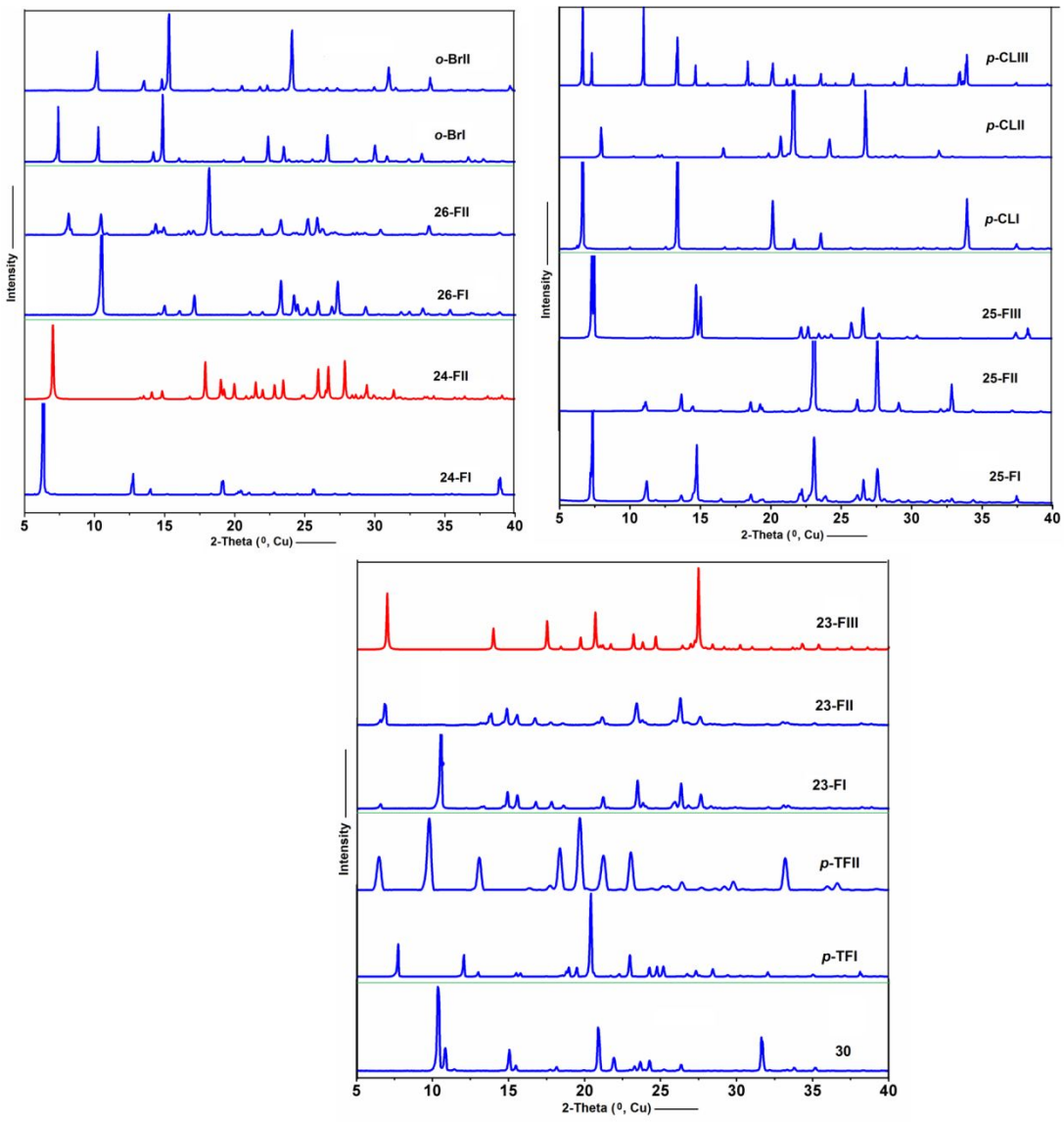


Figure S2. Experimental (at 298 K, room temperature) PXRD patterns (blue) of all the molecules alongwith their polymorphic modifications. Simulated PXRD patterns for **23FIII** and **24-FII** (red) were provided due to lack of sufficient quantity of crystals required for experimental powder diffraction (difficulty in obtaining polymorphs).

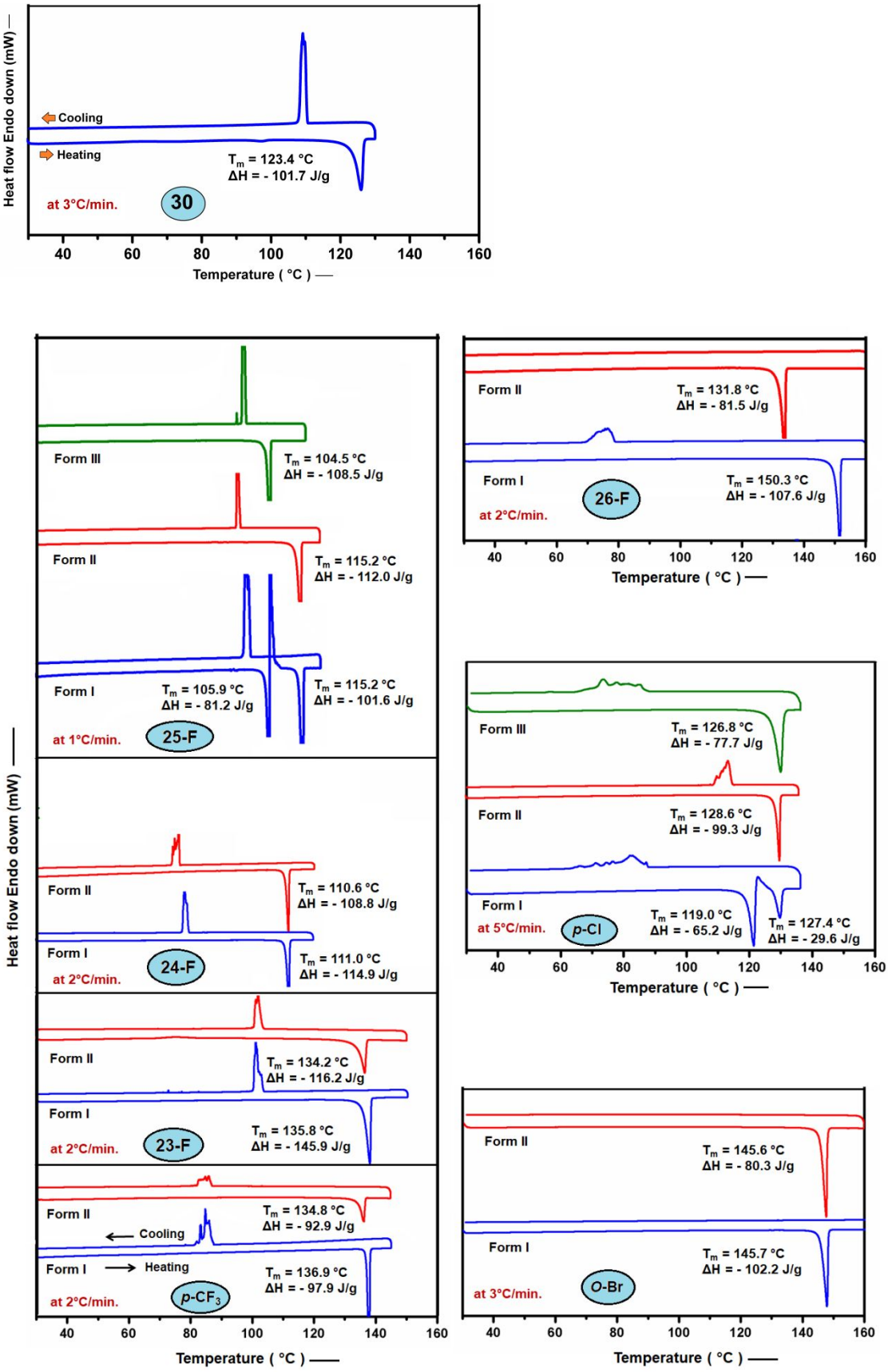


Figure S3. Differential scanning calorimetry traces of monomorphic 30 and all seven polymorphic compounds.

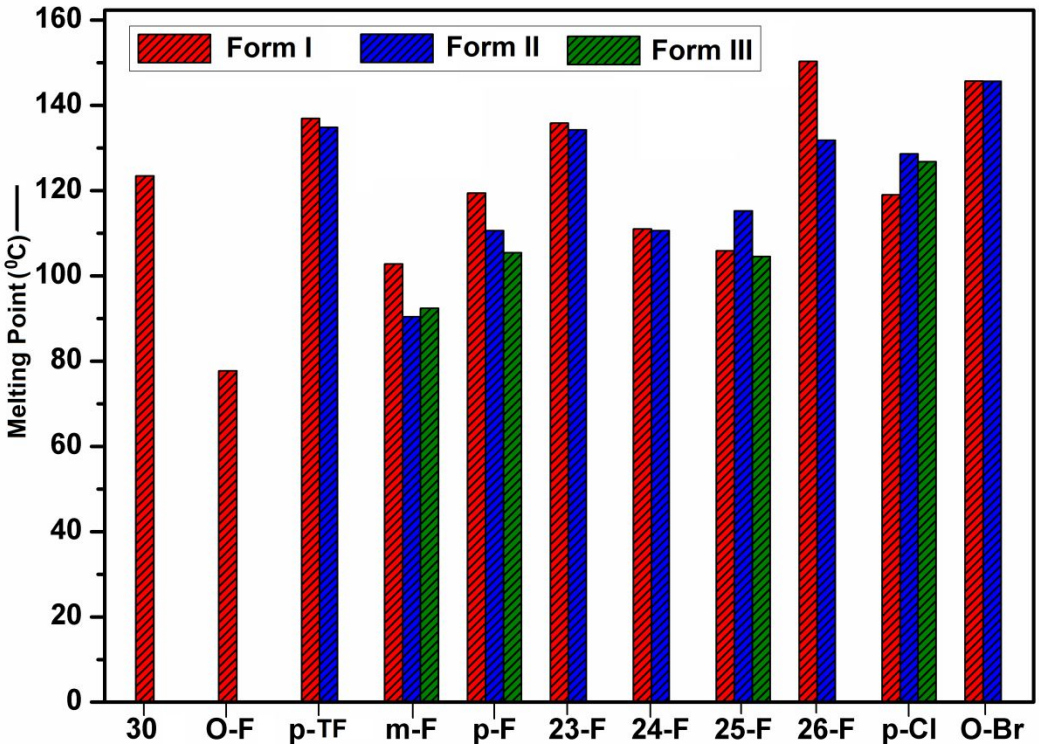


Figure S4. Comparison of available melting points obtained from the DSC experiments for all structures discussed in this study.

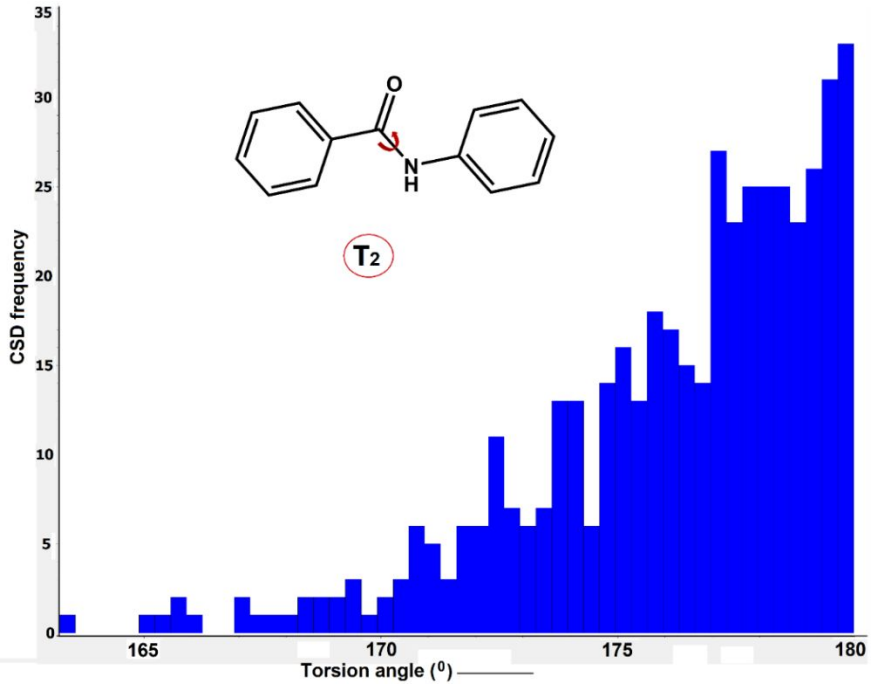


Figure S5. Distribution of T_2 torsion angles in all CSD structures showing only one maximum near to 180° and hence only one conformer is expected in the solid-state.

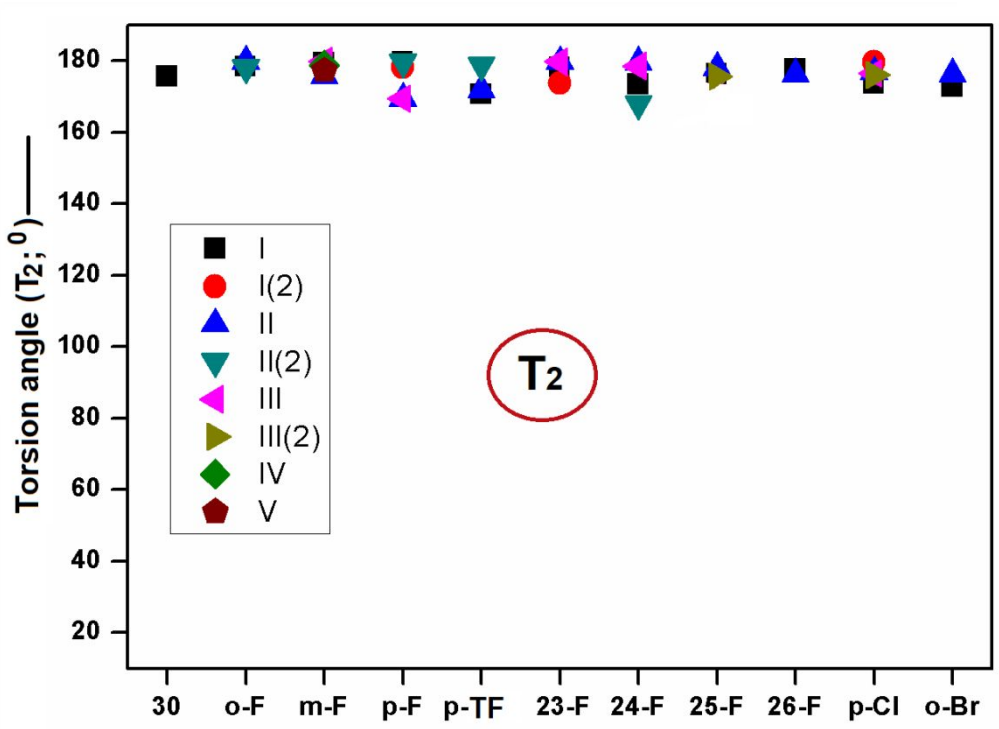


Figure S6. Plot of T_2 torsion angle close to 180° in all crystal structures.

Table S3. List of selected torsion angles in all crystal structures.

Compounds	Torsions			
	Polymorphic Form	T_1 (C6-C1-N1-C13 / C21-C16-N2-C28)	T_2 (C7-C13-N1-C1 / C22-C28-N2-C16)	T_3 (C12-C7-C13-N1 / C27-C22-C28-N2)
30	I	158.2(2)	175.6 (2)	154.6 (2)
o-F	I	162.3(2)	178.4(2)	168.8(2)
	II	174.8(2) /177.9(2)	179.8(2) /178.0(2)	176.1 (2)/ 168.4(2)
m-F	I	145.4(3)	179.5(2)	149.0(2)
	II	35.4(2)	175.8(1)	33.8(2)
	III	148.2(1)	179.9(1)	150.4(1)
	ID	147.1(2)	178.8(3)	38.7(4)
	IID	161.0(2)	177.2(4)	155.5(3)
p-F	I	42.5(7)/ 141.8(1)	179.7(1)/ 178.3(1)	151.8(1)/ 148.7(1)
	II	31.7(3)/ 139.0(2)	169.5(2)/ 179.6(2)	25.3(3)/ 142.8(2)
	III	37.1(3)	169.4(2)	27.9(3)
p-CF_3	I	42.9(2)	170.6(1)	37.3(2)
	II	44.8(2)/ 32.8(2)	171.8(1)/ 178.8(1)	37.7(2)/ 29.5(2)
23-F	I	145.3(4)/ 38.3(5)	178.2(3)/ 173.8(3)	144.1(3)/ 38.4(5)
	II	152.7(1)	179.7(1)	152.3(1)
	III	151.2(3)	179.7(3)	152.8(3)
24-F	I	146.0(2)	173.4(2)	151.9(2)
	II	148.5(4)/ 36.9(6)	179.5(3)/ 167.8(4)	150.2(3)/ 145.1(3)
25-F	I	167.5(2)	176.3(1)	166.4(1)
	II	165.9(2)	178.0(1)	170.6(1)
	III	165.9(4)/ 164.4(3)	172.7(3)/ 175.6(3)	166.8(3)/ 170.2(3)
26-F	I	142.9(2)	177.7(1)	130.5(2)
	II	42.0(4)	176.2(2)	51.2(4)

p-Cl	I	29.8(3)/ 133.6(2)	173.5(2)/ 179.6(2)	24.7(3)/ 47.2(2)
	II	37.7(2)	176.8(1)	35.9(2)
	III	153.4(4)/ 153.8(5)	176.5(4)/ 176.0(4)	157.3(4)/ 157.3(4)
o-Br	I	150.0(3)	172.6(2)	116.9(3)
	II	149.1(4)	176.3(3)	113.2(4)

Table S4. List of all possible intra and intermolecular interactions [**Cg1**- C1> C6, **Cg2**- C7> C12, **Cg1'**- C16> C21, **Cg2'**- C22> C27]

Motifs	Symmetry	Possible Interactions	Geometry (Å/ º)
		30	
I (*Synthon* A)	**x-1/2, -y+1, z**	**N1-H1···O1 C6-H6···O1 C8-H8···O1 Cg1··· Cg2 stacking**	**1.89, 163 2.56, 127 2.54, 122 4.122(3)**
II	**-x+2, -y+1, z+1/2**	**C15-H15···C8 (ring)**	**2.62, 169**
III	**x-1/2, -y+2, z**	**C5-H5···C14 (triple bond)**	**2.75, 142**
IV	**-x+1, -y+1, z+1/2**	**C10-H10···C4(ring)**	**2.79, 139**
V	**-x+3/2, y-1, z-1/2**	**C4-H4···C10(ring)**	**2.88, 154**
VI	**x, y+1, z**	**C12-H12···C5(ring) C12(π)···C6(π) C12(π)···C5(π)**	**2.70, 139 3.575(3) 3.585(3)**
VII	**x, y, z (intra)**	**C2-H2···O1**	**2.32, 112**
		***o*-FI**	
I	**2-x+2, -y, 1-z**	**Cg1··· Cg2 stacking**	**4.563 (2)**
II	**1-x, -y, 1-z**	**Cg1··· Cg2 stacking C6-H6...N1**	**5.206 (2) 2.90, 120**
III (*Synthon* D)	**1+x, y, z**	**C6 -H6 ...O1 C12-H12...F1 C5-H5...π(C14/C15)**	**2.42, 150 2.51, 128 2.88, 134**
IV	**2-x, 1-y, 1-z**	**Cg1··· Cg2 stacking**	**3.722 (3)**
V	**3/2-x, -1/2+y, 3/2-z**	**(C15)π...π(C6/C1)**	**3.487 (2)**
VI	**5/2-x, 1/2+y, 3/2-z**	**C15-H15...O1**	**2.08, 170**
VII	**-1/2+x, 1/2-y, 1/2+z**	**C10-H10.... π(C4/C5)**	**2.71, 151**
VIII	**1/2+x, 1/2-y, 1/2+z**	**C9-H9... π(C14) C10-H10... π(C15)**	**3.02, 134 2.93, 125**
IX	**1-x, 1-y, 1-z**	**C9-H9...F1**	**2.78, 131**
X	**x, y, z (intra)**	**N1-H1...F1 C2-H2...O1**	**1.88, 135 2.25, 115**
		***o*-FII**	
I	**1-x, -y, 2-z**	**Cg1...Cg2**	**3.765 (3)**
II	**2-x, -y, 2-z**	**Cg1...Cg2**	**4.637 (3)**
III	**x, 1/2-y, -1/2+z**	**Cg1'...Cg2'**	**3.659 (3)**
IV (*Synthon* D)	**x, y, z**	**C21 -H21 ...O1 C20-H20...π (C14) C12-H12...F2**	**2.44, 144 2.92, 148 2.66, 113**
V	**-1+x, 1/2-y, -1/2+z**	**C15-H15...O2 C27-H27... π (C15)**	**2.19, 154 2.68, 140**
VI	**x, 1/2-y, -1/2+z**	**C30-H30...O1 C12-H12... π (C30)**	**2.63, 143 2.68, 154**
VII	**2-x, -y, 2-z**	**C6-H6 ...F2 F1...F2 C9-H9... π (C21)**	**2.80, 145 2.99 (2) 2.90, 139**

VIII	1-x, 1/2+y, 3/2-z	C30 -H30...F1 C5-H5...O2 C6-H6... π (C14/C15)	2.63, 119 2.71, 124 2.89, 131
IX	-1+x, 1/2-y, -1/2+z	Cg1'...Cg2'	3.742 (3)
X	1-x, -y, 1-z	(C4)π... π(C14)	3.799 (3)
XI	-1+x, y, -1+z	C10-H10... π (C14/C15)	2.77, 142
XII	x+1, y, z+1	C25-H25... π (C29/C30)	2.77, 141
XIII	2-x, -1/2+y, 5/2-z	C26-H26...F1	2.64, 150
XIV	-x, -y, 1-z	(C4)π...π(C15)	3.668 (3)
XV	x, y, z (intra)	N1-H1...F1 N2-H2 ...F2 C2-H2A...O1 C17-H17...O2	1.88, 137 1.89, 135 2.18, 118 2.19, 118
	***m*-FI**		
I (*Synthon* A)	x, -y, z+1/2	N1-H1···O1 Cg1...Cg2 stacking	1.85, 160 3.928(3)
II	x-1/2, -y-1/2, z+1/2	C10-H10···O1 C2-H2···π(C11) C11-H11···π(C14)	2.56, 133 3.00, 153 2.81, 170
III	x+1/2, y+1/2, z	(C11/C12)π···π(C5/C6)	3.449(3)
IV	x-1/2, -y+1/2, z+1/2	C6-H6···π(C15/C14) C5-H5···F1	2.96, 150 2.86, 163
V	x-1/2, y-1/2, z+1	C4-H4···π(C10)	3.15, 119
VI	x-1, y, z+1	(*sp*)C15-H15···F1	2.26, 167
VII	x, y, z (intra)	C2-H2···O1	2.41, 106
	***m*-FII**		
I (*Synthon* A)	x, -y+1/2, z+1/2	N1-H1···O1 C8-H8··· π(C11) C2-H2··· π(C6) C12-H12···O1	2.08, 160 2.74, 174 2.95, 163 2.59, 127
II	-x+1, -y, -z	(C11)π···π(C1) (C10)π···π(C2)	3.500(2) 3.539(2)
III	-x+1, -y+1, -z	(C5)π···π(C8/C9)	3.355(2)
IV	-x+1, y-1/2, -z-1/2	C10-H10···π(C15) C11-H11···π(C2/C3)	2.92, 132 2.70, 163
V	-x+1, y-1/2, -z+1/2	C5-H5···F1 C5-H5···π(C9)	2.30, 160 2.71, 139
VI	x-1, -y+1/2, z -1/2	C10-H10···π(C15)	2.98, 115
VII	x-1, y, z-1	(*sp*)C15-H15···F1	2.15, 176
VIII	-x, y-1/2, -z-1/2	C4-H4···π(C15)	3.07, 137
IX	x, y, z (intra)	C6-H6···O1	2.39, 108
	***m*-FIII**		
I (*Synthon* B)	x, y-1, z	N1-H1···O1 Cg1...Cg1 Cg2...Cg2	1.92, 150 4.885(2) 4.885(2)
II	-x+3/2, -y-1/2, -z+1	C12-H12···O1 C11-H11···π(C14/C15) H2···H11	2.50, 145 2.84, 155 2.361(1)
III	-x+3/2, -y+1/2 , -z+1	(C2)π···π(C11)	3.339(2)
IV	-x+3/2, y-1/2, -z+3/2	C8-H8···π(C5) C6-H6···π(C6) C5-H5···π(C8) C6-H6···N1	2.71, 154 3.00, 168 2.90, 161 2.88, 138
V	-x+1, y, -z+3/2	C4-H4···π(C14)	2.95, 153
VI	-x+2, -y+1, -z+1	C10-H10···F1	2.58, 161
VII	x-1/2, y-3/2, z	(*sp*)C15-H15···F1	2.29, 161
VIII	x-1/2, y-1/2, z	(C15)π···π(C9) F1··· π(C15)	3.488(2) 3.338(2)
IX	x, y, z	C2-H2···O1	2.34, 108
	***m*-FIV**		
I (*Synthon* A)	x, -y+1/2, z-1/2	N1-H1...O1 Cg1...Cg2 stacking	1.86, 161 3.970(3)

II	-x+1, y+1/2, -z+1/2	C4-H4...O1 C15-H15...F1A C5-H5… π(C14/C15) C8A-H8A… π(C14/C15)	2.64, 144 2.55, 122 2.84, 175 2.71, 156
III	-x, -y, -z+1	Cg2···Cg2 stacking	3.824(*)
IV	-x, y-1/2, -z+3/2	C12A-H12A… π(C9A/C10A) C11A-H11A…F1A C12A-H12A…F1A	3.31, 154 2.68, 137 2.59, 120
V	-x+1, -y+1, -z	C4-H4... π(C4) C4-H4... π(C14)	3.43, 115 3.47, 114
VI	-x, -y, -z+2	C10A-H10A… π(C11A/C10A)	3.16, 125
VII	x-1, -y+1/2, z+1/2	C11A...C15	3.9540(4)
VIII	x, y, z (intra)	C2-H2...O1	2.40, 107
	m-FV		
I (*Synthon* A)	x-1/2, -y+1, z	N1-H1 ...O1 C6-H6 ...O1 C8A-H8A ...O1 Cg1···Cg2 stacking	1.92, 161 2.62, 127 2.55, 121 4.139(3)
II	x, y+1, z	C6-H6 ...F1A C12A-H12A···π(C5)	2.60, 129 2.76, 139
III	-x+1, -y+1, z-1/2	C10A-H10A··· π(C4) C9A-H9A··· π(C3)	2.90, 138 3.17, 139
IV	x+1/2, -y+2, z	C5-H5···π(C14) (C4)π···π(C5)	2.71, 146 3.574(3)
V	-x+3/2 , y, z-1/2	C9A-H9A··· π(C15) C8A-H8A··· π(C15) (C8A)π···π(C15)	2.96, 127 3.14, 119 3.784(3)
VI	-x+3/2, y-1, z+1/2	C4-H4··· π(C10A) C14...F1A	2.87, 155 3.374(3)
VII	-x+2, -y+1, z-1/2	C15-H15···π(C8A)	2.64, 164
VIII	x-1/2, -y, z	(C10A)π···π(C12A) F1A... π(C10A)	3.787(3) 3.310(3)
IX	x, y, z (intra)	C2-H2...O1	2.28, 114
	p-FI		
I (*Synthon* B)	x-1, y, z	N1-H1···O1 C2-H2···O1 Cg1...Cg1 Cg2...Cg2	2.06, 150 2.60, 121 5.209(2) 5.209(2)
II (*Synthon* B)	x-1, y, z	N2-H2A···O2 C21-H21···O2 Cg1'...Cg1' Cg2'...Cg2'	2.04, 153 2.63, 119 5.209(2) 5.209(2)
III	-x+1, -y, -z+1	C27-H27···O1 π(C2)···π(C26) π(C11)···π(C17) F1···π(C29)	2.84, 129 3.573(2) 3.395(2) 3.328(2)
IV	-x+2, -y, -z+1	C23-H23···π(C16) C24-H24···π(C20)	2.80, 124 2.74, 149
V	-x+1, -y, -z+2	C5-H5···F1 C6-H6···π(C9/C10)	2.83, 148 2.70, 156
VI	-x, -y, -z+2	C8-H8···N1 C9-H9···π(C5) C9-H9···π(C6)	2.95, 137 2.65, 161 2.70, 135
VII	-x+1, -y, -z +1	C20-H20···F2 C21-H21···π(C23)	2.66, 140 2.92, 153
VIII	-x+2, -y, -z+1	C11-H11···π(C29)	2.60, 162
IX	-x, -y, -z+1	(*sp*)C15-H15···F2 C26-H26···π(C15)	2.64, 112 2.89, 146
X	-x-1, -y+1, -z+1	π (C15)···π(C15)	3.313(2)

XI	-x, -y+1, -z+1	C19-H19···π(C14) C4-H4···π(C20)	2.87, 128 3.08, 151
XII	-x+1, -y+1, -z+1	C4-H4···π(C29/C30)	2.89, 123
XIII	x-2, y+1, z	(*sp*)C15-H15···F2	2.47, 159
XIV	-x+2, -y+1, -z	π(C30)···π(C30)	3.363(2)
XV	x-1, y-1, z +1	(*sp*)C30-H30···F1	2.32, 164
	***p*-FII**		
I (*Synthon* C)	x, y, z	NI-H1···O2 C12-H12···O2 Cg1··· Cg2' Cg2··· Cg1' stacking	1.88, 169 2.50, 116 4.893(2) 4.806(2)
II (*Synthon* C)	x-1, y, z+1	N2-H2A···O1 C8-H8···π(C16) C5-H5···F2 Cg1··· Cg2' Cg2··· Cg1' stacking	1.92, 155 2.89, 125 2.88, 141 5.088(2) 5.176(2)
III	x, y, z+1	C27-H27···O1 C17-H17···π(C9) C26-H26···π(C6)	2.58, 128 2.86, 122 2.87, 129
IV	x-1, y, z	C21-H21···N1 (C20) π ··· π (C8)	2.88, 113 3.499(2)
V	x-1, y, z	C21-H21···O2 C20-H20···π(C29)	2.40, 156 2.74, 144
VI	x+1, y, z	C12-H12···O1 C11-H11···O1 C5-H5···π(C14) C11-H11···π(C8)	3.10, 110 3.00, 113 2.98, 132 2.96, 145
VII	-x+1, y-1/2, -z+1	C4-H4···F1 C9-H9···π(C15)	2.48, 165 2.83, 160
VIII	-x, y+1/2, -z+2	C19-H19···F2 C24-H24···π(C30)	2.35, 155 2.76, 158
IX	-x, y-1/2, -z+2	C15-H15···π(C19)	3.03, 143
X	-x+1, y+1/2, -z+2	(*sp*)C30-H30···F2	2.44, 157
XI	-x+1, y-1/2, -z+2	C30-H30···π(C15)	3.34, 111
XII	-x, y+1/2, -z+1	(*sp*)C15-H15···F1	2.54, 128
	x, y, z (intra)	C6-H6···O1 C17-H17···O2	2.38, 109 2.49, 102
	***p*-FIII**		
I (*Synthon* A)	x+1/2, -y+1/2, z+1/2	N1-H1···O1 C2-H2···O1 C12-H12···O1 Cg1···Cg2 stacking	1.98, 151 2.37, 131 2.45, 136 3.876(2)
II	x-1, y, z	C5-H5···π(C2) C2-H2···π(C5) C8-H8···π(C11) C11-H11···π(C8) H12···H6	2.86, 121 2.89, 119 3.02, 115 2.99, 117 2.373(2)
III	x-1/2, -y+1/2, z+1/2	Cg1···Cg2	3.873(2)
IV	-x+1, -y, -z	C9-H9···F1	2.53, 163
V	-x, -y+1, -z	C4-H4···π(C15/C14)	3.07, 158
VI	-x+3/2, y+1/2, -z+1/2	(*sp*) C15-H15···F1	2.23, 154
VII	-x+1, -y+1, -z	C15(π) ··· C15(π)	3.660(2)
VIII	x, y, z (intra)	C6-H6···O1	2.44, 106
	23-FI		
I (*Synthon* A)	x, y, z	N2-H2A···O1 C17-H17···O1 C27-H27···O1 Cg1··· Cg2'	1.86, 166 2.85, 118 2.71, 114 3.756 (4)

		stacking	
II (*Synthon* A)	x+1, y, z	N1-H1···O2 Cg1'··· Cg2 stacking F1…O2	1.85, 156 3.716(5) 2.943(3)
III	x-1/2, -y, z+1/2	C5-H5···F1 C4-H4···F1	2.88, 119 2.65, 128
IV	x-1/2, -y, z+1/2	C21-H21···F4 C25-H25···O2 C26-H26···F3 C25-H25···F3	2.50, 146 2.48, 136 2.51, 120 2.54, 118
V	x+1/2, -y+1, z-1/2	C10-H10…O1 C12-H12···F2 C11-H11···C15 (triple bond)	2.59, 136 2.86, 157 2.86, 155
VI	x-1, y, z-1	C15-H15···F2	2.29, 158
VII	x, y+1, +z	C30-F30···F3 C30-F30···F4	2.50, 152 2.34, 137
VIII	x, y, z (intra)	C2-H2···O1 C21-H21···O2 N1-H1···F1	2.44, 106 2.48, 105 2.27, 114
23-FII			
I (*Synthon* B)	x+1, y, z	C6-H6···O1 N1-H1···O1 Cg1··· Cg1 Cg2··· Cg2 stacking	2.785, 109 2.074, 143 5.133(2) 5.133(2)
II	-x+1, -y+1, -z+1	C6-H6···F1 C6-H5···F1 C5-H5···F2	2.70, 117 2.49, 126 2.58, 170
III	-x-1, -y, -z+1	C12-H12···O1 C11-H11···C14 (triple bond)	2.53, 146 2.79, 169
IV	x-1, y, z+1	C15-H15···F2	2.210, 164
V	-x, -y, 1-z	C11 (π)···C1 (π) C10 (π)···C2 (π)	3.485(2) 3.476(2)
VI	-x, 1-y, 1-z	C5 (π)···C8 (π)	3.266 (2)
V	x, y, z (intra)	N1-H1···F1 C2-H2···O1	2.12, 120 2.30, 111
23-FIII			
I (*Synthon* B)	x, y+1, z	N1-H1···O1 Cg1··· Cg1 Cg2··· Cg2 stacking	2.02, 144 5.084(4) 5.084(4)
II	x+1, y+1, z	C6-H6···O1 C11-H11···F2 C11-H11···F1 C12-H12···F1 C5-H5···C14 (triple bond)	2.72, 144 2.53, 179 2.56, 118 2.42, 124 2.89, 161
III	x, y-1, z+1	C15-H15···F2	2.22, 166
IV	1+x, y, z	C8 (π)···C11 (π) C2 (π)···C5 (π)	3.238(4) 3.285(5)
V	1+x, y, 1+z	C10-H10···C14 (triple bond)	2.85, 163
VI	x, y, z (intra)	N1-H1···F1 C2-H2···O1	2.130, 119 2.349, 110
24-FI			
I (*Synthon* B)	x, y-1, z	N1-H1···O1 Cg1··· Cg1 Cg2··· Cg2 stacking	1.96, 153 4.994(4) 4.994 (4)
II	-x+2, y-1/2, -z+1/2	C5-H5···F2 C9-H9···C5 (ring) C6-H6···C8 (ring) C13···F1	2.79, 152 2.75, 174 2.71, 157 3.221 (3)
III	-x+2, -y+2, -z	C12-H12···O1 C11-H11···C14 (triple bond)	2.407, 151 2.85, 174
IV	x+1, y+1, +z	C15-H15···F2	2.320, 156
V	-x+2, -y+1, -z	C8 (π)···C11 (π)	3.338 (4)
VI	-x+3, y+1/2, -z+1/2	C4-H4···C14 (triple bond)	2.87, 135

VII	-x+3, -y+2, -z	C15 (π)···C15 (π)	3.461
VIII	x, y, z (intra)	N1-H1···F1 C2-H2···O1	2.20, 113 2.36, 108
	24-FII		
I (*Synthon* C)	x, y, z (inter)	N2-H2···O1 Cg1··· Cg2' Cg2··· Cg1' stacking	1.88, 169 4.643(6) 4.799(5)
II (*Synthon* C)	x+1. y, z-1	N1-H1···O2 Cg1··· Cg2' Cg2··· Cg1' stacking	1.98, 146 5.306(6) 5.137(5)
III	-x+2, y-1/2, -z	C4-H4···F2 C9-H9···C15 (triple bond)	2.28, 165 2.78, 162
IV	x+1, y, z	C6-H6···O1 C5-H5···C14 (triple bond) C12-H12···F1 C11-H11···F1	2.47, 151 2.96, 153 2.58, 119 2.61, 117
V	x-1, +y, +z	C21-H21···F3A C26-H26A···O2	2.32, 170 2.72, 128
VI	x, +y, +z-1	C12-H12···O2 C11 (π)···C16 (π) C2 (π)···C25A (π)	2.61, 131 3.372(5) 3.299(6)
VII	-x+1, +y-1/2, -z	C15-H15···F2	2.43, 154
VIII	-x+1, +y+1/2, -z+1	C19-H19···F4A C24A-H24A···C29 (triple bond)	2.72, 159 2.95, 159
IX	-x+2, y+1/2, -z+1	C30-H30···F4A	2.54, 131
	-x+2, y+1/2, -z	C30-H30···C4(ring)	2.90, 130
X	x, y, z (intra)	N1-H1···F1 N2-H2···F3A C2-H2A···O1 C21-H21···O2	2.17, 117 2.27, 106 2.35, 108 2.46, 107
	25-FI		
Motif	Symmetry	Possible interactions	Geometry (Å/ º)
I	-x, y, -z+1/2	Cg1··· Cg2 stacking	3.841(2)
II	-x, -y, -z+1	Cg1··· Cg2 stacking	4.759(3)
III	-x, +y+1, -z+1/2	C5-H5···F2 C5-H5···C11(ring)	2.94, 115 3.12, 135
IV (*Synthon* D)	x, +y+1, +z	C9-H9···F2 C12-H12···F1 C6-H6···O1 C5-H5···C14 (triple bond)	2.48, 134 2.43, 136 2.39, 153 2.87, 146
V	x-1/2, -y-1/2, +z-1/2	C15-H15···F2	2.43, 140
VI	x, y, z (intra)	N1-H1···F1 C2-H2···O1	1.85, 136 2.28, 116
	25-FII		
I	-x, -y+1, -z+1	stacking Cg1··· Cg2	 4.716(2)
II	-x+1, -y+1, -z+1	stacking Cg1··· Cg2	 5.183(2)
III	-x, -y, -z+1	stacking Cg2··· Cg2	 3.676 (2)
IV (*Synthon* D)	x+1, y, z	C9-H9···F2 C6-H6···O1 C5-H5···C14 (triple bond) C12-H12···F1	2.49, 136 2.52, 154 2.93, 150 2.46, 136
V	-x+1, -y, -z+1	C9-H9···F1	2.81, 127
VI	-x-1/2, y+1/2, -z+1/2	C15-H15···O1	2.08, 169
VII	x-1/2, -y+1/2, z+1/2	C10-H10···C5(ring)	2.82, 144

VIII	x+1/2, -y+1/2, z+1/2	C10-H10···C15 (triple bond)	2.89, 130
IX	x, y, z (intra)	N1-H1···F1 C2-H2···O1	1.87, 136 2.22, 116
25-FIII			
I	x, y, z	stacking Cg1··· Cg2' Cg1'··· Cg2	 4.736(4) 4.424(5)
II	x-1/2, -y+3/2, z	stacking Cg1··· Cg2' Cg1'··· Cg2	 4.485(5) 4.598 (5)
III (*Synthon* D)	x, y+1, z	C6-H6···O1 C9-H9···F2 C12-H12···F1 C5-H5···C14 (triple bond)	2.35, 159 2.53, 133 2.45, 135 2.79, 149
		C21-H21···O2 C24-H24···F4 C27-H27···F3 C20-H20···C29 (triple bond)	2.33, 158 2.46, 130 2.41, 131 2.79, 147
IV	-x+3/2 , -y-1/2, z+1/2	C15-H15···C18(ring)	2.96, 156
V	-x+1, -y+1, z+1/2	C15-H15···F2	2.94, 106
VI	-x+3/2, y+1/2, z+1/2	C25-H25···F2	2.45, 135
VII	x, y, z (intra)	N1-H1···F1 N2-H2···F3 C2-H2A···O1 C17-H17···O2	1.84, 137 1.87, 136 2.27, 116 2.24, 116
26-FI			
I (*Synthon* A)	x, -y+1, z+1/2	N1-H1···O1 Cg1··· Cg2 stacking	1.801, 168 4.039(2)
II	x-1/2, y+1/2, z	C4-H4···O1 Cg1··· Cg2 stacking	2.67, 126 3.890(2)
III	x+1/2, -y+1/2, z+1/2	C9-H9···F2 C10-H10···F2 C10-H10···O1 C11-H11···C14 (triple bond) C2-H2···C11 (ring)	2.70, 117 2.50, 125 2.77, 128 2.84, 154 2.98, 151
IV	x-1/2, -y+1/2+1, z-1/2	C4-H4···F1 C6-H6···C14 (triple bond)	2.69, 127 3.10, 147
V	x, y, z (intra)	N1-H1···F1 C2-H2···O1	2.51, 102 2.48, 105
26-FII			
I (*Synthon* B')	x-1, y, z	N1-H1···O1 Cg1··· Cg1 Cg2··· Cg2 stacking C12···O1	1.81, 164 4.758(4) 4.758(4) 3.127(3)
II	-x+2, -y, -z+1	C5-H5···O1 C5-H5···F1	2.82, 133 2.38, 160
III	x+1/2, -y+1/2, z+1/2	C9-H9···F2 C2-H2···C10 (ring)	2.35, 118 3.06, 171
IV	-x+1, -y, -z	C4-H4···C15 (triple bond)	2.92, 161
V	x-1/2, -y+1/2, z+1/2	C10-H10···F2 C10-H10···N1 C11-H11···C3 (ring)	2.89, 137 2.97, 156 2.83, 160
VI	x-1, y, z-1	C15-H15···F1	2.43, 168
VII	x, y, z (intra)	N1-H1···F2 C6-H6···O1	2.51, 98 2.51, 103
o-BrI			
I (*Synthon* A)	-x+1/2, y-1/2, z	N1-H1···O1 C6-H6···O1 Br1A···C11A (π) C3(π)···C15 (π)	1.85, 162 2.63, 122 3.885(3) 3.505(5)

I	x+1/2, y, -z+3/2	C4-H4···O1 C5-H5··· C2 (ring)	2.47, 157 2.98, 127
II	x, -y+1/2, +z+1/2	C15-H15···Br1A	2.82, 146
III	-x, -y, -z+1	Cg2··· Cg2	4.372(4)
IV	x-1/2, -y-1/2, -z+1	C9A-H9A···Br1A	2.99, 129
V	-x+1, y+1/2, -z+3/2	C5-H5··· C3 (ring) C5-H5···C14 (triple bond)	2.91, 132 2.86, 133
VI	x, y, z (intra)	C2-H2···01	2.41, 109
	o-BrII		
I (*Synthon* A)	x-1/2, -y+3/2, z	N1-H1···O1 C6-H6···O1 Br1···C11(π) C3(π)···C15 (π)	1.833, 165 2.728, 119 3.453(3) 3.506(6)
II	x+1/2, -y+3/2, z-1	C15-H15···Br1 C11-H11···C15(triple bond)	2.92, 140 2.72, 133
III	-x+1/2, y+1/2, z-1/2	C4-H4···O1 C4-H4··· C7 (ring) C4(π)···C12 (π)	2.49, 158 2.92, 130 3.460(5)
IV	-x, -y+1, z+1/2	C10-H10···O1 C2-H2··· C10 (ring)	2.57, 149 2.87, 147
V	x, y, z (intra)	C2-H2···O1	2.40, 109
	p-CLI		
I (*Synthon* C)	x, y, z	N1-H1···O2 C2-H2···O2 C12-H12···O2 Cg1··· Cg2' Cg2··· Cg1' stacking	1.97, 165 2.80, 123 2.53, 124 5.200(3) 4.788(3)
II (*Synthon* C)	x+1, y+1, z	N2-H2A···O1 Cg1··· Cg2' Cg2··· Cg1' stacking	1.95, 152 4.873(3) 5.294(2)
III	x+1, y, z	C21-H21···O2 C20-H20···C29(triple bond)	2.37, 162 2.79, 136
IV	x, y+1, z	C23-H23···O1 C17(π)···C10 (π) C24(π)···C1 (π)	2.56, 139 3.471(3) 3.590(3)
V	-x+2, -y+12, -z+1	C15-H15···Cl2	2.92, 150
VI	-x+2, -y, -z+2	Cl1···Cl1	3.655(1)
VII	-x+1, -y+1, -z+1	C4-H4···C15(triple bond)	3.04, 119
VIII	-x+2, -y+1, -z+2	C19-H19···C30(triple bond)	2.85, 156
IX	-x+1, -y+1, -z+2	C30-H30···Cl1 C30-H30··· C10 (ring)	2.90, 148 3.06, 157
X	x, y, z (intra)	C6-H6···O1 C17-H17···O2	2.35, 109 2.63, 99
	p-CLII		
I (*Synthon* B')	x-1, y, z	N1-H1···O1 C2-H2···O1 C12-H12···O1 Cg1··· Cg1 Cg2··· Cg2 stacking	1.99, 157 2.765, 118 2.744, 128 5.174(2) 5.174(2)
II	-x, -y+2, -z+1	C4-H4···C14(triple bond)	2.99, 134
III	-x, -y+1, -z+1	C12-H12···N1 C11-H11··· C6 (ring)	2.82, 135 2.64, 143
IV	x-1, y+1, z	C15-H15···C11	2.80, 158
V	-x+1, y-1/2, -z+3/2	C9-H9··· C2 (ring) Cl1··· C13	2.60, 150 3.632(2)

VI	-x+1, -y+1, -z+1	C5-H5···C11 C6-H6···C12 (ring)	3.08, 149 2.63, 164
VII	-x, y+1/2, -z+3/2	C2-H2···Cl1	2.97, 158
VIII	x, y-1, z	Cl1··· C15	3.488(2)
IX	x, y, z	C6-H6···O1	2.42, 106
p-CLIII			
I (*Synthon* A)	x+1/2, -y+2, z	N1-H1···O1 C8-H8···O1 C6-H6···O1 C2-H2···C6 (ring) C15(π)···C3 (π)	1.87, 163 2.33, 134 2.59, 125 2.96, 146 3.470(9)
II (*Synthon* A)	x+1/2, -y+1, z	N2-H2A···O2 C23-H23···O2 C21-H21···O2 C17-H17···C21 (ring) C18(π)···C30 (π)	1.88, 164 2.38, 133 2.61, 125 2.96, 146 3.434(7)
III	x, y, z	C24-H24···Cl1 C10···Cl2	2.91, 154 3.580(4)
IV	x+1/2, -y+1, z	C24···Cl1	3.479(4)
V	x, y+1, z	C2(π)···C5 (π) C11(π)···C8 (π)	3.480(6) 3.523(6)
VI	-x, -y+1, z-1/2	C15-H15···C29(triple bond)	2.99, 163
VII	-x, -y+2, z+1/2	C30-H30···C14(triple bond)	2.93, 159
VIII	x, y+1, z	C20(π)···C17(π) C23(π)···C26(π)	3.506(6) 3.514(6)
IX	x, y-1, z	Cl2···Cl1	3.688(2)
X	x-1/2, -y, z	C20-H20···C29(triple bond)	2.60, 152
XI	x-1/2, -y+1, z	C11···Cl1 C11···C10	3.508(7) 3.572(7)
XII	x, y, z (intra)	C2-H2···O1 C17-H17···O2	2.31, 112 2.31, 112
p-TFI			
I (*Synthon* B')	x+1, y, z	N1-H1···O1 C2-H2···O1 C12-H12···O1 C9-H9···F3 Cg1··· Cg1 Cg2··· Cg2 stacking	1.99, 153 2.67, 118 2.85, 125 2.70, 131 5.154(2) 5.154(2)
II	-x+3/2, y+1/2, -z+1/2	C2-H2···F3	2.47, 150
II	-x, -y, -z	C5-H5···F2 C6-H6···C12(ring)	2.432, 162 2.68, 169
IV	-x+1/2, y-1/2, -z+1/2	C9-H9···C2(ring) F1···C14	2.79, 150 3.024(2)
V	-x+1, -y, -z	C12-H12···N1 C11-H11···C5(ring)	2.683, 140 2.85, 160
VI	x+1, +y+1, +z	C16-H16···F2 C16-H16···F1	2.679, 130 2.507, 158
VII	x, y, z (intra)	C6-H6···O1	2.485, 104
p-TFII			
I (*Synthon* B)	x, y+1, z	N1-H1···O1 C12-H12···O1 C11-H11···O2 C2-H2···O1 Cg1··· Cg1 Cg2··· Cg2 stacking	1.86, 162 2.75, 116 2.76, 133 2.90, 114 5.010(2) 5.010(2)

II (*Synthon* B)		N2-N2A···O2 C28-H28···O2 Cg1'··· Cg1' Cg2'··· Cg2' stacking	1.97, 151 2.86, 113 5.010(2) 5.010(2)
III	x, y, z	Cg1··· Cg1' Cg2··· Cg2' stacking F3···C25	4.877(2) 4.975(2) 3.289(2)
IV	-x+1, y+1/2, -z+3/2	C16-H16···C32(triple bond)	2.71, 151
V	-x+1, y+1/2, -z+3/2	C32-H32···C16(triple bond)	2.62, 144
VI	x, -y+3/2, z+1/2	C18-H18···C5(ring) F3···C10	2.79, 162 3.257(2)
VII	x, y+1, z	C24-H24···F3 C11-H11··O2	2.53, 138 2.85, 135
VIII	x, -y+1/2, z+1/2	C8-H8···F6 C9-H9···F5 C8-H8···C26(ring) C5-H5···C18(ring)	2.70, 130 2.93, 118 2.83, 138 2.86, 158
IX	x, y-1, z	C25-H25···F4 C24-H24···F3 C9-H9···F1	2.72, 138 2.44, 136 2.77, 140
X	-x+2, -y+1, -z+2	C9-H9···F1	2.81, 146
XI	-x+2, y-1/2, -z+3/2	C25-H25···F4	2.53, 141
XII	-x+2, y+1/2, -z+3/2	F5···F1 F5···F3	3.099(2) 3.015(2)
XIII	x, -y+3/2, z-1/2	C28-H28···N1	2.91, 125
XIV	x, y, z (intra)	C6-H6···O1 C22-H22···O2	2.53, 102 2.36, 109

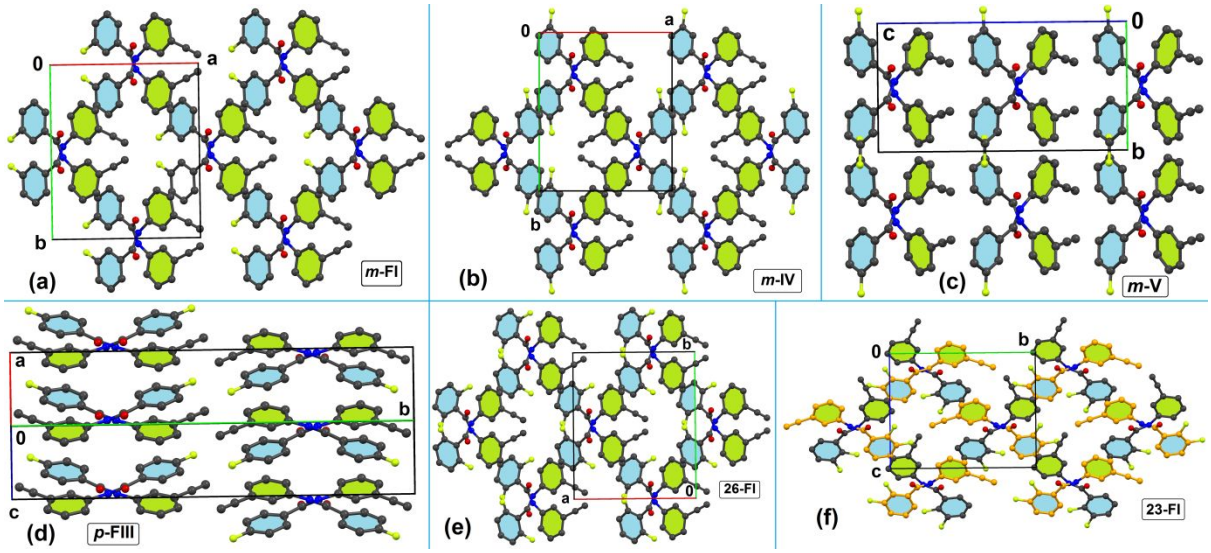


Figure S7. Selectivity of the crisscross hydrogen bonding *synthon* A patterns by molecules to form a layered supramolecular structure in ***m*-F** (**I**, **IV** and **V**) polymorphs, ***p*-FIII, 26-FI** and **23-FI.**

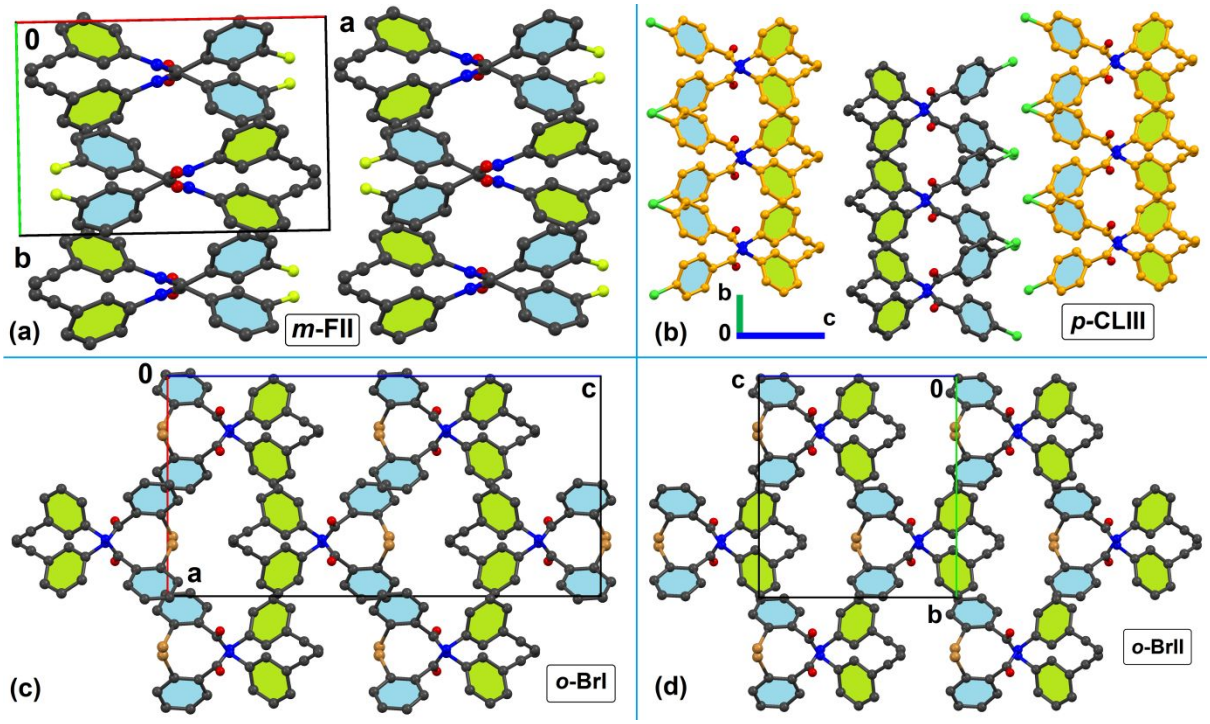


Figure S8. Similar crisscross pattern of molecules found in ***m*-FII, *p*-CLIII** and two ***o*-Br** polymorphs (**I** and **II**) forming a layered packing.

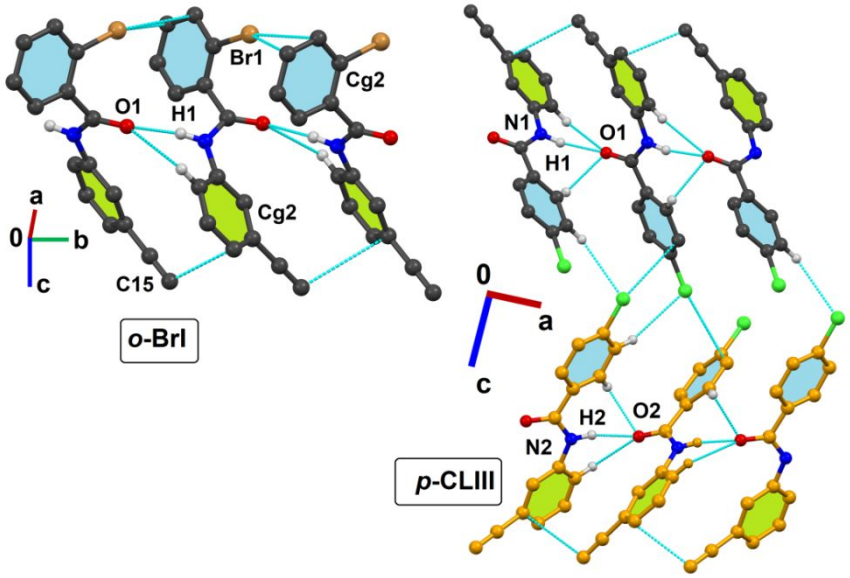


Figure S9. *Synthon* A type primary recognition topology of molecules formed mainly by N-H···O=C hydrogen bonding chains in ***o*-BrI** and ***p*-CLIII** structures.

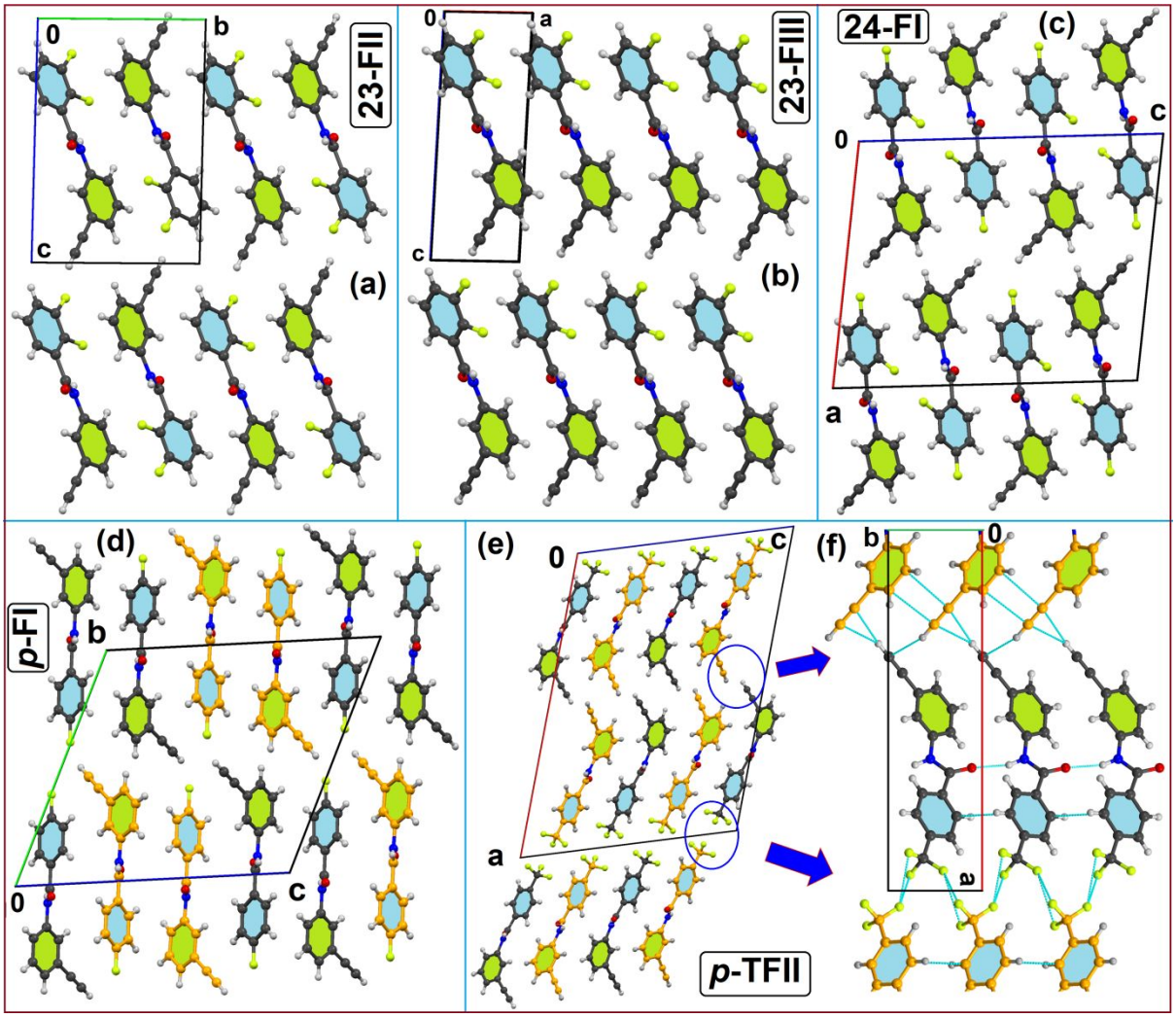


Figure S10. Parallel layered topology of molecules directed by the *synthon* B patterns in **23-FII**, **23-FIII**, **24-FI**, ***p*-TFII**, and ***p*-FI** structures.

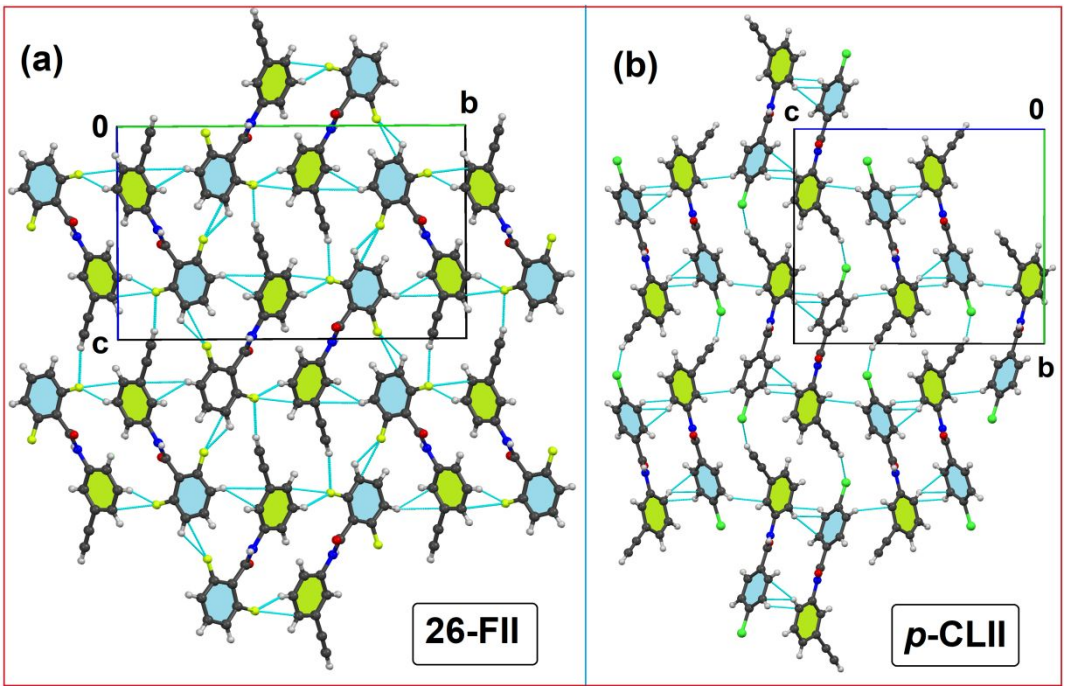


Figure S11. The *synthon* B′ mediated similar layered supramolecular architectures in **26-FII** and ***p*-CLII** crystals.

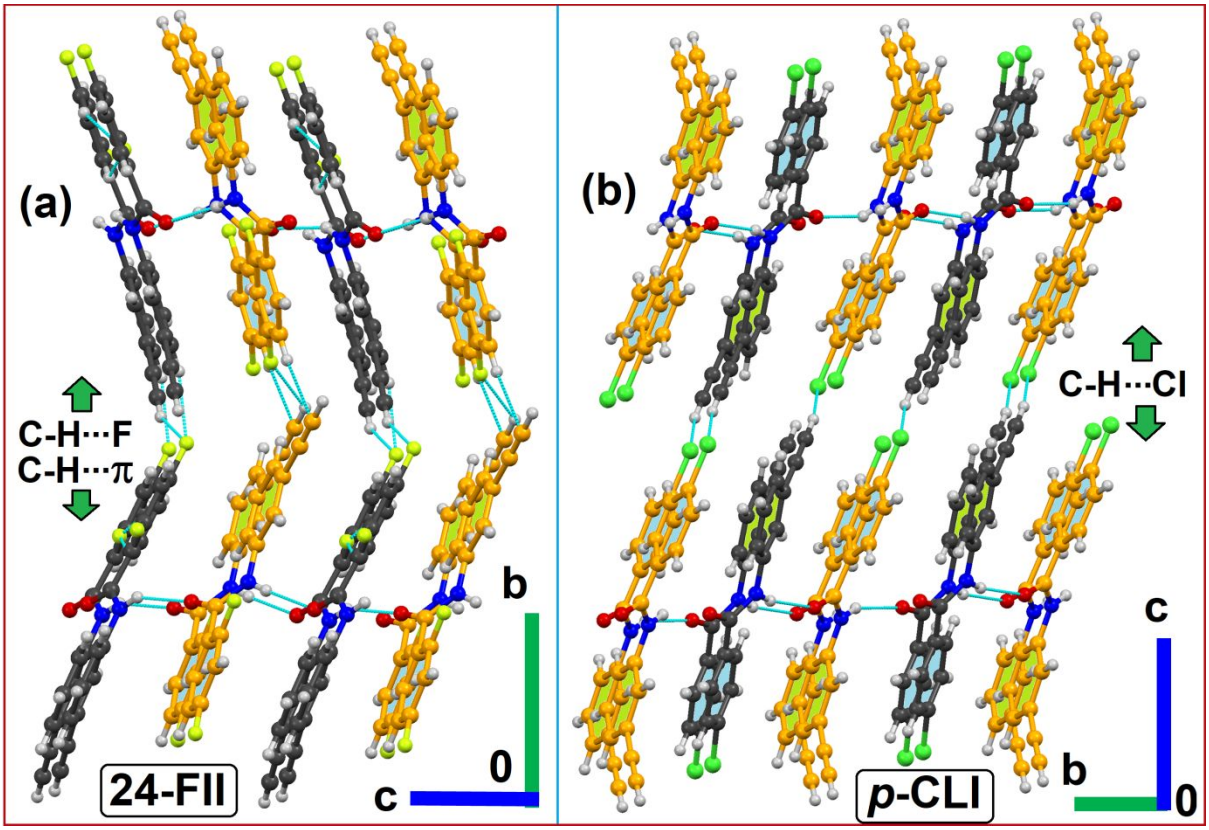


Figure S12. The *synthon* C array of molecules in **24-FII** and ***p*-CLI** crystal structures show comparable packing arrangements.

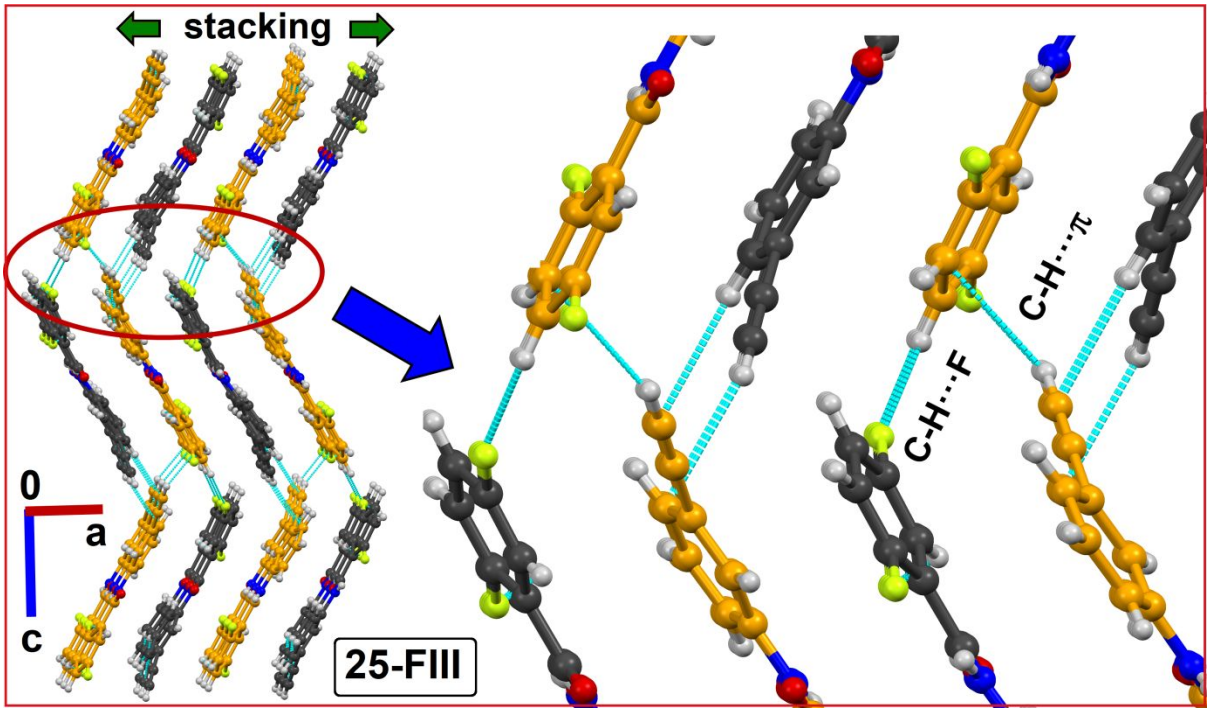


Figure S13. Columnar π···π stacking constructed alongwith weak C-H···π, and C-H···F interaction supported supramolecular topology of molecules in the **25-FIII** crystal.

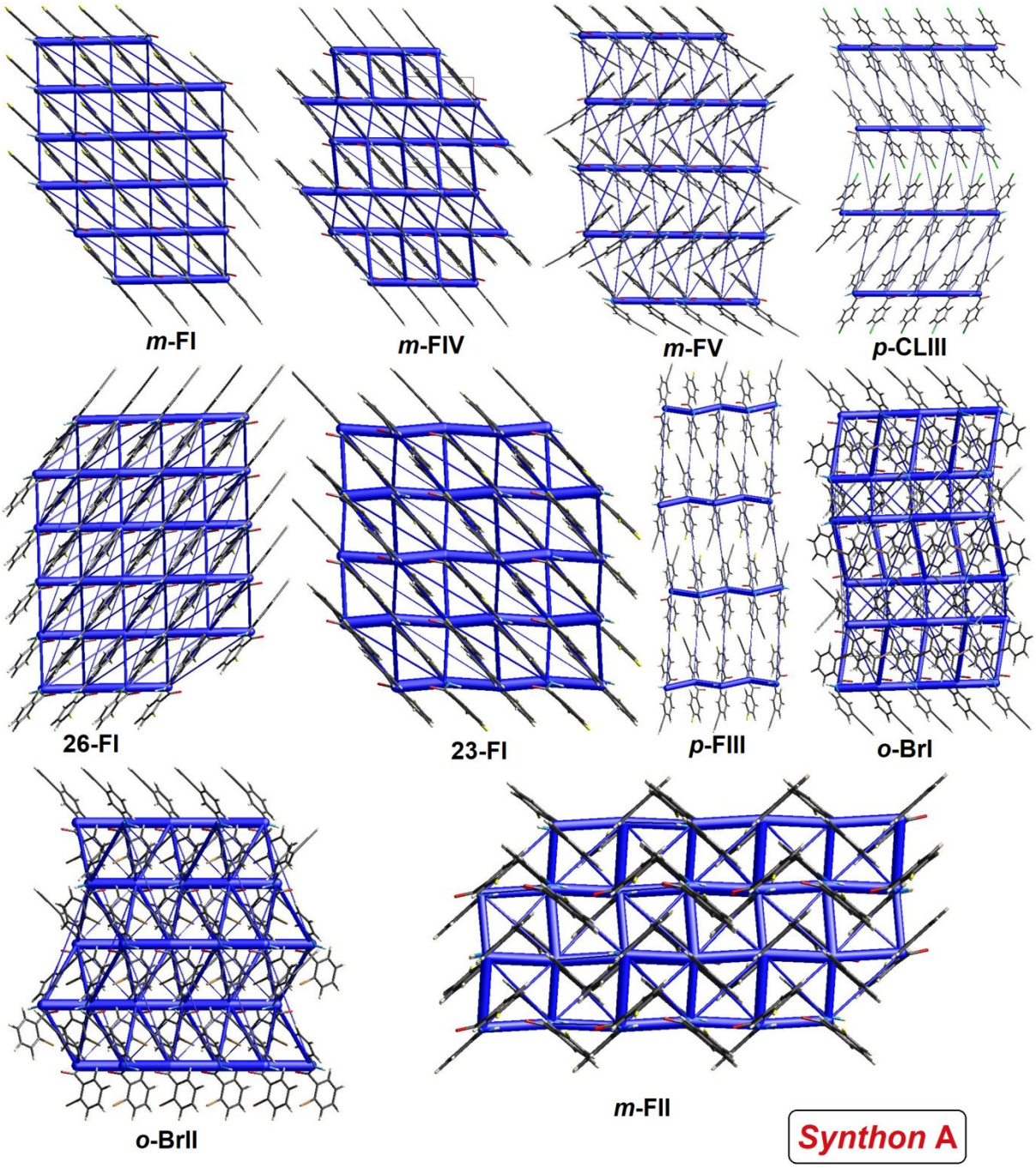


Figure S14. Parallel pillar like interaction topologies as depicted by the energy frameworks for all *synthon* A governed crystal structures.

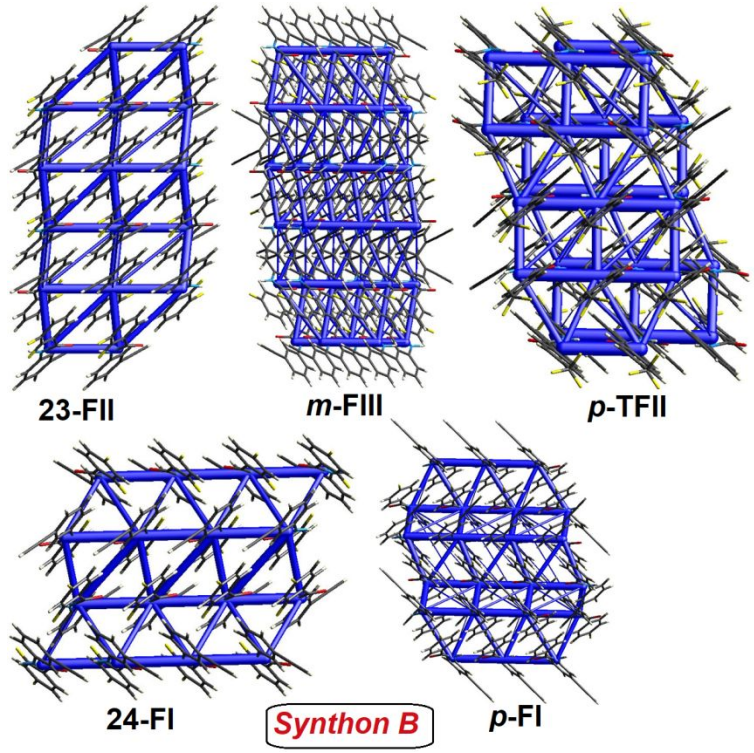


Figure S15. Obtained energy frameworks by molecules in all *synthon* B directed structures.

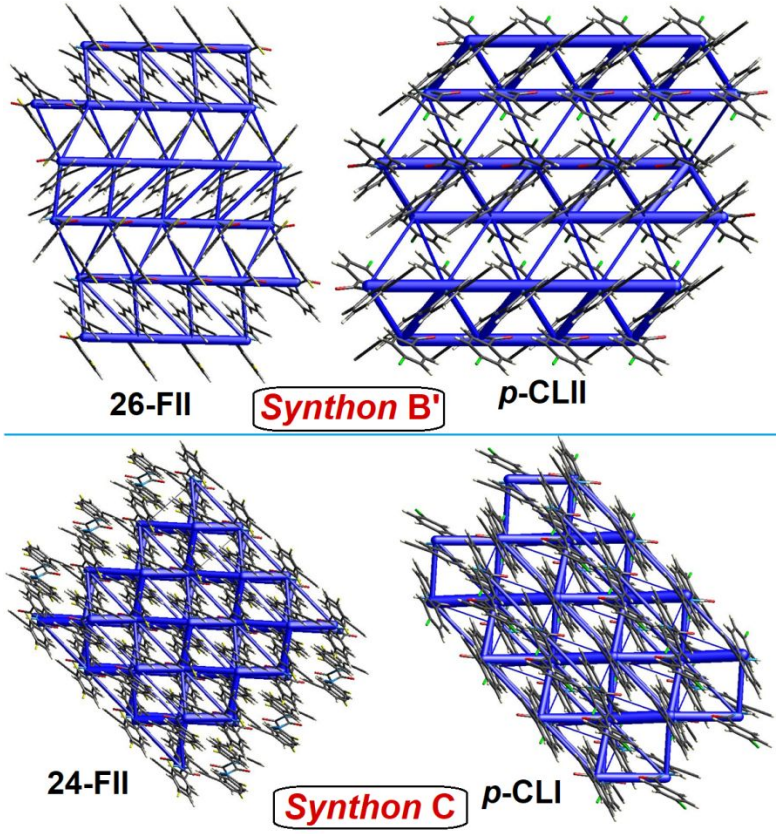


Figure S16. Interaction topologies of all *synthons* B′ and C stabilized supramolecular structures.

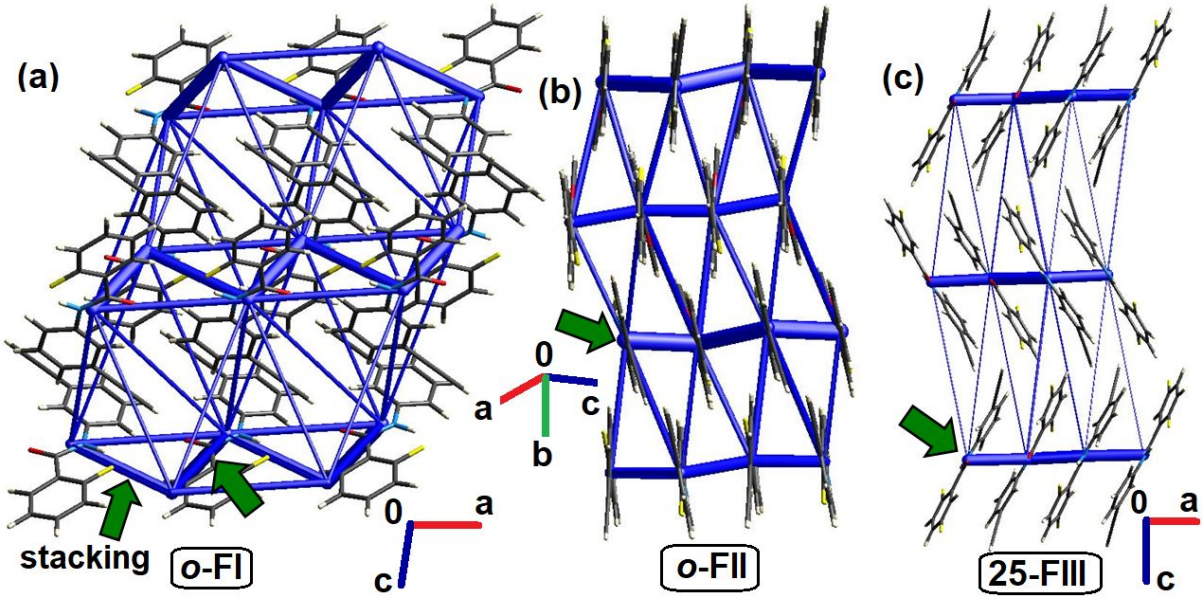


Figure S17. Stacking interaction (green arrows) dominated supramolecular structures (*synthon* D category) showing the construction of pillar like energy frameworks.

Table S5. Top 100 predicted structures in the CSP according to their energy ranks (kJ/mol)

Rank	Space group	Cell volume	Density	Total energy	Length a	Length b	Length c	Angle alpha	Angle beta	Angle gamma
1	C2/C	2.18E+03	1.345478	-128.466	30.83602	5.161557	17.02954	90	126.2954	90
2	C2/C	2.20E+03	1.337525	-127.660	28.82607	5.223203	37.91239	90	157.3577	90
3	P21	551.8317	1.3316	-127.604	7.841294	5.298473	13.3024	90	93.16259	90
4	P21/C	1.11E+03	1.32921	-127.573	12.98719	5.272429	31.14782	90	148.7752	90
5	C2/C	2.17E+03	1.353132	-127.543	27.41208	5.519393	15.20154	90	109.1871	90
6	C2/C	2.21E+03	1.331738	-127.450	28.25527	5.129947	19.53537	90	128.7899	90
7	PC	552.1879	1.330741	-127.418	4.627452	5.084953	24.8813	90	109.411	90
8	C2/C	2.22E+03	1.32346	-127.362	45.37251	5.049462	30.42733	90	161.4225	90
9	P-1	549.7335	1.336682	-127.305	13.11288	8.049718	5.239544	92.73129	84.40054	89.40965
10	P-1	549.5115	1.337222	-127.303	17.59491	9.790389	5.24876	54.88711	59.78911	94.10721
11	PNA21	1.11E+03	1.326216	-127.296	7.684197	27.77655	5.191817	90	90	90
12	P21/C	1.10E+03	1.330935	-127.292	5.231804	24.72053	8.540791	90	88.47586	90
13	P-1	549.8718	1.336346	-127.292	14.69463	7.97698	5.246924	87.26824	116.4429	89.85432
14	P21/C	1.10E+03	1.331593	-127.287	5.234499	24.76665	13.3304	90	140.3098	90
15	P-1	542.9693	1.353334	-127.252	13.15459	7.491103	5.512443	90.77334	91.48211	89.65058
16	P-1	551.6259	1.332097	-127.214	9.757281	12.54873	5.25094	86.1373	120.2414	87.21129
17	P-1	551.4688	1.332476	-127.213	5.25448	13.26992	9.751658	75.8397	59.7414	70.59942
18	P1	273.147	1.345098	-127.207	6.677627	12.62918	5.284527	89.94384	41.26948	75.84768

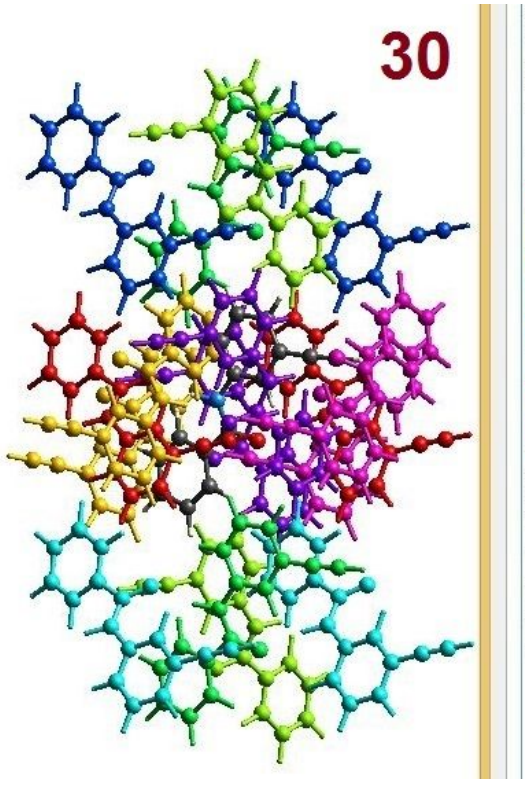
19	P1	273.1484	1.345091	-127.204	14.80592	6.673835	4.402512	127.7453	127.4032	67.06618
20	P1	273.0739	1.345458	-127.199	12.78012	4.409963	6.668645	127.7689	73.38232	87.76368
21	P1	273.1893	1.34489	-127.196	13.69747	4.421045	5.282011	86.29151	67.23883	108.5101
22	P-1	551.8354	1.331591	-127.177	15.47532	9.719971	13.94967	81.82984	147.4946	125.6064
23	P1	272.9365	1.346135	-127.171	6.689649	13.32088	12.78661	160.5725	73.57354	118.5167
24	P-1	548.7862	1.338989	-127.16	5.393836	13.97291	13.22846	134.0599	95.22386	113.2039
25	P21	542.6607	1.354104	-127.15	13.14227	10.86757	4.059548	90	69.38047	90
26	P-1	545.2589	1.347651	-127.148	6.444603	10.11275	15.0425	57.4818	42.8194	57.81586
27	P-1	545.4899	1.347081	-127.139	6.442818	8.619532	38.69057	157.2054	100.0949	97.06985
28	P-1	544.869	1.348616	-127.131	8.622976	25.13667	6.421799	93.15255	97.25653	23.53681
29	PCA21	1.11E+03	1.324713	-127.125	25.13613	4.233523	10.42529	90	90	90
30	P21/C	1.10E+03	1.333725	-127.104	26.7846	7.840672	26.52999	90	168.5932	90
31	P-1	552.5018	1.329985	-127.103	8.096879	13.15628	5.188298	89.46505	91.31343	89.64534
32	PBCA	2.23E+03	1.315382	-127.059	25.33606	8.71745	10.11719	90	90	90
33	P21/C	1.12E+03	1.310564	-127.034	7.767264	5.181714	30.61765	90	114.4954	90
34	PCA21	1.12E+03	1.309157	-127.011	8.81253	8.022589	15.87828	90	90	90
35	P21/C	1.10E+03	1.331914	-126.986	5.235817	26.552	9.584225	90	124.0934	90
36	P21/C	1.09E+03	1.353275	-126.983	5.404433	12.95266	15.52745	90	87.58827	90
37	PC	554.589	1.324979	-126.969	4.256578	12.52313	10.41636	90	87.2016	90
38	P21	558.0953	1.316655	-126.967	4.577292	23.77382	6.749529	90	130.5491	90
39	P21	558.3791	1.315986	-126.966	4.593936	23.72023	6.751821	90	130.6296	90
40	P21/C	1.12E+03	1.313381	-126.96	13.03383	8.600562	26.10719	90	157.5207	90
41	P21/C	1.11E+03	1.318256	-126.941	14.73273	8.59323	10.20213	90	59.67078	90
42	P21/C	1.12E+03	1.307281	-126.94	15.02556	8.689348	10.10418	90	58.44768	90
43	P1	274.6706	1.337637	-126.928	4.233439	17.68428	5.381687	89.79512	93.06583	43.1601
44	PBCA	2.26E+03	1.300634	-126.897	9.607076	9.542998	24.64957	90	90	90
45	P21/C	1.12E+03	1.310901	-126.893	15.02821	8.743027	10.02851	90	58.3004	90
46	C2/C	2.20E+03	1.335955	-126.882	25.71235	5.334052	28.93916	90	146.3358	90
47	PNA21	1.12E+03	1.309061	-126.879	8.496236	8.272188	15.97362	90	90	90
48	P-1	546.1249	1.345514	-126.866	12.70399	5.236445	8.477728	84.7113	76.84972	91.64518
49	P-1	559.9285	1.312344	-126.840	5.197936	8.738743	13.20352	89.04463	69.13346	87.62008
50	C2/C	2.24E+03	1.310914	-126.809	65.41025	6.61565	60.16177	90	175.0593	90
51	P21/C	1.11E+03	1.319841	-126.801	13.97409	8.608513	10.16696	90	65.56465	90
52	CC	1.09E+03	1.347887	-126.793	4.151298	24.85475	11.40084	90	112.0453	90
53	P21/C	1.14E+03	1.29132	-126.764	15.37264	8.766628	10.0136	90	57.495	90
54	C2/C	2.21E+03	1.328716	-126.756	18.51367	5.181271	24.78842	90	111.5158	90
55	P21	550.2536	1.335419	-126.755	4.367557	23.82886	6.998839	90	49.06306	90
56	P21/C	1.12E+03	1.316718	-126.735	14.08584	8.741554	10.02204	90	64.75081	90
57	PCA21	1.12E+03	1.315341	-126.678	27.91536	5.22725	7.656943	90	90	90
58	P1	279.2545	1.31568	-126.674	12.19361	4.568408	5.09486	88.76016	80.34362	86.51752
59	P1	278.9793	1.316977	-126.671	6.767213	4.541685	14.442	104.9772	57.41764	131.0276
60	P21/C	1.09E+03	1.352983	-126.661	4.000457	10.62692	25.70035	90	96.1882	90
61	P21	553.22	1.328258	-126.639	13.57427	7.603177	5.372882	90	86.07313	90
62	P21/C	1.11E+03	1.326699	-126.632	5.123935	46.68401	6.738023	90	136.5848	90
63	P21	556.8158	1.31968	-126.624	26.52265	4.841336	5.065187	90	58.88355	90
64	P-1	555.3011	1.32328	-126.619	24.65042	4.93757	5.065157	94.92374	72.53858	109.2054

65	P1	278.3121	1.320135	-126.608	12.71996	5.120781	4.443003	90.4415	91.52476	105.8157
66	PBCA	2.20E+03	1.337274	-126.591	27.72818	7.689506	10.30861	90	90	90
67	P21	561.1674	1.309447	-126.583	14.02943	7.675211	5.362112	90	103.6122	90
68	P1	279.2856	1.315533	-126.582	5.129635	12.63254	4.558186	106.7595	90.99744	98.34189
69	P21/C	1.10E+03	1.338523	-126.571	5.451824	15.52151	12.97869	90	88.64072	90
70	C2/C	2.19E+03	1.34075	-126.554	64.09278	5.605968	42.35928	90	171.7183	90
71	P21/C	1.13E+03	1.304006	-126.552	9.339953	5.214699	24.15588	90	73.32147	90
72	P21/C	1.11E+03	1.323208	-126.543	5.265899	17.67193	12.39997	90	105.7386	90
73	PC	554.6744	1.324775	-126.541	24.19953	5.242749	25.47232	90	170.1172	90
74	C2/C	2.21E+03	1.331801	-126.541	34.10942	5.182897	17.54748	90	45.35237	90
75	P-1	556.1194	1.321333	-126.534	10.59027	4.826833	30.10187	57.60003	49.28432	28.63818
76	PBCA	2.24E+03	1.311643	-126.511	21.16225	12.82254	8.258265	90	90	90
77	P-1	551.7274	1.331852	-126.492	5.363132	12.87818	11.62059	45.12748	99.70445	89.70263
78	P-1	545.0423	1.348187	-126.490	5.424869	16.33868	9.308743	121.7497	121.1419	91.91177
79	P21	552.1091	1.330931	-126.482	4.3913	5.313936	26.10651	90	64.99746	90
80	C2/C	2.25E+03	1.30769	-126.474	46.4451	6.63263	7.579148	90	105.699	90
81	P21/C	1.13E+03	1.298267	-126.472	13.91492	9.021428	9.910497	90	65.49185	90
82	P-1	546.9948	1.343375	-126.462	14.01297	14.1113	5.282815	141.2356	112.4894	87.00062
83	P-1	564.0338	1.302792	-126.460	12.93521	8.027496	5.517179	89.67143	99.7668	92.53183
84	C2/C	2.24E+03	1.313595	-126.439	6.78985	7.382255	45.06747	90	97.89251	90
85	P-1	563.84	1.30324	-126.437	22.55776	8.156331	5.493262	89.74539	109.5856	139.5255
86	P21/C	1.14E+03	1.287515	-126.433	14.94757	9.014656	9.87073	90	59.11515	90
87	C2/C	2.24E+03	1.314574	-126.431	6.792265	7.374487	48.86034	90	113.9935	90
88	PNA21	1.11E+03	1.329868	-126.427	16.04665	12.98126	5.305187	90	90	90
89	P21/C	1.11E+03	1.323111	-126.426	22.6529	10.12803	19.1355	90	165.3447	90
90	P21/C	1.12E+03	1.308227	-126.421	10.67786	20.59852	12.47881	90	155.8396	90
91	PBCA	2.20E+03	1.336893	-126.417	26.45038	7.481175	11.11071	90	90	90
92	P1	276.1214	1.330608	-126.416	4.303539	13.05863	6.736302	106.3625	50.44067	107.6244
93	P21	555.2032	1.323514	-126.409	23.54152	4.635669	5.159969	90	80.38658	90
94	C2/C	2.23E+03	1.316504	-126.402	7.346981	6.747335	45.12781	90	93.61964	90
95	P1	272.7843	1.346886	-126.398	5.332829	15.40522	4.177203	61.84683	88.2905	111.4994
96	P-1	559.196	1.314063	-126.388	23.34186	4.965	5.066032	84.63281	77.46098	99.96277
97	P21/C	1.11E+03	1.319918	-126.385	5.133901	46.96932	6.727631	90	136.6589	90
98	P21/C	1.09E+03	1.348507	-126.373	12.7066	16.15923	13.88046	90	157.5184	90
99	P21/C	1.09E+03	1.349414	-126.366	12.70881	16.0647	13.88949	90	157.4145	90
100	C2/C	2.24E+03	1.313516	-126.362	6.769754	7.420939	46.30714	90	105.869	90

Interaction energy calculations and Energy framework analysis

The energy framework analysis has been performed to visualize the interaction topology. The pairwise intermolecular interaction energies were estimated from B3LYP/6-31G(d,p)molecular wave functions calculations by *CrystalExplorer17.5* for the crystals. For, two ***o*-Br** polymorphs CE-B3LYP/ DGDZVP molecular wave functions were used to generate energy frameworks due to the high polarization effect of Br-atoms. [reference number 44 in the main manuscript]. The energy cut-off and tube size were 5 and 80 kJ/mol respectively, for generating the energy framework of each structure.

Output of interaction energy calculations for all structures using *CrystalExplorer17.5*:



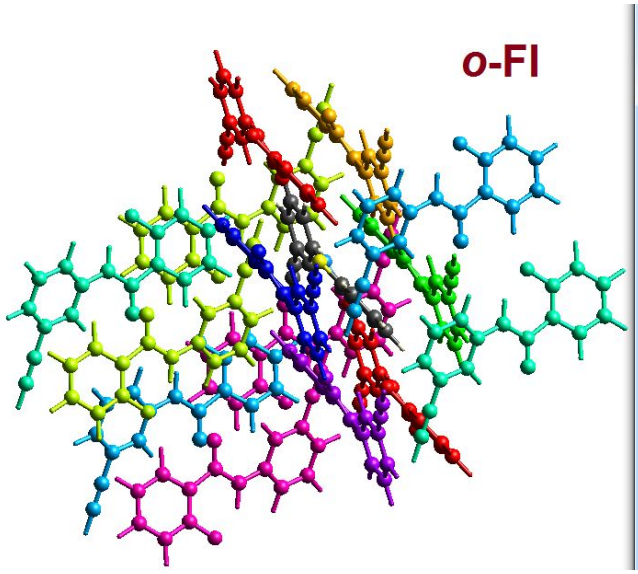
Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x+1/2, -y, z	4.31	B3LYP/6-31G(d,p)	-41.2	-10.8	-50.9	64.4	-56.2
	2	-x, -y, z+1/2	8.88	B3LYP/6-31G(d,p)	-4.5	-0.7	-13.9	9.3	-11.6
	2	-x+1/2, y, z+1/2	11.60	B3LYP/6-31G(d,p)	-4.6	-0.6	-11.1	7.1	-10.5
	2	x, y, z	8.33	B3LYP/6-31G(d,p)	-1.6	-1.1	-16.2	13.7	-8.1
	2	x+1/2, -y, z	9.49	B3LYP/6-31G(d,p)	-2.1	-0.8	-10.0	4.5	-8.7
	2	x+1/2, -y, z	9.28	B3LYP/6-31G(d,p)	-4.3	-0.8	-15.3	12.2	-10.9
	2	-x+1/2, y, z+1/2	8.06	B3LYP/6-31G(d,p)	-3.1	-0.9	-9.6	5.2	-9.1
	2	-x, -y, z+1/2	9.40	B3LYP/6-31G(d,p)	-3.3	-1.1	-13.0	12.6	-7.8

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618



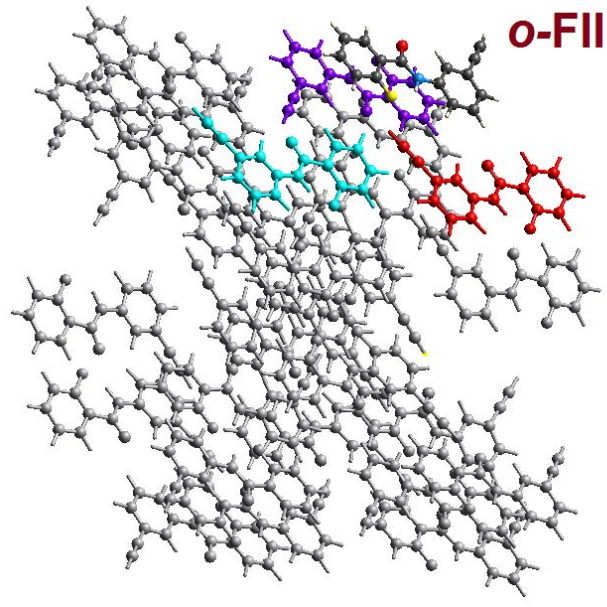
Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	6.66	B3LYP/6-31G(d,p)	-9.7	-2.8	-22.2	17.5	-20.8
	1	-x, -y, -z	5.46	B3LYP/6-31G(d,p)	-8.0	-1.5	-38.8	20.9	-30.5
	2	-x+1/2, y+1/2, -z+1/2	7.96	B3LYP/6-31G(d,p)	-1.9	-1.1	-22.1	12.7	-14.2
	1	-x, -y, -z	4.30	B3LYP/6-31G(d,p)	-7.3	-4.1	-54.9	32.4	-38.6
	2	x+1/2, -y+1/2, z+1/2	9.31	B3LYP/6-31G(d,p)	-3.9	-0.9	-12.5	8.6	-10.3
	2	x+1/2, -y+1/2, z+1/2	9.00	B3LYP/6-31G(d,p)	-5.5	-1.0	-9.8	6.6	-11.0
	1	-x, -y, -z	9.63	B3LYP/6-31G(d,p)	-1.2	-0.3	-7.8	2.5	-6.8
	1	-x, -y, -z	9.03	B3LYP/6-31G(d,p)	-4.3	-0.6	-24.5	12.0	-18.9
	2	-x+1/2, y+1/2, -z+1/2	9.51	B3LYP/6-31G(d,p)	-14.8	-3.0	-7.9	20.5	-12.1

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

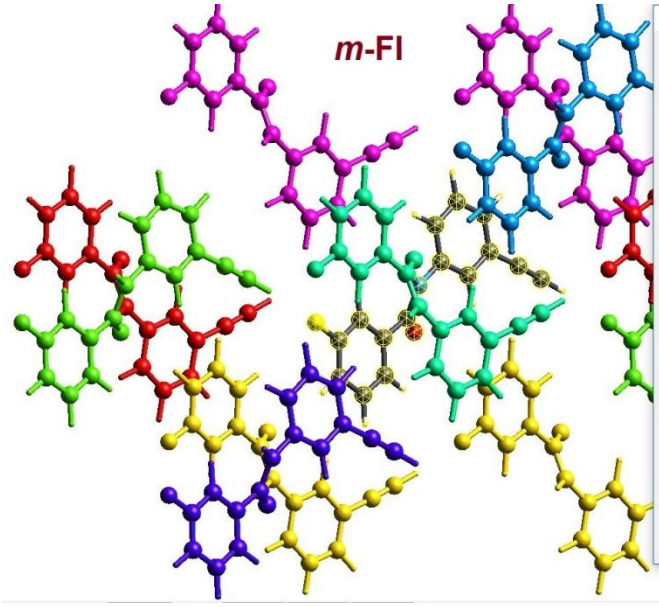


Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	7.93	B3LYP/6-31G(d,p)	-4.8	-1.8	-20.6	14.0	-15.8
	0	-	6.54	B3LYP/6-31G(d,p)	-7.4	-2.2	-24.8	18.7	-19.5
	0	-	9.56	B3LYP/6-31G(d,p)	-16.5	-3.3	-11.0	17.0	-18.9
	0	-	12.06	B3LYP/6-31G(d,p)	-0.8	-0.1	-4.5	1.0	-4.3
	0	-	6.89	B3LYP/6-31G(d,p)	-4.5	-1.1	-23.4	15.1	-16.7
	0	x, -y+1/2, z+1/2	8.45	B3LYP/6-31G(d,p)	-3.3	-1.2	-30.1	16.2	-20.6
	0	x, -y+1/2, z+1/2	6.55	B3LYP/6-31G(d,p)	-8.4	-2.5	-52.3	33.2	-35.7
	0	x, y, z	13.27	B3LYP/6-31G(d,p)	-3.0	-1.0	-10.8	10.5	-6.8
	1	-	10.61	B3LYP/6-31G(d,p)	-1.1	-0.5	-8.0	3.5	-6.3
	0	-	9.72	B3LYP/6-31G(d,p)	-18.3	-3.6	-11.1	20.2	-19.2
	0	-	13.90	B3LYP/6-31G(d,p)	-0.4	-0.2	-1.9	0.3	-2.1
	0	x, y, z	13.27	B3LYP/6-31G(d,p)	-2.9	-1.0	-10.8	10.3	-6.8
	1	-x, -y, -z	3.86	B3LYP/6-31G(d,p)	-14.7	-3.6	-76.3	46.6	-55.9
	0	-x, -y, -z	12.02	B3LYP/6-31G(d,p)	-0.3	-0.7	-10.4	5.1	-6.7
	0	-x, -y, -z	5.25	B3LYP/6-31G(d,p)	-11.3	-1.8	-61.7	33.2	-46.5
	0	-x, -y, -z	9.99	B3LYP/6-31G(d,p)	1.8	-1.1	-14.7	4.6	-8.8

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)



Information

Crystal | Atoms | Surface | Energies

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R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	x, -y, z+1/2	11.66	B3LYP/6-31G(d,p)	1.0	-0.1	-5.0	0.6	-3.0
2	x+1/2, -y+1/2, z+1/2	9.19	B3LYP/6-31G(d,p)	-7.2	-2.0	-19.4	17.6	-15.1
2	x, y, z	13.71	B3LYP/6-31G(d,p)	-4.2	-0.4	-3.4	5.2	-4.5
2	x, -y, z+1/2	4.17	B3LYP/6-31G(d,p)	-44.5	-11.0	-59.5	71.0	-63.1
2	x+1/2, y+1/2, z	8.40	B3LYP/6-31G(d,p)	-2.7	-1.9	-27.8	19.0	-16.7
2	x+1/2, y+1/2, z	11.84	B3LYP/6-31G(d,p)	-2.7	-0.5	-10.9	4.5	-10.0
2	x+1/2, -y+1/2, z+1/2	9.58	B3LYP/6-31G(d,p)	-1.6	-1.6	-16.2	11.2	-10.1

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

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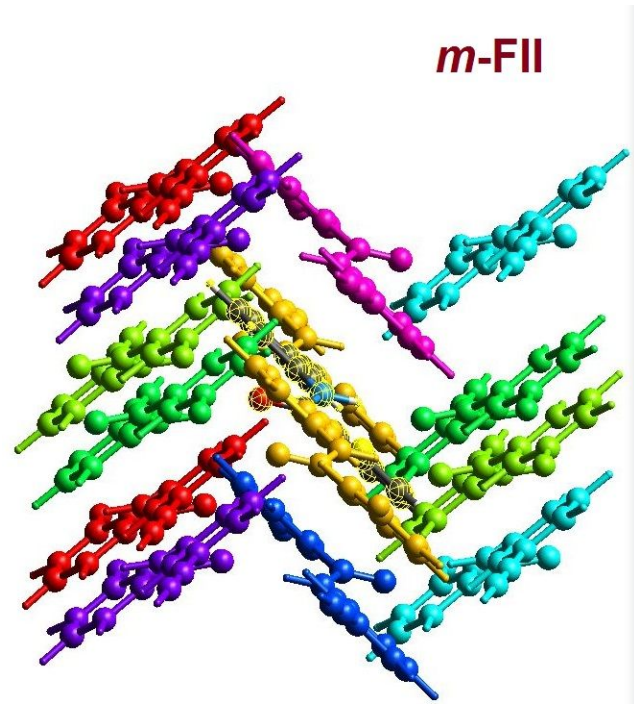

Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
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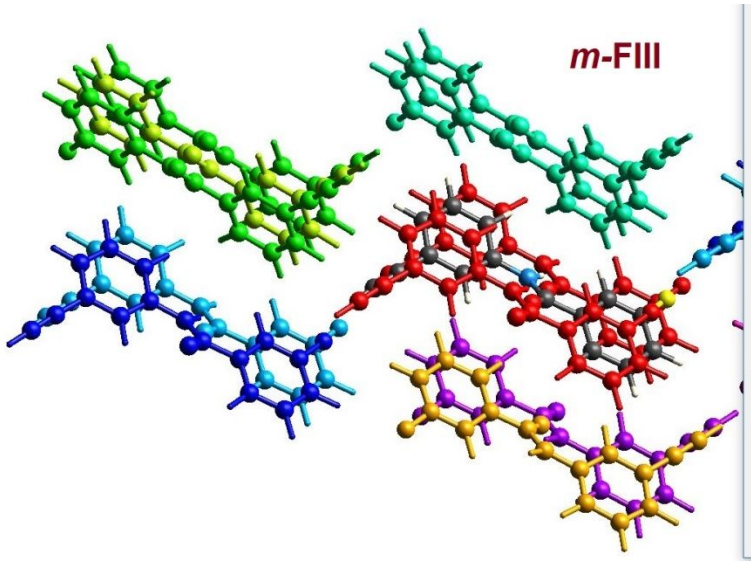
N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	-x, y+1/2, -z+1/2	12.97	B3LYP/6-31G(d,p)	-0.5	-0.3	-5.1	2.0	-3.9
2	x, y, z	14.63	B3LYP/6-31G(d,p)	-5.4	-0.6	-3.3	8.2	-4.1
2	x, -y+1/2, z+1/2	12.96	B3LYP/6-31G(d,p)	-0.8	-0.5	-9.6	5.6	-6.1
2	x, -y+1/2, z+1/2	5.20	B3LYP/6-31G(d,p)	-31.4	-7.8	-33.2	36.7	-45.2
2	-x, y+1/2, -z+1/2	6.93	B3LYP/6-31G(d,p)	-4.5	-1.5	-16.7	14.8	-11.3
1	-x, -y, -z	4.69	B3LYP/6-31G(d,p)	-15.6	-3.1	-52.8	30.4	-45.9
2	-x, y+1/2, -z+1/2	6.79	B3LYP/6-31G(d,p)	-5.0	-1.0	-15.8	13.0	-11.8
1	-x, -y, -z	4.26	B3LYP/6-31G(d,p)	-6.2	-1.0	-54.3	31.2	-35.4

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618



Crystal | Atoms | Surface | Energies

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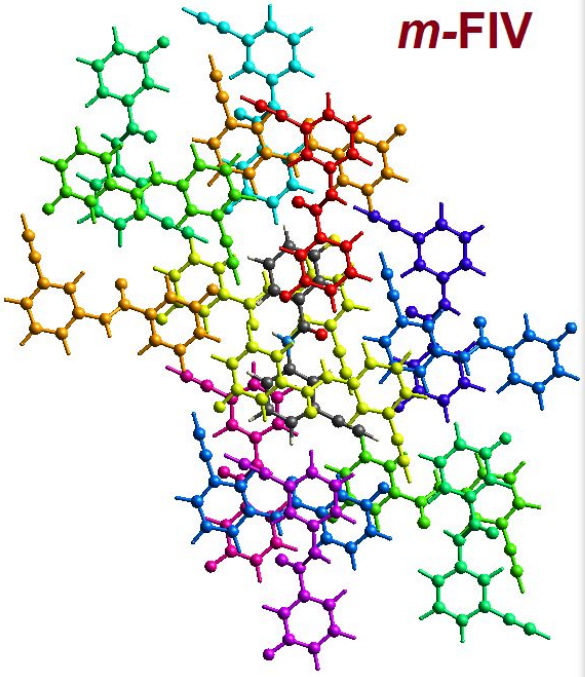
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	x, y, z	4.89	B3LYP/6-31G(d,p)	-33.6	-9.7	-45.7	53.4	-49.5
1	-x+1/2, -y+1/2, -z	6.47	B3LYP/6-31G(d,p)	-14.7	-3.9	-29.2	26.0	-27.8
1	-x, y, -z+1/2	12.43	B3LYP/6-31G(d,p)	-3.6	-0.8	-13.6	9.8	-10.1
2	-x, y, -z+1/2	13.35	B3LYP/6-31G(d,p)	1.1	-0.2	-4.9	2.0	-2.0
2	-x+1/2, y+1/2, -z+1/2	5.82	B3LYP/6-31G(d,p)	-3.6	-3.1	-32.3	20.3	-21.6
2	x+1/2, y+1/2, z	11.64	B3LYP/6-31G(d,p)	-0.4	-0.3	-8.4	4.2	-5.3
2	x+1/2, y+1/2, z	13.53	B3LYP/6-31G(d,p)	-3.7	-0.4	-3.4	4.8	-4.3
1	-x+1/2, -y+1/2, -z	5.10	B3LYP/6-31G(d,p)	-7.8	-1.2	-46.0	26.8	-32.7
1	-x, -y, -z	13.20	B3LYP/6-31G(d,p)	-4.4	-0.6	-8.3	6.1	-8.6

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618



Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-x, -y, -z	8.18	B3LYP/6-31G(d,p)	-10.8	-2.5	-34.0	20.7	-30.1
2	-x, y+1/2, -z+1/2	10.08	B3LYP/6-31G(d,p)	-1.1	-1.3	-13.0	9.1	-7.8
2	x, -y+1/2, z+1/2	4.26	B3LYP/6-31G(d,p)	-44.2	-11.1	-58.8	69.8	-63.0
2	x, -y+1/2, z+1/2	11.69	B3LYP/6-31G(d,p)	-1.0	-0.3	-4.5	0.8	-4.7
2	x, y, z	13.70	B3LYP/6-31G(d,p)	1.9	-0.4	-2.4	1.2	0.3
1	-x, -y, -z	12.16	B3LYP/6-31G(d,p)	-2.4	-0.3	-8.2	5.0	-6.8
2	-x, y+1/2, -z+1/2	8.82	B3LYP/6-31G(d,p)	-9.6	-1.8	-22.3	22.4	-17.1
1	-x, -y, -z	7.41	B3LYP/6-31G(d,p)	0.7	-0.2	-4.8	0.2	-3.4
1	-x, -y, -z	11.71	B3LYP/6-31G(d,p)	-1.8	-0.6	-10.6	2.7	-9.9
1	-x, -y, -z	8.92	B3LYP/6-31G(d,p)	-3.2	-1.0	-22.8	15.0	-14.7

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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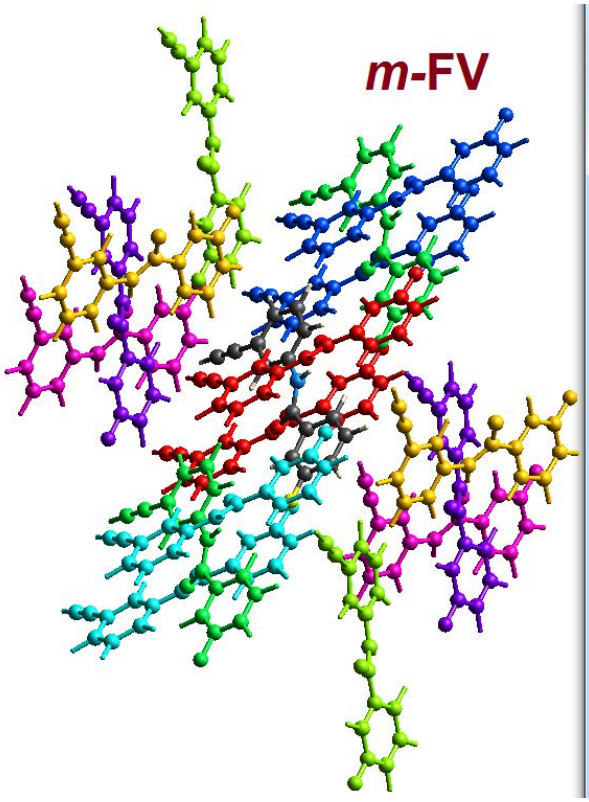

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	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x+1/2, -y, z	4.39	B3LYP/6-31G(d,p)	-38.7	-9.9	-50.9	59.2	-55.9
	2	-x, -y, z+1/2	8.91	B3LYP/6-31G(d,p)	-4.5	-0.9	-12.2	6.3	-12.2
	2	-x+1/2, y, z+1/2	11.67	B3LYP/6-31G(d,p)	-1.0	-0.6	-11.9	6.8	-7.6
	2	x, y, z	8.36	B3LYP/6-31G(d,p)	-4.5	-1.0	-17.3	12.9	-12.5
	2	x+1/2, -y, z	8.89	B3LYP/6-31G(d,p)	2.0	-0.5	-11.9	4.2	-6.1
	2	x+1/2, -y, z	9.97	B3LYP/6-31G(d,p)	-4.3	-0.9	-15.1	12.5	-10.6
	2	-x+1/2, y, z+1/2	8.14	B3LYP/6-31G(d,p)	-3.3	-0.9	-9.1	4.5	-9.3
	2	-x, -y, z+1/2	9.57	B3LYP/6-31G(d,p)	-2.6	-0.9	-12.2	10.2	-7.7

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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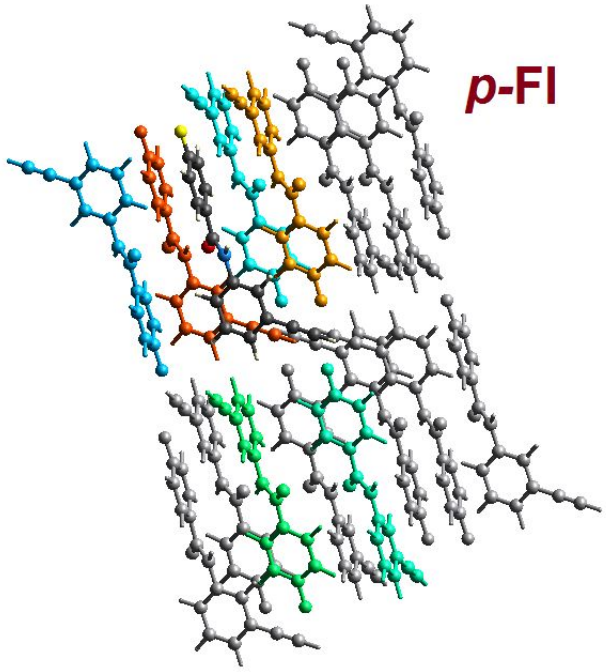

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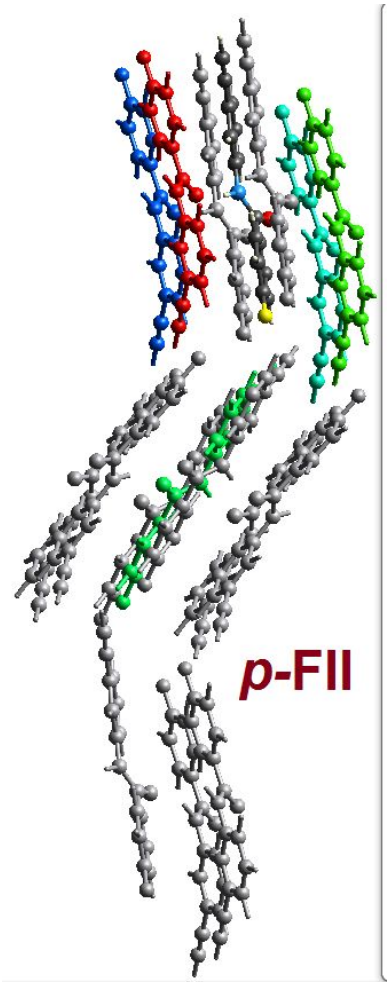
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	0	x, y, z	5.21	B3LYP/6-31G(d,p)	-34.8	-8.8	-42.8	50.4	-49.5
	1	x, y, z	5.21	B3LYP/6-31G(d,p)	-33.8	-9.1	-41.9	47.5	-49.6
	1	-	4.18	B3LYP/6-31G(d,p)	-8.5	-2.4	-54.8	29.3	-40.4
	0	-x, -y, -z	5.03	B3LYP/6-31G(d,p)	-10.1	-3.3	-40.3	32.4	-28.2
	0	-x, -y, -z	14.50	B3LYP/6-31G(d,p)	-6.6	-0.6	-6.1	9.0	-7.2
	0	-	12.65	B3LYP/6-31G(d,p)	-3.0	-0.6	-12.8	9.8	-8.7
	0	-	14.64	B3LYP/6-31G(d,p)	-3.4	-0.4	-4.6	3.1	-5.9
	0	-	6.98	B3LYP/6-31G(d,p)	-2.8	-1.2	-12.4	9.0	-9.0
	1	-	12.42	B3LYP/6-31G(d,p)	-3.5	-0.6	-11.7	8.7	-8.9
	1	-	13.77	B3LYP/6-31G(d,p)	1.8	-0.1	-3.5	0.4	-0.9
	1	-	6.36	B3LYP/6-31G(d,p)	-7.3	-1.8	-17.5	15.2	-14.9
	1	-x, -y, -z	5.27	B3LYP/6-31G(d,p)	-13.4	-1.3	-41.7	27.5	-34.4
	0	-x, -y, -z	15.13	B3LYP/6-31G(d,p)	0.9	-0.1	-1.7	0.1	-0.6
	0	-	13.68	B3LYP/6-31G(d,p)	2.0	-0.2	-4.3	0.7	-1.3
	0	-	14.35	B3LYP/6-31G(d,p)	-4.2	-0.5	-4.4	5.0	-5.5
	0	-	14.83	B3LYP/6-31G(d,p)	0.1	-0.0	-0.8	0.0	-0.6
	0	-x, -y, -z	5.59	B3LYP/6-31G(d,p)	-8.3	-1.5	-36.5	23.8	-27.0
	0	-x, -y, -z	4.79	B3LYP/6-31G(d,p)	-13.0	-3.2	-45.9	31.9	-36.3
	0	-x, -y, -z	13.97	B3LYP/6-31G(d,p)	-5.6	-0.5	-5.7	7.6	-6.6
	0	-x, -y, -z	15.26	B3LYP/6-31G(d,p)	0.8	-0.1	-1.5	0.0	-0.4



Information

Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	4.46	B3LYP/6-31G(d,p)	-44.4	-12.0	-53.2	69.6	-59.1
	0	x, y, z	6.51	B3LYP/6-31G(d,p)	-4.6	-2.3	-24.4	16.3	-17.7
	0	-x, y+1/2, -z	14.07	B3LYP/6-31G(d,p)	-2.1	-0.2	-3.4	2.4	-3.9
	0	-	13.01	B3LYP/6-31G(d,p)	-2.4	-0.4	-5.7	2.4	-6.4
	1	-	4.47	B3LYP/6-31G(d,p)	-7.3	-2.0	-58.5	38.6	-36.4
	1	-x, y+1/2, -z	12.60	B3LYP/6-31G(d,p)	-5.4	-0.6	-9.4	9.3	-8.6
	1	-	5.61	B3LYP/6-31G(d,p)	-38.3	-9.0	-35.3	47.9	-48.3
	0	-	12.75	B3LYP/6-31G(d,p)	-1.0	-0.2	-3.9	0.5	-4.2
	1	-	5.04	B3LYP/6-31G(d,p)	-0.9	-2.4	-42.0	21.5	-26.0
	0	-	12.70	B3LYP/6-31G(d,p)	-1.4	-0.2	-4.9	1.6	-5.0
	0	x, y, z	6.51	B3LYP/6-31G(d,p)	-6.7	-3.7	-26.5	22.9	-18.7
	0	-x, y+1/2, -z	12.65	B3LYP/6-31G(d,p)	-4.1	-0.7	-9.5	10.4	-6.7
	0	-x, y+1/2, -z	13.73	B3LYP/6-31G(d,p)	-2.1	-0.5	-5.1	3.8	-4.6

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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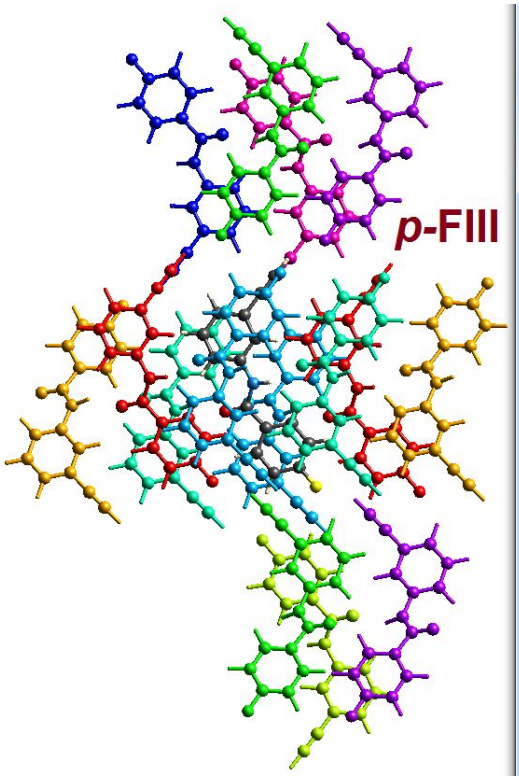

Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	5.85	B3LYP/6-31G(d,p)	-3.9	-1.8	-33.4	20.8	-21.6
	2	x+1/2, -y+1/2, z+1/2	9.56	B3LYP/6-31G(d,p)	-0.2	-0.3	-3.8	1.3	-2.9
	1	-x, -y, -z	13.37	B3LYP/6-31G(d,p)	-5.0	-0.4	-7.0	5.4	-8.4
	2	-x+1/2, y+1/2, -z+1/2	13.18	B3LYP/6-31G(d,p)	-0.7	-0.2	-6.2	2.7	-4.6
	2	x+1/2, -y+1/2, z+1/2	4.83	B3LYP/6-31G(d,p)	-41.6	-11.7	-50.2	67.1	-54.9
	2	x+1/2, -y+1/2, z+1/2	4.87	B3LYP/6-31G(d,p)	0.9	-1.6	-32.0	13.0	-20.1
	1	-x, -y, -z	13.15	B3LYP/6-31G(d,p)	-4.0	-0.6	-11.5	10.4	-8.2
	2	-x+1/2, y+1/2, -z+1/2	14.45	B3LYP/6-31G(d,p)	-4.5	-0.5	-3.7	6.6	-4.3
	1	-x, -y, -z	13.20	B3LYP/6-31G(d,p)	-1.7	-0.3	-4.4	1.9	-4.7

Scale factors for benchmarked energy models
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Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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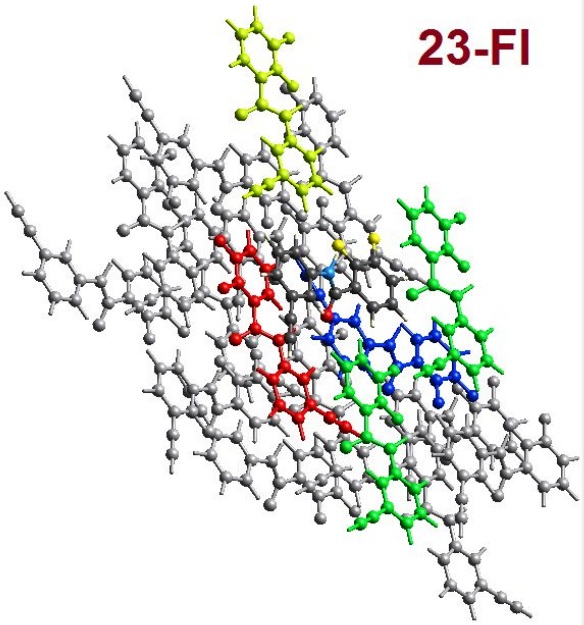

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	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	4.22	B3LYP/6-31G(d,p)	-45.2	-11.0	-60.5	70.6	-65.0
	0	-	11.91	B3LYP/6-31G(d,p)	-2.7	-0.7	-10.5	4.7	-9.6
	0	x, y, z	13.46	B3LYP/6-31G(d,p)	-3.8	-0.4	-3.8	5.1	-4.4
	1	x+1/2, -y, z+1/2	9.71	B3LYP/6-31G(d,p)	-2.5	-1.0	-15.3	9.4	-10.9
	0	-	8.44	B3LYP/6-31G(d,p)	-1.8	-1.7	-30.6	18.9	-18.2
	2	x+1/2, -y, z+1/2	9.23	B3LYP/6-31G(d,p)	-6.8	-2.0	-18.1	13.5	-16.1
	0	-	4.28	B3LYP/6-31G(d,p)	-42.0	-9.8	-57.1	68.1	-59.2
	0	-	11.33	B3LYP/6-31G(d,p)	-1.1	-0.3	-4.3	0.6	-4.7
	0	-	8.56	B3LYP/6-31G(d,p)	1.7	-0.6	-8.5	3.4	-3.9
	1	-	8.52	B3LYP/6-31G(d,p)	-5.2	-1.8	-35.7	24.7	-22.7
	0	-	12.01	B3LYP/6-31G(d,p)	-0.6	-0.3	-7.1	1.9	-5.9
	0	x+1/2, -y, z+1/2	9.82	B3LYP/6-31G(d,p)	-1.5	-1.4	-14.4	8.9	-9.7
	0	x+1/2, -y, z+1/2	9.13	B3LYP/6-31G(d,p)	-11.6	-2.9	-17.5	16.5	-19.4
	0	x, y, z	13.32	B3LYP/6-31G(d,p)	-5.1	-0.8	-6.8	7.7	-7.1

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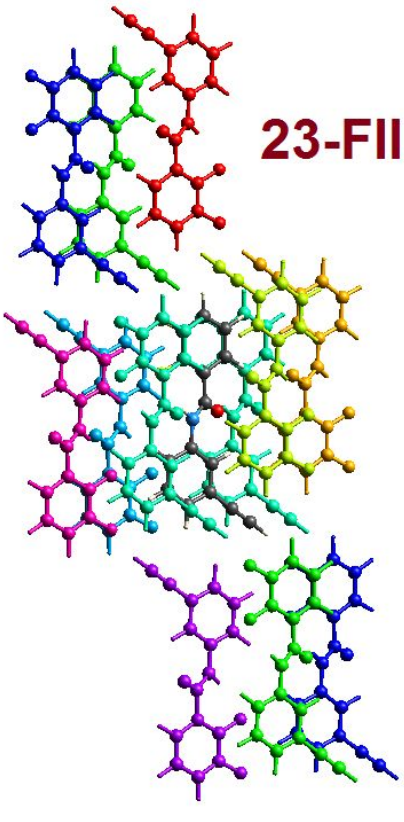

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	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	13.81	B3LYP/6-31G(d,p)	0.0	-0.3	-3.1	0.6	-2.5
	1	-x, -y, -z	6.57	B3LYP/6-31G(d,p)	-16.4	-4.0	-31.7	30.8	-28.9
	1	-x, -y, -z	4.46	B3LYP/6-31G(d,p)	-10.8	-1.9	-56.8	37.8	-38.9
	2	x, y, z	12.87	B3LYP/6-31G(d,p)	-1.4	-0.3	-7.2	3.9	-5.6
	2	x, y, z	5.13	B3LYP/6-31G(d,p)	-25.0	-7.0	-43.4	39.5	-45.0
	1	-x, -y, -z	4.42	B3LYP/6-31G(d,p)	-10.4	-1.6	-55.9	30.8	-41.8
	2	x, y, z	14.09	B3LYP/6-31G(d,p)	-4.2	-0.4	-3.5	6.7	-3.7
	1	-x, -y, -z	13.25	B3LYP/6-31G(d,p)	-4.8	-0.8	-13.4	13.5	-8.9
	1	-x, -y, -z	7.00	B3LYP/6-31G(d,p)	-5.8	-1.1	-20.5	15.0	-15.5

Scale factors for benchmarked energy models
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Energy Model	k_ele	k_pol	k_disp	k_rep
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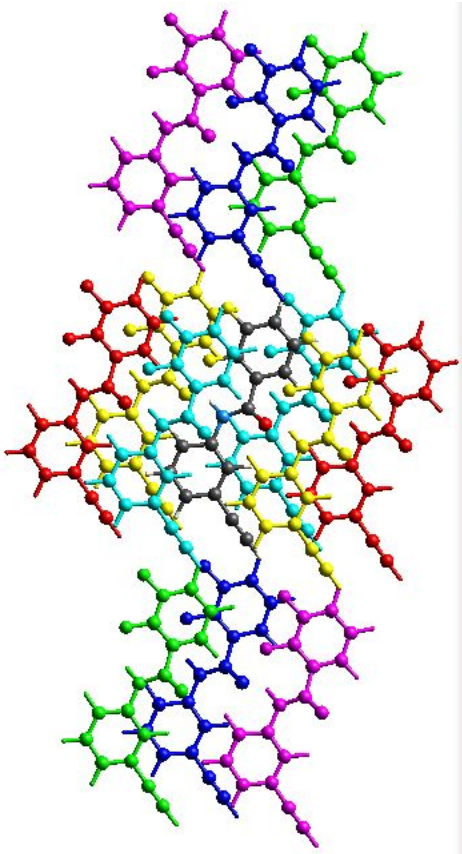

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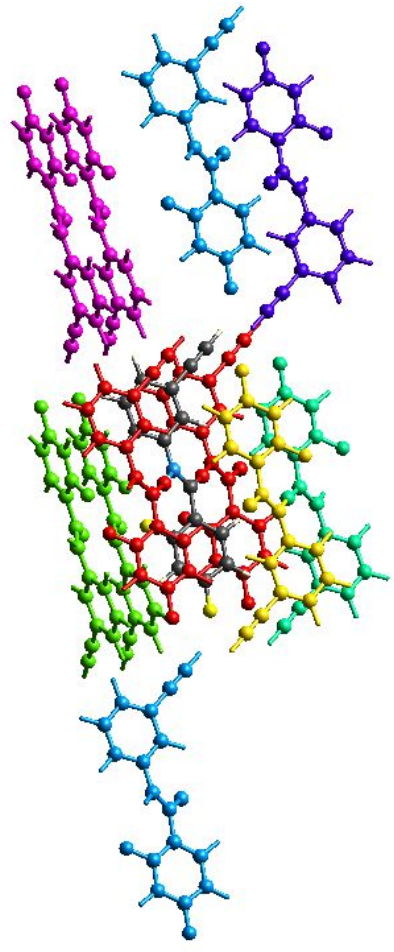
	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	6.79	B3LYP/6-31G(d,p)	-9.2	-2.2	-26.0	21.5	-20.7
	2	x, y, z	5.08	B3LYP/6-31G(d,p)	-26.5	-7.4	-43.4	41.0	-46.0
	2	x, y, z	13.35	B3LYP/6-31G(d,p)	-4.3	-1.0	-9.9	9.3	-8.1
	2	x, y, z	4.51	B3LYP/6-31G(d,p)	-4.3	-1.7	-55.0	31.5	-34.2
	2	x, y, z	12.73	B3LYP/6-31G(d,p)	-1.1	-0.3	-7.2	3.6	-5.4
	2	x, y, z	14.03	B3LYP/6-31G(d,p)	-4.1	-0.4	-3.5	6.3	-3.8

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

23-FIII



Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

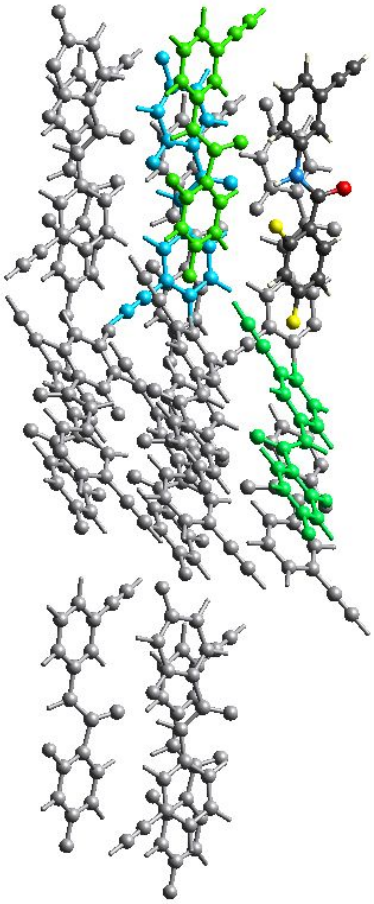
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	4.99	B3LYP/6-31G(d,p)	-29.0	-7.8	-42.5	43.9	-46.4
	1	-x, -y, -z	4.58	B3LYP/6-31G(d,p)	-3.2	-1.4	-49.3	25.7	-31.5
	2	-x, y+1/2, -z+1/2	5.22	B3LYP/6-31G(d,p)	-6.1	-1.6	-37.0	24.6	-24.7
	1	-x, -y, -z	6.22	B3LYP/6-31G(d,p)	-22.3	-4.6	-32.0	32.2	-35.0
	2	x, y, z	14.79	B3LYP/6-31G(d,p)	-3.6	-0.3	-3.9	4.7	-4.6
	1	-x, -y, -z	14.29	B3LYP/6-31G(d,p)	-4.4	-0.4	-5.0	5.2	-6.1
	2	-x, y+1/2, -z+1/2	12.72	B3LYP/6-31G(d,p)	-3.5	-0.6	-12.8	9.7	-9.4

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

24-FI



Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

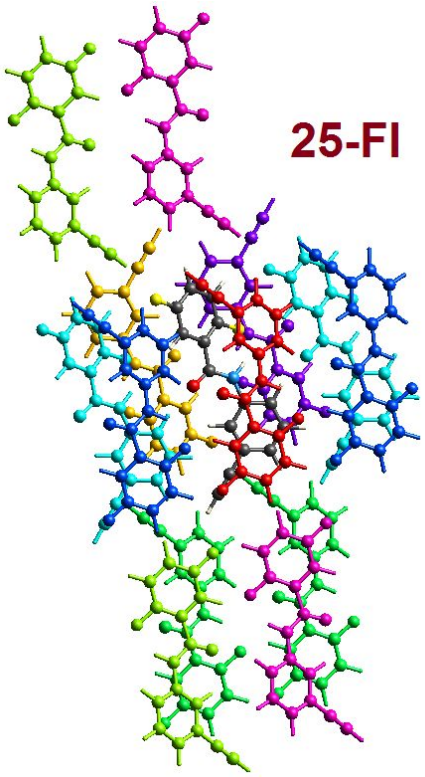
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	0	-	4.33	B3LYP/6-31G(d,p)	-40.4	-9.8	-57.1	65.4	-59.4
	0	-	12.91	B3LYP/6-31G(d,p)	-1.7	-0.3	-5.4	1.8	-5.6
	0	-	4.28	B3LYP/6-31G(d,p)	-8.2	-1.9	-64.5	40.3	-41.4
	0	-x, y+1/2, -z	13.82	B3LYP/6-31G(d,p)	-1.7	-0.5	-5.3	4.2	-4.2
	1	x, y, z	6.79	B3LYP/6-31G(d,p)	-7.2	-2.6	-23.9	17.8	-19.3
	1	-x, y+1/2, -z	12.61	B3LYP/6-31G(d,p)	-5.9	-0.7	-9.5	11.5	-7.9
	0	-	13.10	B3LYP/6-31G(d,p)	-0.8	-0.2	-3.5	0.3	-3.8
	1	-	5.69	B3LYP/6-31G(d,p)	-30.8	-7.6	-33.4	38.1	-43.7
	0	-	5.36	B3LYP/6-31G(d,p)	0.1	-1.2	-38.9	17.2	-24.1
	0	-	13.07	B3LYP/6-31G(d,p)	-2.8	-0.4	-6.5	3.8	-6.6
	0	x, y, z	6.79	B3LYP/6-31G(d,p)	-4.4	-2.0	-23.5	17.9	-15.5
	0	-x, y+1/2, -z	12.59	B3LYP/6-31G(d,p)	-4.7	-0.6	-9.1	7.5	-8.7
	0	-x, y+1/2, -z	13.96	B3LYP/6-31G(d,p)	-1.6	-0.2	-3.3	2.3	-3.3

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

24-FII



25-FI

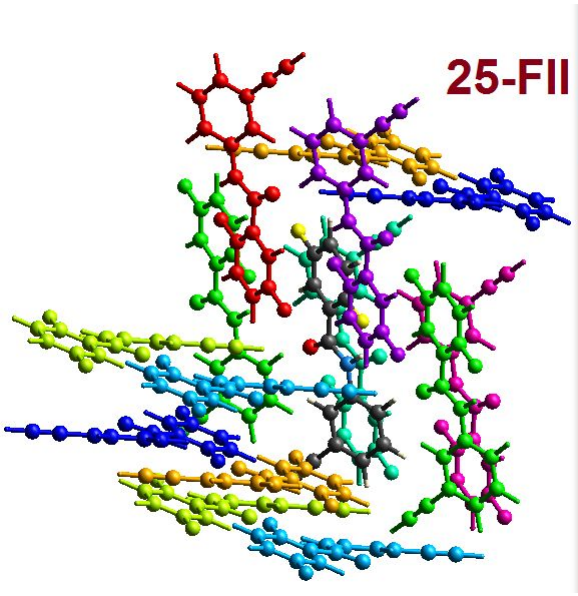
Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, y, -z+1/2	3.51	B3LYP/6-31G(d,p)	-6.1	-3.5	-80.5	44.3	-51.8
	1	-x, -y, -z	4.19	B3LYP/6-31G(d,p)	-13.7	-3.2	-59.1	35.6	-46.4
	2	x+1/2, -y+1/2, z+1/2	14.53	B3LYP/6-31G(d,p)	-2.6	-0.4	-4.2	3.7	-4.4
	2	-x+1/2, y+1/2, -z+1/2	12.99	B3LYP/6-31G(d,p)	-2.5	-0.5	-7.8	4.1	-7.2
	2	x, y, z	6.63	B3LYP/6-31G(d,p)	-14.9	-2.5	-25.5	23.7	-25.1
	2	-x, y, -z+1/2	7.50	B3LYP/6-31G(d,p)	-3.5	-0.6	-12.8	7.6	-10.7
	1	-x, -y, -z	5.43	B3LYP/6-31G(d,p)	-8.4	-1.4	-39.9	21.7	-31.3
	2	x+1/2, -y+1/2, z+1/2	13.38	B3LYP/6-31G(d,p)	-1.8	-1.0	-8.8	5.6	-6.8

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618



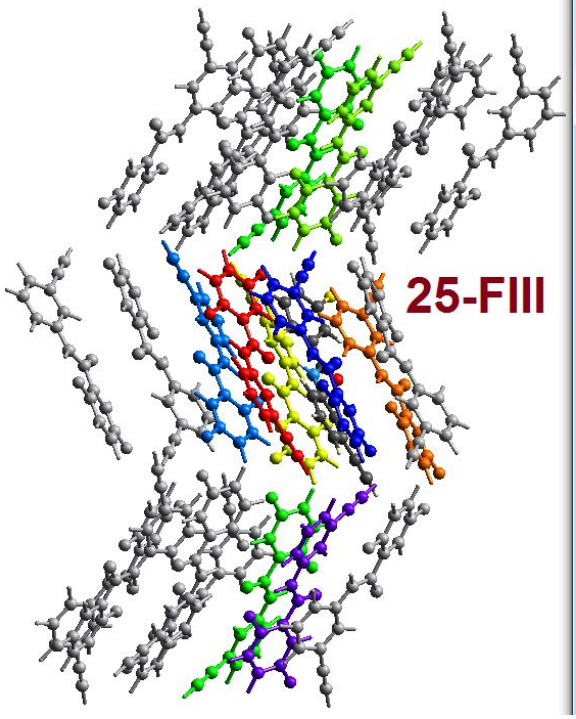
Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	8.49	B3LYP/6-31G(d,p)	-6.5	-0.6	-30.1	15.9	-23.7
	2	x+1/2, -y+1/2, z+1/2	9.02	B3LYP/6-31G(d,p)	0.0	-1.0	-14.3	8.7	-7.8
	2	-x+1/2, y+1/2, -z+1/2	9.58	B3LYP/6-31G(d,p)	-14.7	-2.8	-7.7	20.0	-11.9
	2	x, y, z	6.77	B3LYP/6-31G(d,p)	-12.8	-2.2	-23.4	18.8	-23.9
	1	-x, -y, -z	4.26	B3LYP/6-31G(d,p)	-8.4	-3.1	-55.6	29.5	-41.4
	2	-x+1/2, y+1/2, -z+1/2	8.29	B3LYP/6-31G(d,p)	-2.9	-1.1	-22.3	12.2	-15.7
	2	x+1/2, -y+1/2, z+1/2	8.61	B3LYP/6-31G(d,p)	-4.9	-1.1	-9.7	5.0	-11.3
	1	-x, -y, -z	9.37	B3LYP/6-31G(d,p)	-0.2	-0.4	-8.5	2.5	-6.3
	1	-x, -y, -z	5.82	B3LYP/6-31G(d,p)	-8.5	-1.8	-42.1	24.5	-31.9

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618



Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	x, y, z	6.62	B3LYP/6-31G(d,p)	-16.0	-2.6	-26.2	26.4	-25.4
	1	-	4.21	B3LYP/6-31G(d,p)	-7.9	-3.5	-74.8	46.6	-47.2
	0	-x, -y, z+1/2	13.03	B3LYP/6-31G(d,p)	0.3	-0.2	-3.3	1.0	-2.2
	1	-	4.01	B3LYP/6-31G(d,p)	-15.4	-3.2	-64.3	39.5	-50.3
	1	-	11.57	B3LYP/6-31G(d,p)	2.2	-0.5	-5.8	1.3	-2.4
	2	-x, -y, z+1/2	11.71	B3LYP/6-31G(d,p)	-4.3	-1.2	-10.5	6.0	-10.8
	0	-	12.84	B3LYP/6-31G(d,p)	-3.1	-0.6	-8.3	6.2	-7.1
	0	-	8.16	B3LYP/6-31G(d,p)	-1.4	-0.5	-6.9	1.5	-6.9
	0	-	11.78	B3LYP/6-31G(d,p)	-2.1	-0.6	-6.3	4.0	-5.6
	1	-	5.68	B3LYP/6-31G(d,p)	-6.5	-1.2	-34.3	16.7	-27.3
	1	-	7.52	B3LYP/6-31G(d,p)	-2.0	-0.8	-11.7	4.6	-9.9
	1	-	12.64	B3LYP/6-31G(d,p)	-4.1	-0.6	-8.7	8.9	-6.8
	0	x, y, z	6.62	B3LYP/6-31G(d,p)	-16.5	-2.7	-27.1	28.4	-25.4
	0	-x+1/2, y+1/2, z+1/2	12.26	B3LYP/6-31G(d,p)	1.9	-0.3	-6.5	2.3	-2.4
	0	-x+1/2, y+1/2, z+1/2	12.26	B3LYP/6-31G(d,p)	-2.3	-0.4	-6.9	5.8	-5.1

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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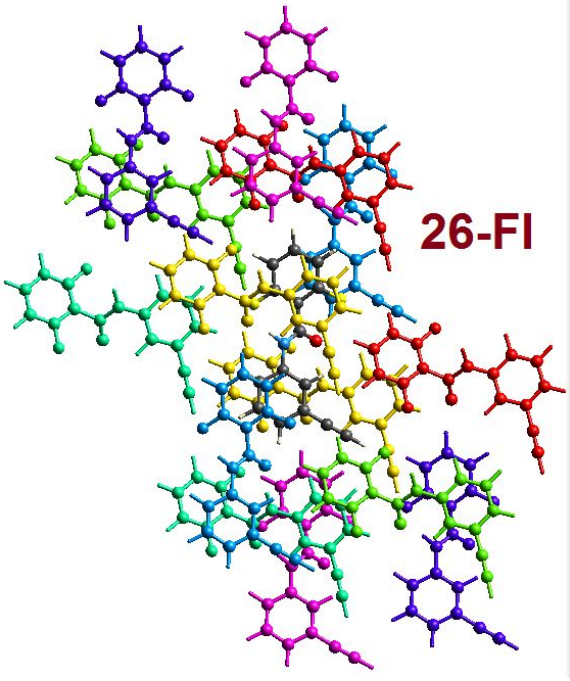

Interaction Energies (kJ/mol)
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	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x+1/2, -y+1/2, z+1/2	8.93	B3LYP/6-31G(d,p)	-9.2	-2.6	-22.7	19.4	-19.4
	2	x, -y, z+1/2	4.27	B3LYP/6-31G(d,p)	-43.2	-11.2	-57.8	71.3	-60.3
	2	x, -y, z+1/2	11.58	B3LYP/6-31G(d,p)	-2.1	-0.4	-6.7	2.4	-6.8
	2	x+1/2, -y+1/2, z+1/2	9.90	B3LYP/6-31G(d,p)	-0.7	-0.9	-14.5	8.3	-8.9
	2	x+1/2, y+1/2, z	8.43	B3LYP/6-31G(d,p)	-2.6	-2.5	-29.9	20.4	-18.0
	2	x, y, z	13.64	B3LYP/6-31G(d,p)	1.7	-0.4	-2.6	1.1	-0.1
	2	x+1/2, y+1/2, z	11.88	B3LYP/6-31G(d,p)	-3.1	-0.7	-9.4	3.8	-9.7

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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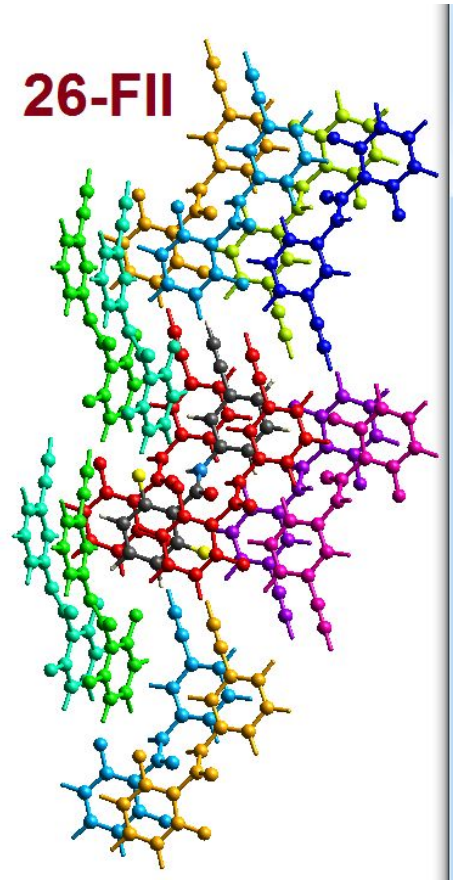

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	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	4.76	B3LYP/6-31G(d,p)	-39.6	-11.4	-43.6	57.9	-52.5
	2	x, y, z	13.22	B3LYP/6-31G(d,p)	-2.4	-0.7	-5.3	4.1	-5.1
	1	-x, -y, -z	14.09	B3LYP/6-31G(d,p)	0.3	-0.2	-3.9	0.6	-2.8
	2	x+1/2, -y+1/2, z+1/2	8.18	B3LYP/6-31G(d,p)	-0.9	-0.9	-17.5	11.8	-9.5
	2	x+1/2, -y+1/2, z+1/2	8.33	B3LYP/6-31G(d,p)	-5.0	-1.6	-20.7	12.8	-16.6
	2	x, y, z	12.54	B3LYP/6-31G(d,p)	-2.0	-0.4	-6.0	3.7	-5.3
	1	-x, -y, -z	13.52	B3LYP/6-31G(d,p)	-1.7	-0.3	-8.3	5.1	-6.1
	1	-x, -y, -z	5.41	B3LYP/6-31G(d,p)	0.7	-1.3	-42.9	20.7	-24.8
	1	-x, -y, -z	7.33	B3LYP/6-31G(d,p)	-11.2	-3.4	-19.8	16.9	-21.2

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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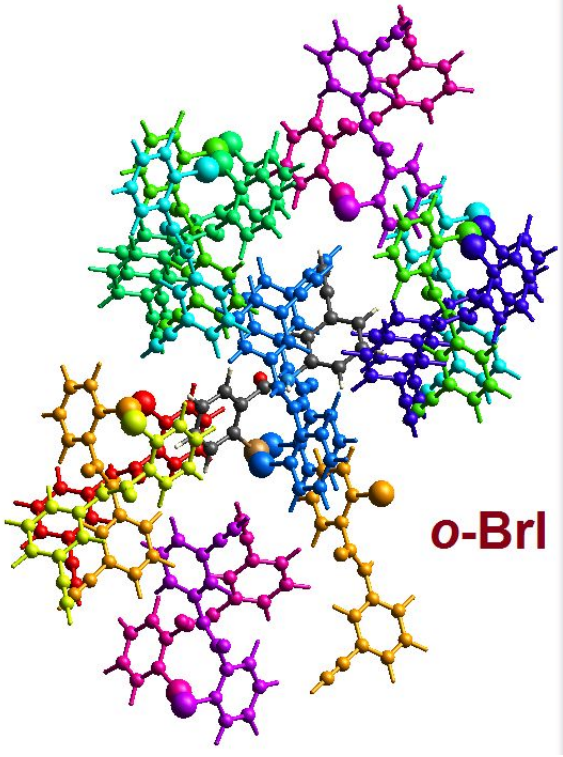

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	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	7.60	B3LYP/DGDZVP	-28.0	-4.7	-36.6	46.5	-36.1
	2	x+1/2, -y+1/2, -z	8.93	B3LYP/DGDZVP	-5.3	-1.4	-13.3	12.8	-10.3
	1	-x, -y, -z	11.30	B3LYP/DGDZVP	-3.6	-0.5	-11.3	12.1	-6.6
	2	x+1/2, y, -z+1/2	8.94	B3LYP/DGDZVP	-5.7	-2.2	-20.1	16.8	-14.7
	2	-x, y+1/2, -z+1/2	9.63	B3LYP/DGDZVP	-2.8	-0.5	-5.4	2.9	-6.2
	2	x+1/2, y, -z+1/2	12.64	B3LYP/DGDZVP	-0.0	-0.1	-1.2	0.0	-1.1
	2	-x+1/2, y+1/2, z	4.51	B3LYP/DGDZVP	-55.1	-11.5	-51.7	80.8	-61.9
	2	-x, y+1/2, -z+1/2	10.38	B3LYP/DGDZVP	-4.6	-1.1	-16.5	15.8	-10.4
	2	-x+1/2, -y, z+1/2	11.92	B3LYP/DGDZVP	-2.1	-0.5	-7.5	4.9	-6.1
	2	x, -y+1/2, z+1/2	12.92	B3LYP/DGDZVP	-5.2	-0.4	-4.9	10.5	-3.6

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
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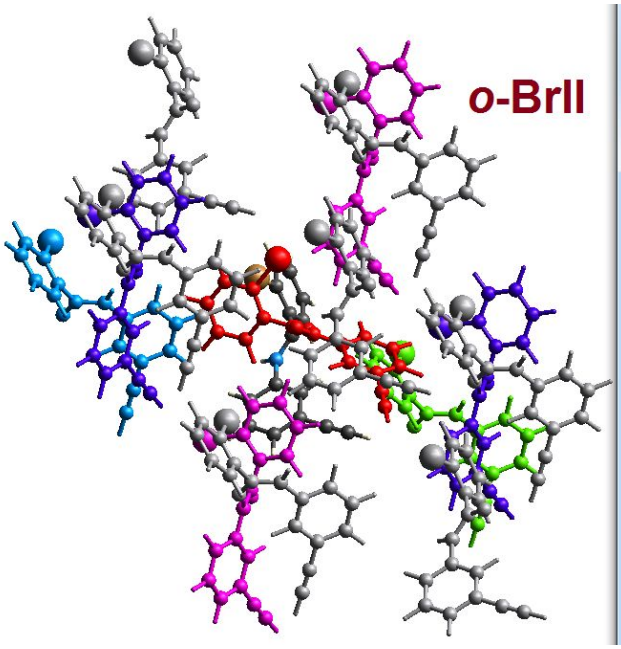

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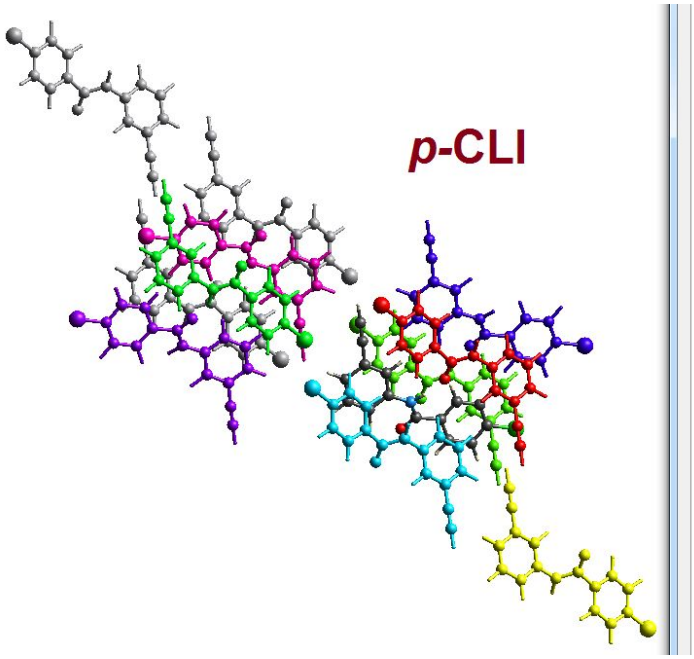
	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	x+1/2, -y+1/2, z	4.44	B3LYP/DGDZVP	-59.5	-12.2	-55.5	89.2	-65.1
	0	-x+1/2, y+1/2, z+1/2	10.69	B3LYP/DGDZVP	-3.1	-0.8	-11.9	12.7	-6.4
	1	-x, -y, z+1/2	8.46	B3LYP/DGDZVP	-13.4	-2.4	-21.5	18.6	-23.2
	0	x+1/2, -y+1/2, z	12.30	B3LYP/DGDZVP	-8.8	-0.9	-10.9	17.9	-8.3
	1	-x, -y, z+1/2	9.19	B3LYP/DGDZVP	-2.2	-0.8	-8.5	3.7	-8.2
	2	-x+1/2, y+1/2, z+1/2	8.96	B3LYP/DGDZVP	1.0	-0.2	-2.6	0.1	-1.3
	2	-x+1/2, y+1/2, z+1/2	8.96	B3LYP/DGDZVP	-16.6	-3.5	-25.3	27.2	-25.3

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

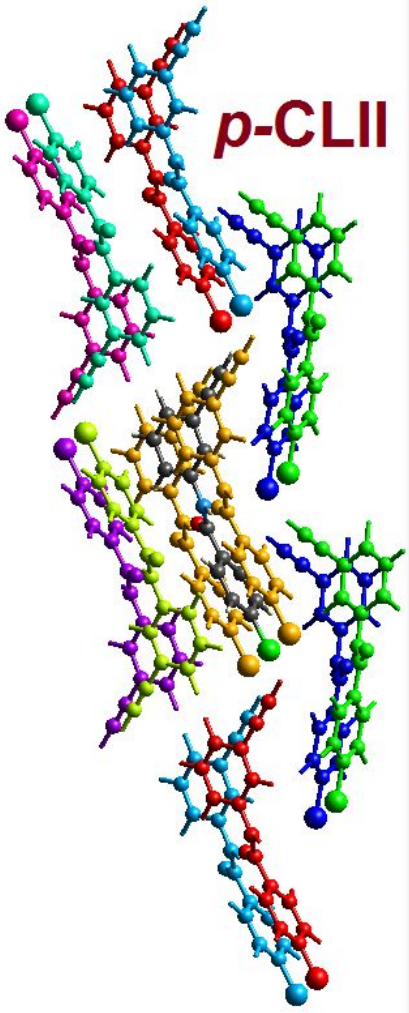


Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	4.64	B3LYP/6-31G(d,p)	-40.8	-10.9	-51.2	56.7	-60.7
	0	x, y, z	6.34	B3LYP/6-31G(d,p)	-8.4	-3.7	-27.1	22.8	-21.2
	0	-x, -y, -z	14.93	B3LYP/6-31G(d,p)	-5.1	-0.5	-5.1	5.5	-6.9
	1	-	13.27	B3LYP/6-31G(d,p)	-2.6	-0.5	-7.6	6.8	-5.5
	0	-x, -y, -z	14.35	B3LYP/6-31G(d,p)	-2.3	-0.4	-9.3	6.8	-6.6
	1	-	4.17	B3LYP/6-31G(d,p)	-6.1	-2.1	-54.4	32.7	-35.3
	1	-	14.71	B3LYP/6-31G(d,p)	0.2	-0.1	-5.9	4.3	-2.4
	0	-	5.53	B3LYP/6-31G(d,p)	-36.1	-8.1	-35.4	43.0	-48.4
	0	-x, -y, -z	13.05	B3LYP/6-31G(d,p)	-1.3	-0.2	-5.7	3.0	-4.6
	1	-	5.35	B3LYP/6-31G(d,p)	-1.2	-2.7	-42.3	19.8	-27.9
	0	-	13.86	B3LYP/6-31G(d,p)	-0.7	-0.1	-5.8	3.2	-3.9
	0	-	14.72	B3LYP/6-31G(d,p)	-2.4	-0.4	-4.0	4.2	-3.7
	1	x, y, z	6.34	B3LYP/6-31G(d,p)	-3.5	-1.9	-25.7	13.6	-19.0
	1	-x, -y, -z	15.50	B3LYP/6-31G(d,p)	0.0	-0.0	-1.1	0.0	-1.0
	0	-x, -y, -z	13.61	B3LYP/6-31G(d,p)	-0.8	-0.1	-2.1	0.1	-2.7
	1	-x, -y, -z	13.69	B3LYP/6-31G(d,p)	-1.3	-0.5	-10.7	6.2	-7.2
	0	-x, -y, -z	15.11	B3LYP/6-31G(d,p)	-0.9	-0.0	-3.0	2.9	-1.8

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)



Crystal | Atoms | Surface | Energies

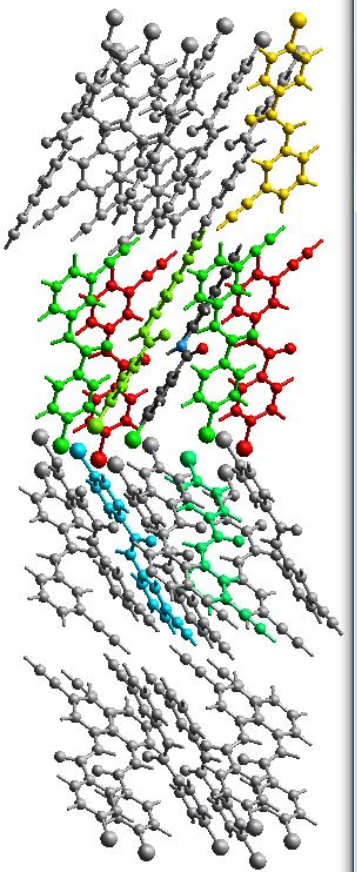
Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	14.19	B3LYP/6-31G(d,p)	-0.7	-0.2	-5.4	5.2	-2.4
	2	x, y, z	5.17	B3LYP/6-31G(d,p)	-37.0	-9.2	-44.1	51.0	-52.9
	1	-x, -y, -z	4.93	B3LYP/6-31G(d,p)	-8.5	-3.7	-41.6	32.2	-28.1
	2	-x, y+1/2, -z+1/2	8.88	B3LYP/6-31G(d,p)	-4.6	-0.7	-17.6	10.4	-14.3
	1	-x, -y, -z	13.51	B3LYP/6-31G(d,p)	-3.1	-0.5	-14.3	9.4	-10.3
	2	x, y, z	15.10	B3LYP/6-31G(d,p)	-3.5	-0.4	-3.9	5.7	-3.8
	2	-x, y+1/2, -z+1/2	8.49	B3LYP/6-31G(d,p)	-4.3	-1.3	-22.8	17.4	-14.6
	1	-x, -y, -z	5.11	B3LYP/6-31G(d,p)	-18.4	-2.1	-48.4	35.7	-41.1
	1	-x, -y, -z	13.57	B3LYP/6-31G(d,p)	-0.3	-0.2	-5.9	1.7	-4.5

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618



Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

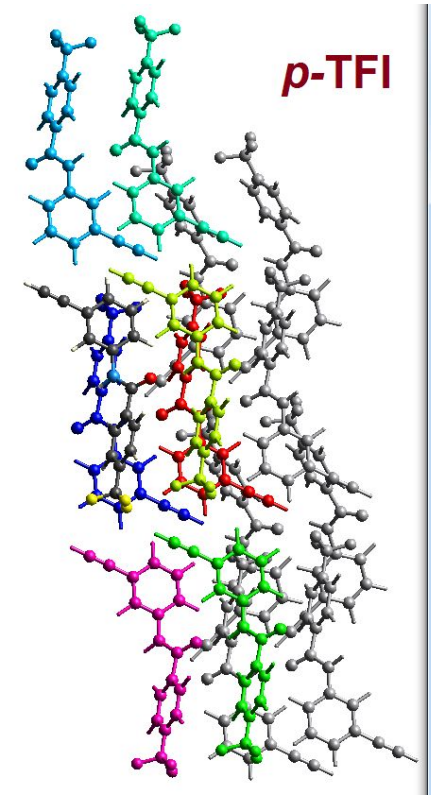
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	x+1/2, -y, z	4.61	B3LYP/6-31G(d,p)	-43.1	-11.1	-42.2	60.6	-53.0
0	x+1/2, -y, z	4.60	B3LYP/6-31G(d,p)	-43.1	-11.2	-42.7	60.4	-53.7
1	-	15.17	B3LYP/6-31G(d,p)	-4.5	-0.6	-5.6	6.0	-6.3
0	-	13.52	B3LYP/6-31G(d,p)	-0.7	-0.1	-5.2	5.3	-2.1
1	x, y, z	5.77	B3LYP/6-31G(d,p)	-3.1	-1.8	-34.9	20.2	-22.5
2	x+1/2, -y, z	6.50	B3LYP/6-31G(d,p)	-1.7	-1.2	-21.1	14.5	-12.1
1	-	11.32	B3LYP/6-31G(d,p)	-4.5	-0.4	-12.0	13.3	-7.3
0	-	13.82	B3LYP/6-31G(d,p)	-1.6	-0.5	-11.2	7.7	-7.1
1	-	11.52	B3LYP/6-31G(d,p)	-0.8	-0.1	-9.1	8.2	-3.8
0	-	11.53	B3LYP/6-31G(d,p)	-4.1	-0.4	-8.4	9.9	-5.9
0	x+1/2, -y, z	8.17	B3LYP/6-31G(d,p)	-4.6	-0.9	-15.5	10.9	-12.3
0	-	15.18	B3LYP/6-31G(d,p)	-4.2	-0.6	-5.8	5.9	-6.3
0	x+1/2, -y, z	8.14	B3LYP/6-31G(d,p)	-5.5	-1.1	-16.0	13.5	-12.3
0	x, y, z	5.77	B3LYP/6-31G(d,p)	-2.5	-1.9	-34.2	19.5	-21.9
0	x+1/2, -y, z	6.53	B3LYP/6-31G(d,p)	-1.2	-1.1	-19.9	11.9	-12.2

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

p-CLIII

Energy Model	k_ele	k_pol	k_disp	k_rep



p-TFI

Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-x, -y, -z	5.40	B3LYP/6-31G(d,p)	-19.3	-2.3	-47.0	32.8	-42.7
0	-x+1/2, y+1/2, -z+1/2	8.48	B3LYP/6-31G(d,p)	-4.7	-1.2	-26.9	13.3	-21.1
1	x, y, z	5.15	B3LYP/6-31G(d,p)	-35.9	-9.3	-46.7	49.8	-54.7
1	x, y, z	15.28	B3LYP/6-31G(d,p)	-2.7	-0.4	-5.7	3.8	-5.7
1	-x, -y, -z	15.21	B3LYP/6-31G(d,p)	0.1	-0.2	-4.2	0.7	-3.2
1	-x, -y, -z	15.10	B3LYP/6-31G(d,p)	-1.8	-0.3	-10.4	4.0	-8.7
1	-x, -y, -z	5.08	B3LYP/6-31G(d,p)	-7.6	-4.4	-45.5	35.1	-29.2
0	-x+1/2, y+1/2, -z+1/2	9.15	B3LYP/6-31G(d,p)	-3.9	-0.5	-14.3	6.6	-12.9
1	x, y, z	14.38	B3LYP/6-31G(d,p)	0.5	-0.2	-6.4	2.1	-3.9

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
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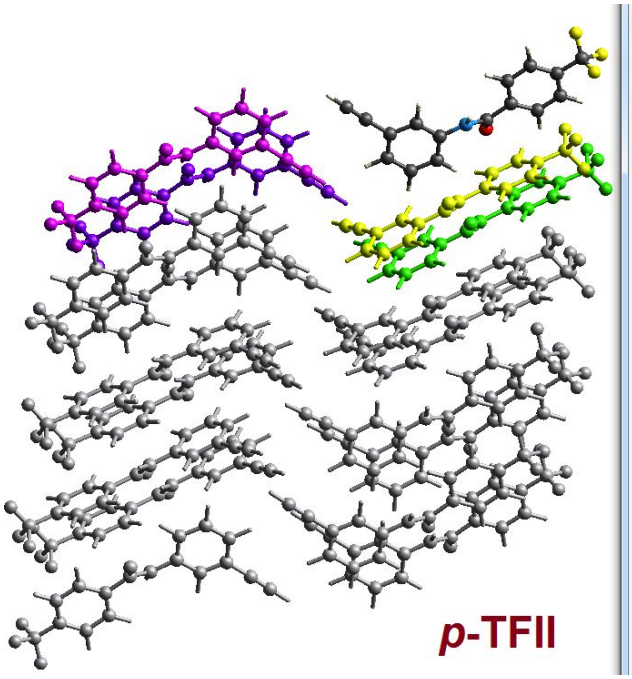

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Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	0	x, y, z	5.01	B3LYP/6-31G(d,p)	-42.4	-10.9	-48.2	60.4	-57.6
	0	x, y, z	5.01	B3LYP/6-31G(d,p)	-34.5	-8.9	-48.8	51.8	-53.6
	0	-	6.96	B3LYP/6-31G(d,p)	-5.6	-2.7	-22.9	16.2	-17.8
	1	-	5.31	B3LYP/6-31G(d,p)	-3.9	-2.8	-38.9	20.5	-27.5
	0	-	4.92	B3LYP/6-31G(d,p)	-5.6	-2.0	-60.1	31.6	-40.2
	1	-	5.66	B3LYP/6-31G(d,p)	-7.8	-2.0	-39.8	22.2	-30.6
	0	-	15.03	B3LYP/6-31G(d,p)	-4.7	-0.8	-5.7	6.3	-6.6
	0	-x, y+1/2, -z+1/2	16.34	B3LYP/6-31G(d,p)	-1.0	-0.4	-6.6	5.1	-3.9
	0	-	15.06	B3LYP/6-31G(d,p)	-4.0	-0.7	-5.8	7.5	-5.2
	0	-	13.99	B3LYP/6-31G(d,p)	0.8	-0.1	-6.0	1.2	-3.8
	0	-x, y+1/2, -z+1/2	11.98	B3LYP/6-31G(d,p)	-2.0	-0.3	-8.5	3.7	-7.4
	0	-	14.02	B3LYP/6-31G(d,p)	0.7	-0.1	-5.1	0.8	-3.3
	1	-x, -y, -z	15.78	B3LYP/6-31G(d,p)	-1.0	-0.2	-5.5	1.1	-5.3
	1	-x, -y, -z	16.41	B3LYP/6-31G(d,p)	1.9	-0.3	-6.5	3.1	-2.0
	0	-x, -y, -z	12.10	B3LYP/6-31G(d,p)	-2.5	-0.3	-10.0	2.5	-10.1
	0	-x, -y, -z	12.92	B3LYP/6-31G(d,p)	0.2	-0.1	-2.5	0.2	-1.9

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep

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