Supporting Information

Supramolecular assemblies in the molecular complexes of 4-cyanophenylboronic acid with different N-donor ligands

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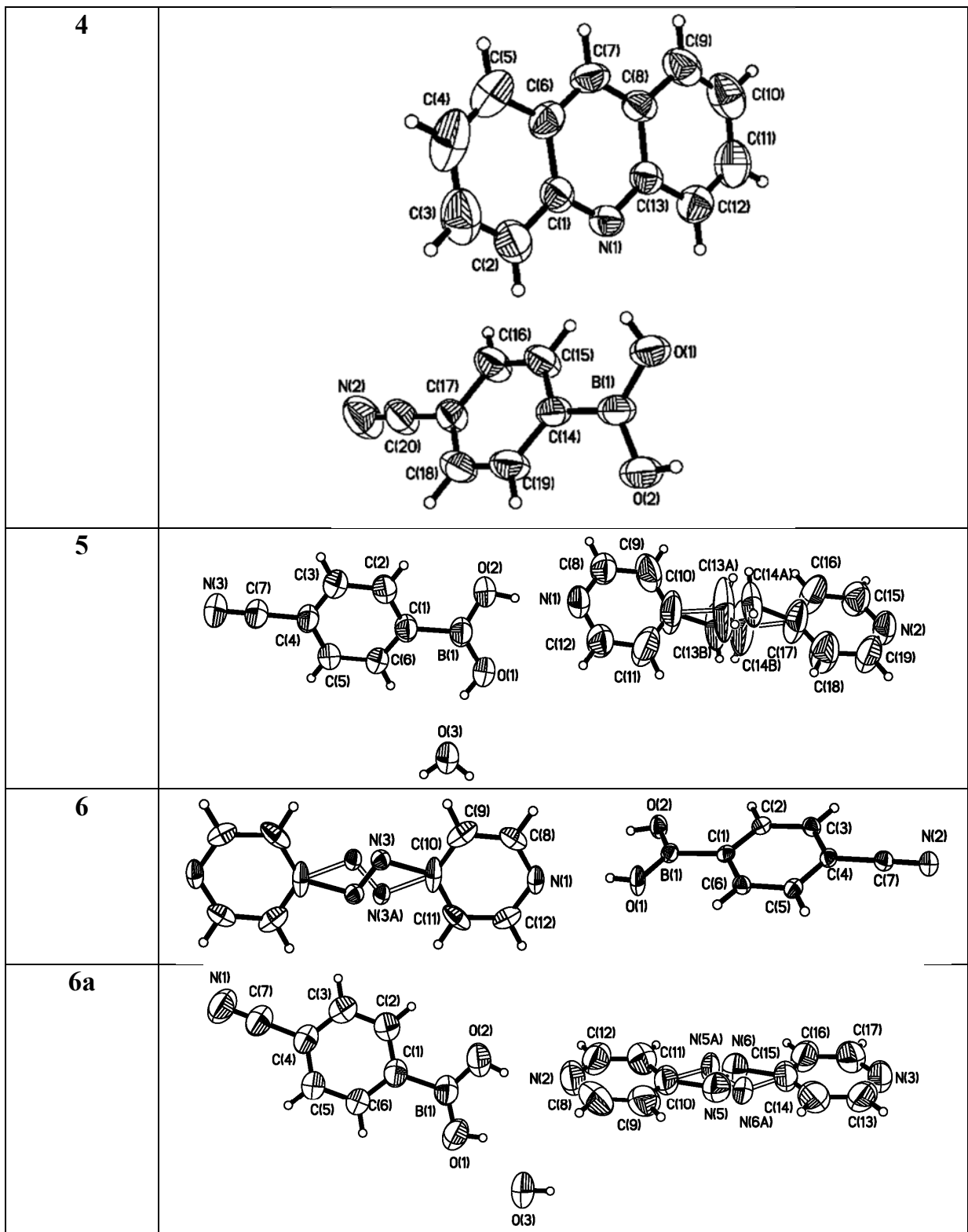**S4. Isostructurility and Isomorphism**
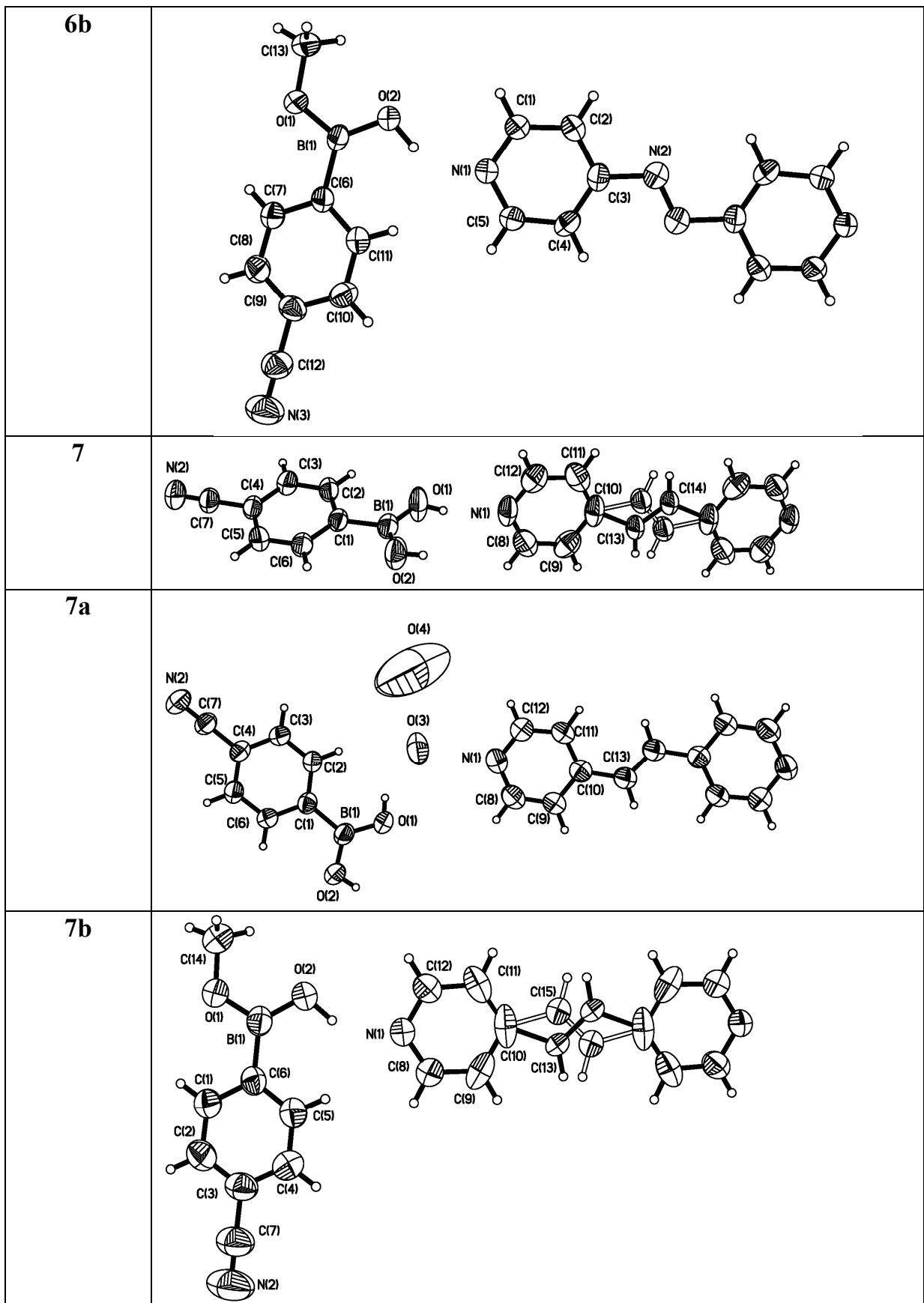
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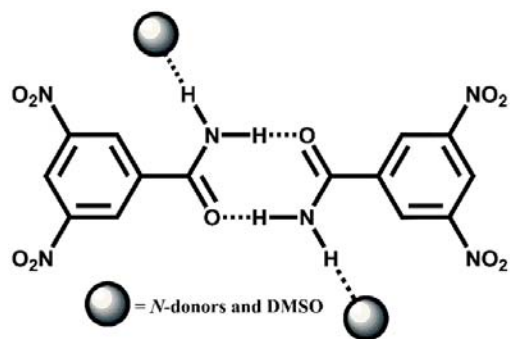
S7. Interaction Energy Calculation

Table S1. ORTEP Representation for all the Co-crystals, 1 – 7, 6a, 6b, 7a and 7b, with all Non-hydrogen Atoms Thermal Ellipsoids are Shown at the 50 % Probability Level

Co-crystals	ORTEP Represntation
1	
2	
3	

4	
5	
6	
6a	

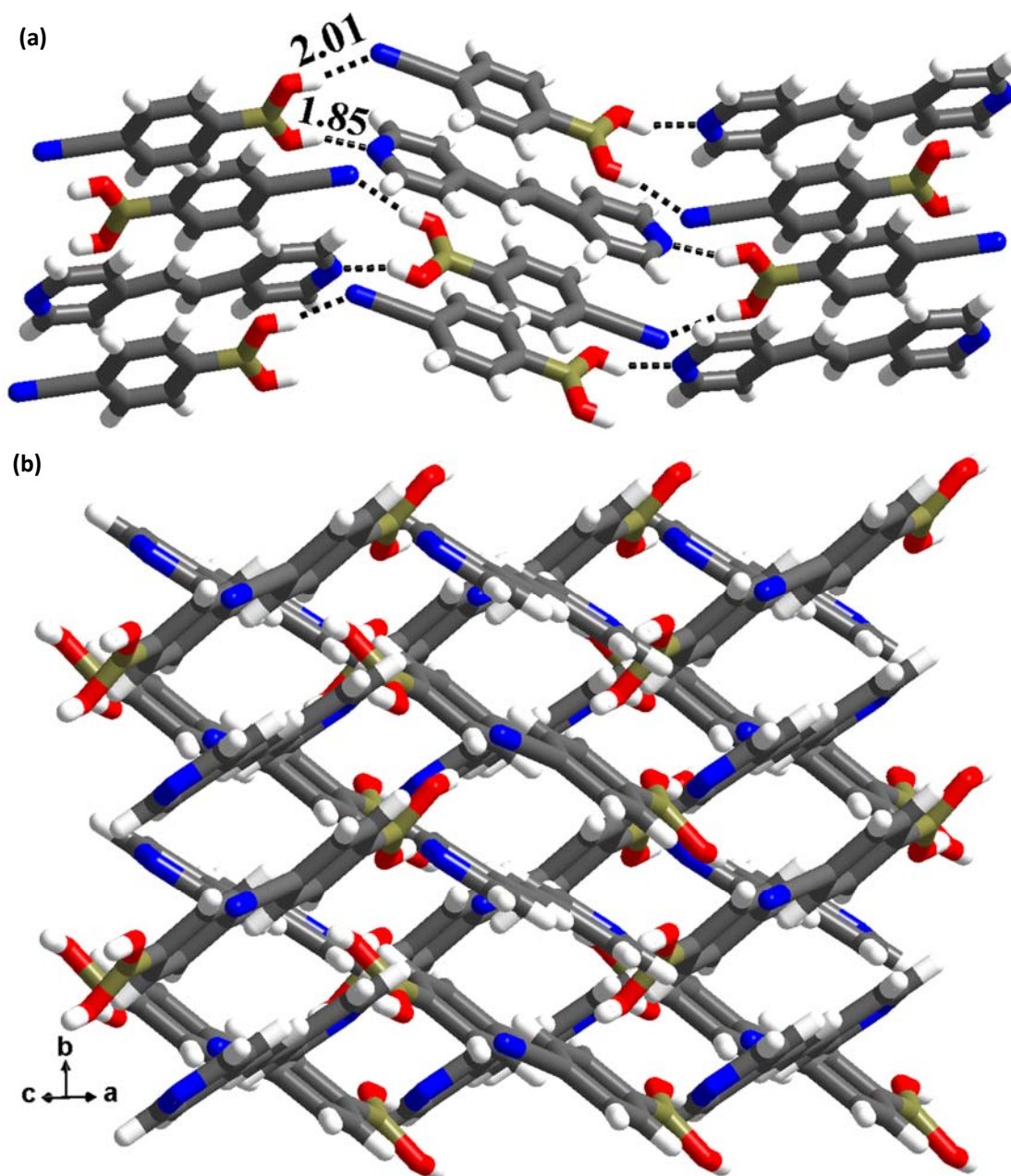|	
6b	
7	
7a	
7b	

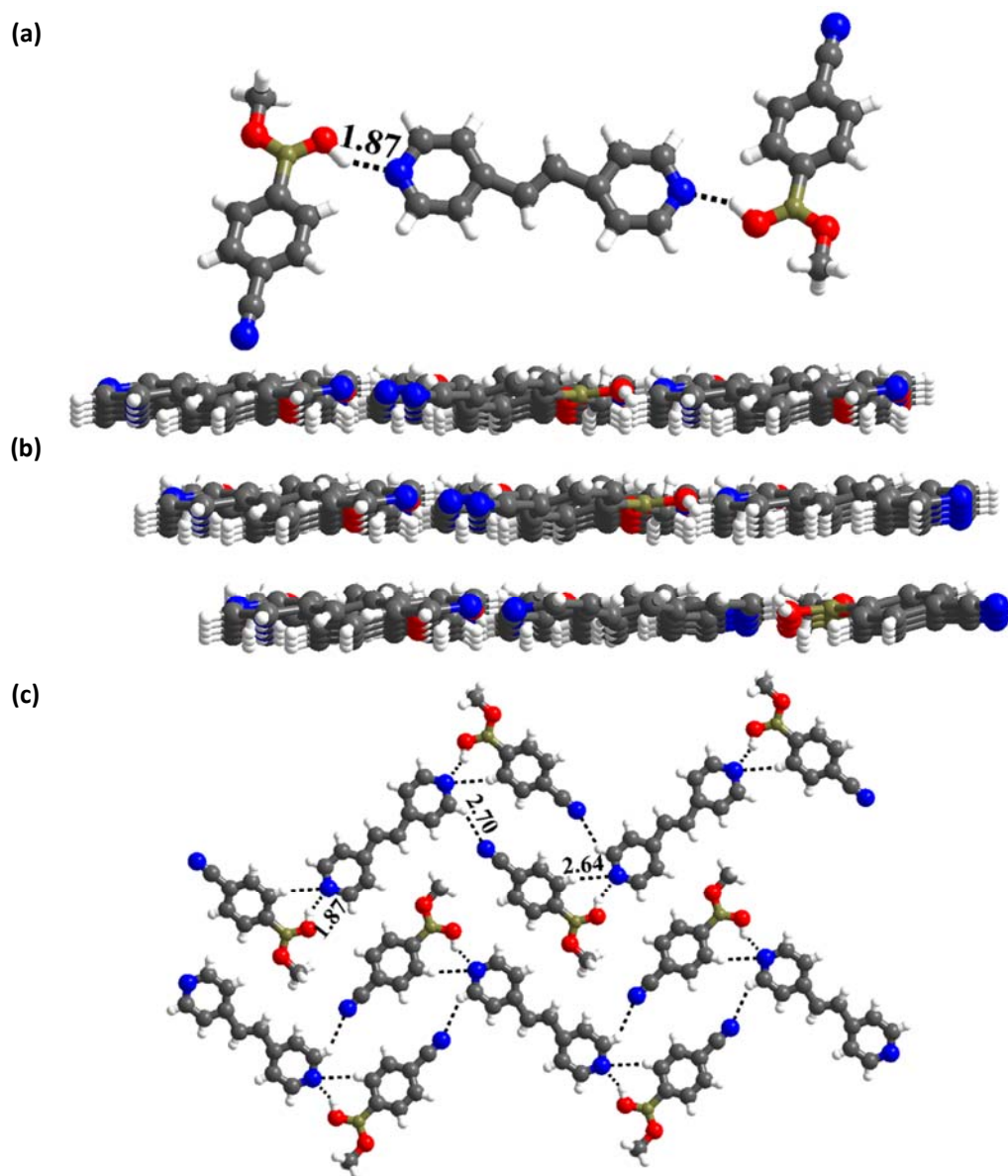**Scheme S1.** A schematic representation of recognition pattern of 3,5-dinitrobenzamide with some co-formers, yielding a tetramer. (J. PrakashaReddy, V. R. Pedireddi, *Tetrahedron* **2004**, *60*, 8817-8827)

S2. Packing Arrangements

(a)

2.01

1.85

(b)

b

c   a

Figure S1. (a) Proparagtion of chain arrangement in the molecular complex, **7**. (b) crossed ribbon arrangement present in the crystal lattice.

(a)

(b)

(c)

Figure S2. (a) Molecular recognition observed in the monoester with *bpyee*. (b) Stacked sheet arrangement found in the molecular complex **7b**. (c) Two-dimensional arrangement of the molecules in the crystal lattice, 7**b**.

S3. PXRD Patterns
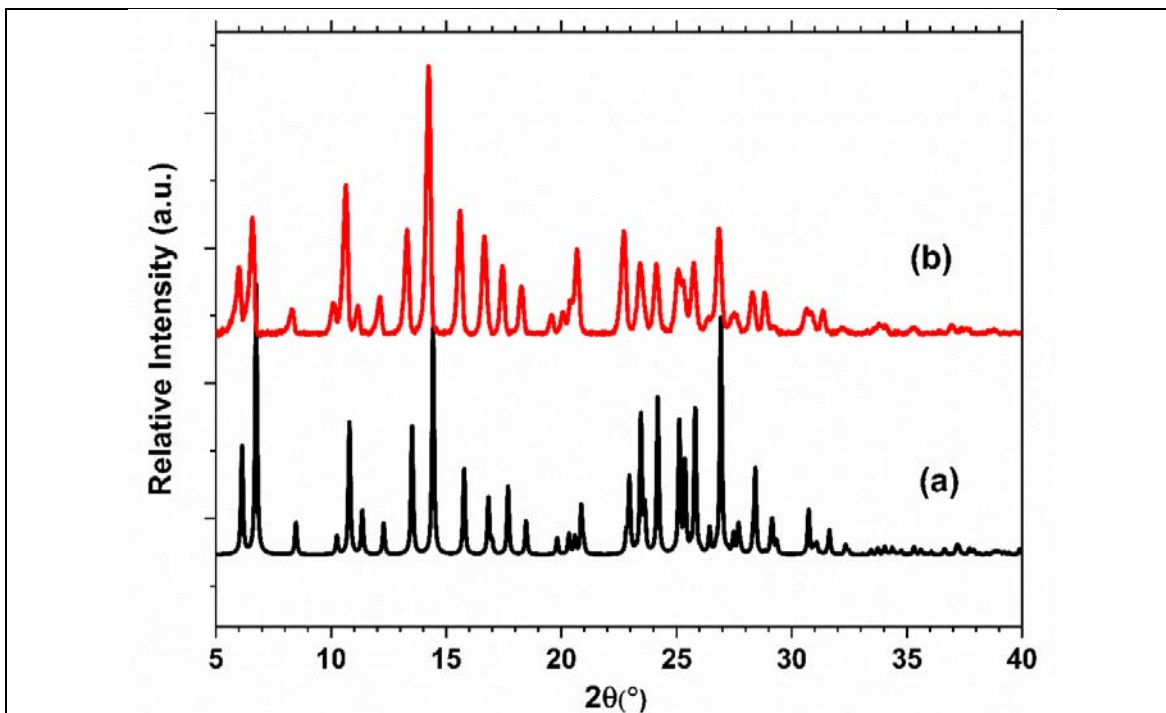
Figure S2a. Powder X-ray diffraction patterns of **1** (a) Simulated patterns. (b) Experimental ground co-crystals.
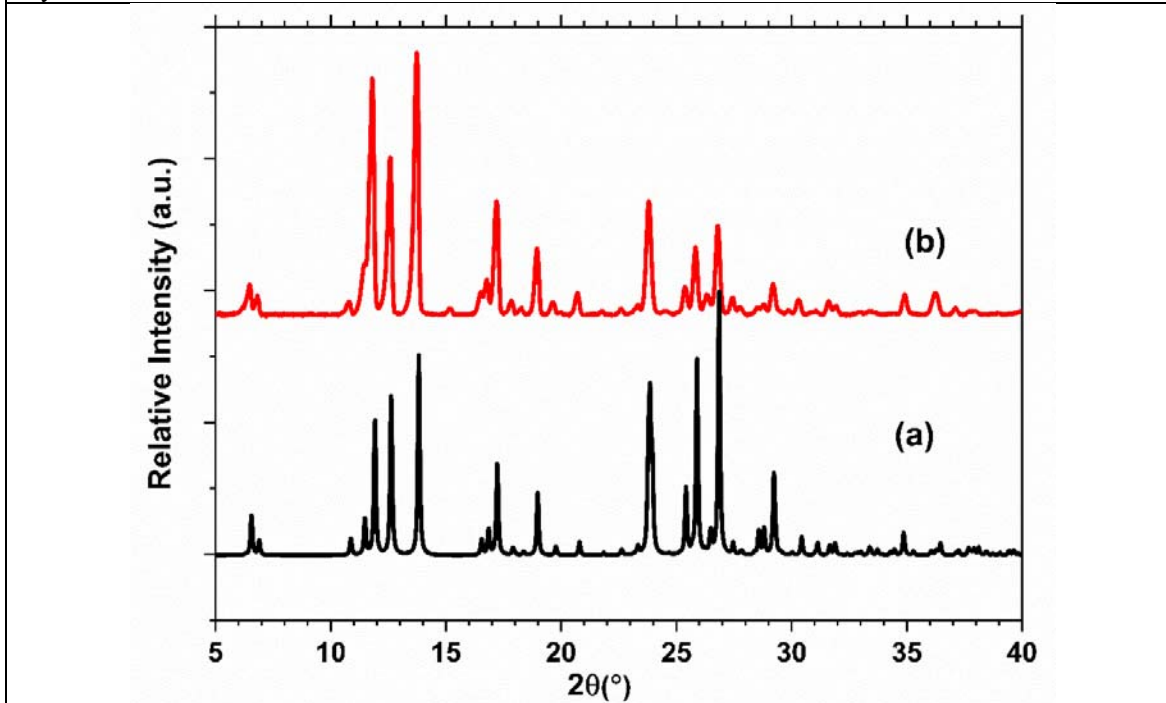
Figure S2b. Powder X-ray diffraction patterns of **2** (a) Simulated patterns (b) Experimental ground co-crystals.

Figure S2c. Powder X-ray diffraction patterns of **3** (a) Simulated patterns (b) Experimental ground co-crystals.

Figure S2d. Powder X-ray diffraction patterns of **4** (a) Simulated patterns (b) Experimental ground co-crystals.

Figure S2e. Powder X-ray diffraction patterns of **5** (a) Simulated patterns (b) Experimental ground co-crystals.

Figure S2f. Powder X-ray diffraction patterns of **6** (a) Simulated patterns (b) Experimental ground co-crystals.

Figure S2g. Powder X-ray diffraction patterns of **6a** (a) Simulated patterns (b) Experimental ground co-crystals.

Figure S2h. Powder X-ray diffraction patterns of **6b** (a) Simulated patterns (b) Experimental ground co-crystals.
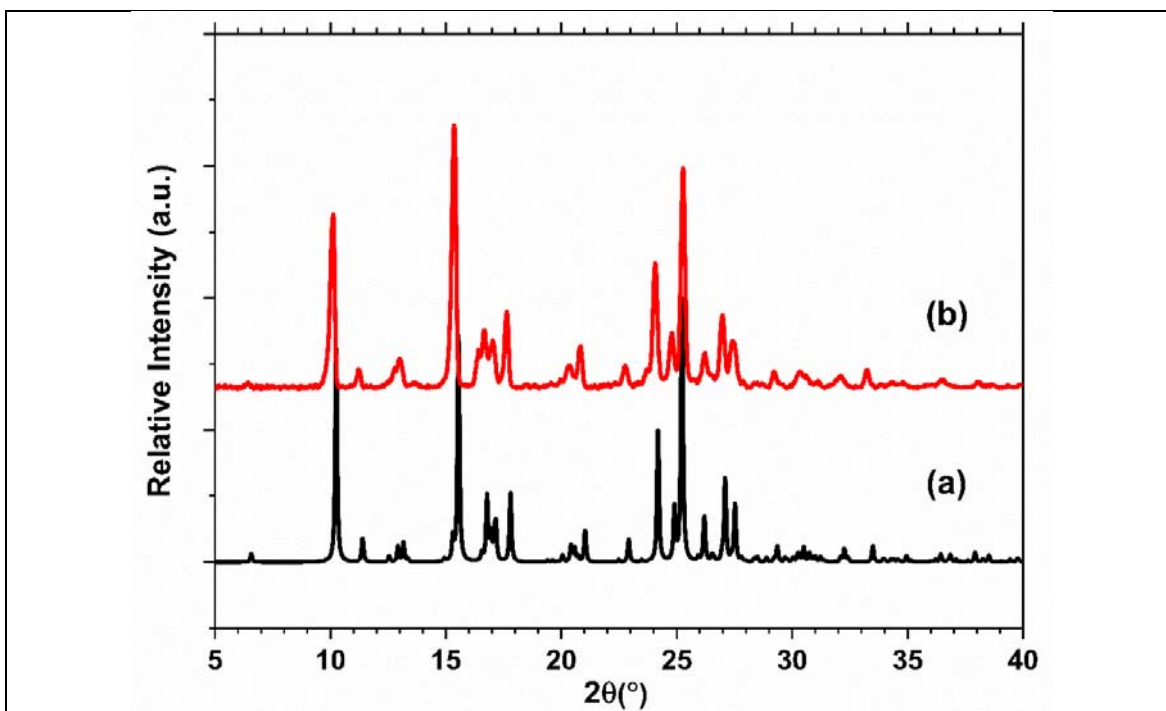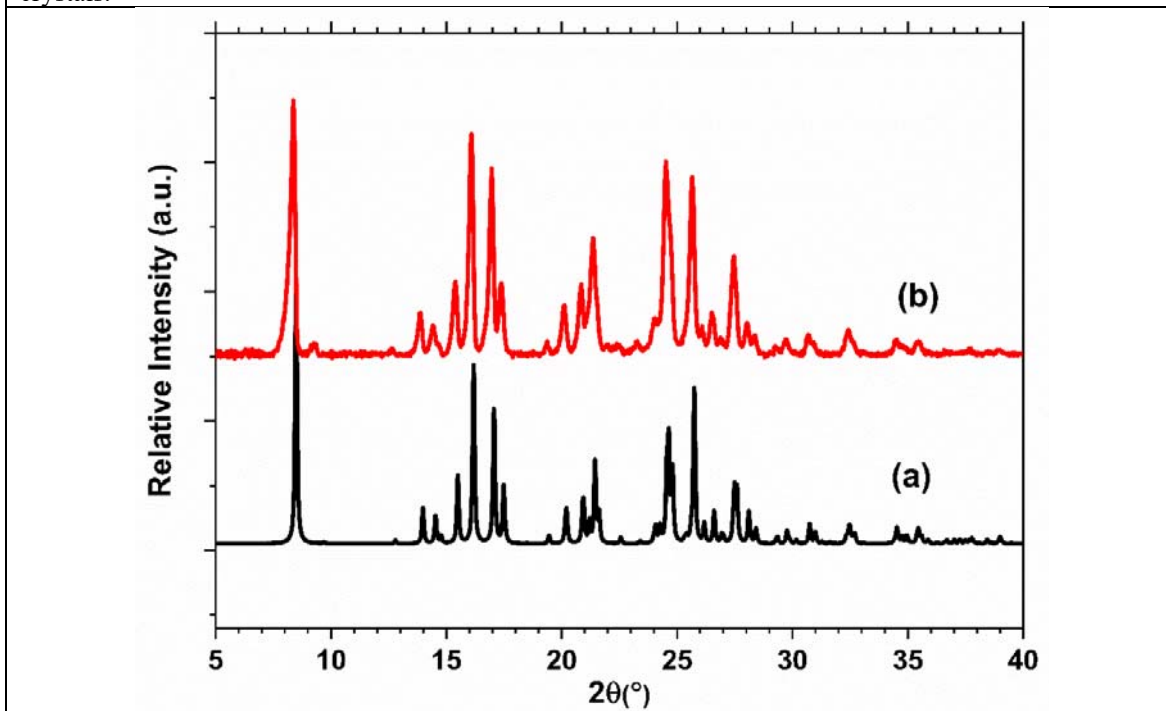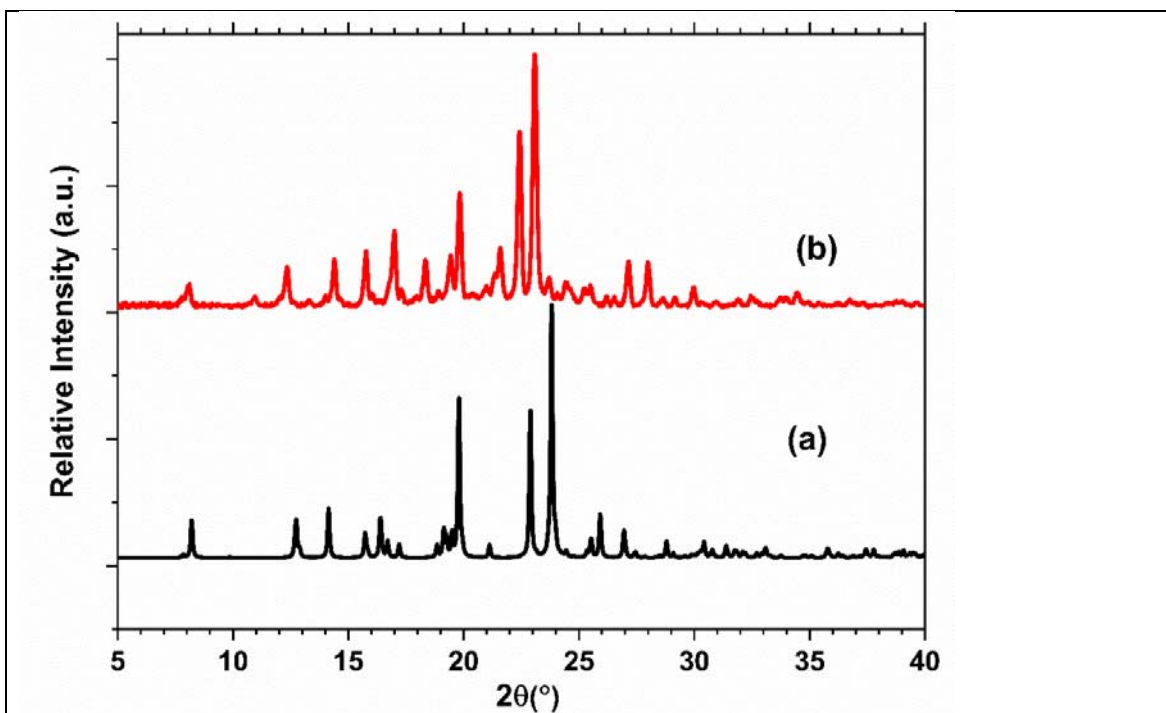
Figure S2i. Powder X-ray diffraction patterns of **7** (a) Simulated patterns (b) Experimental ground co-crystals.
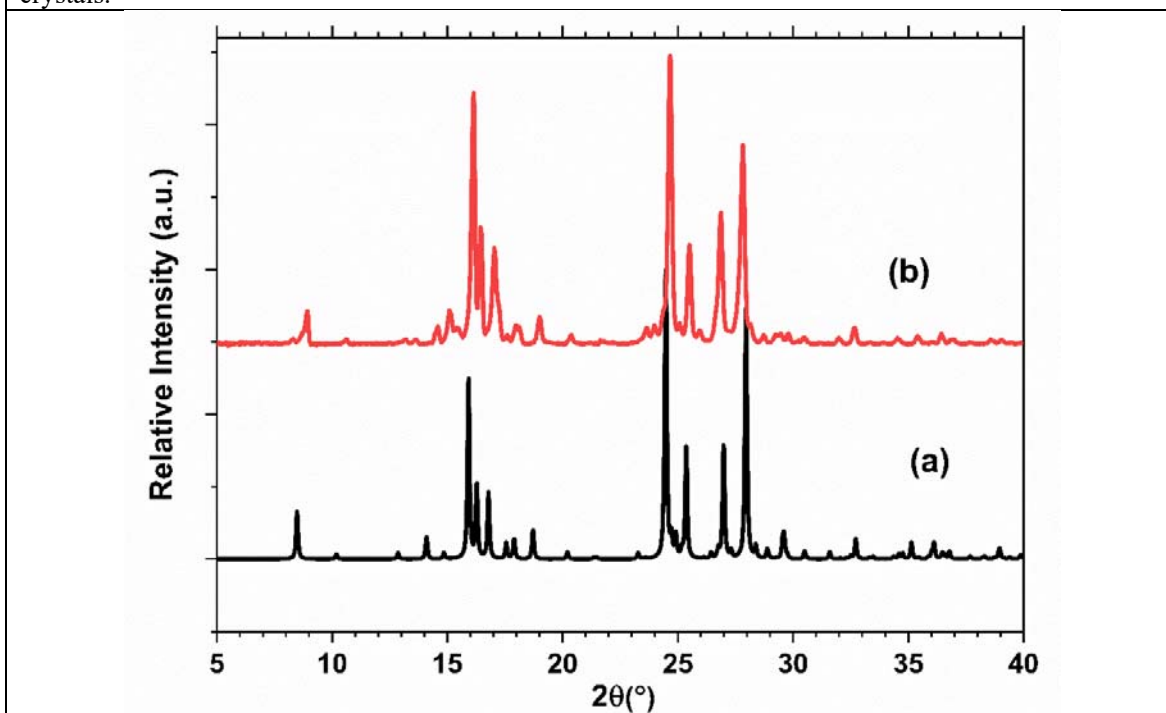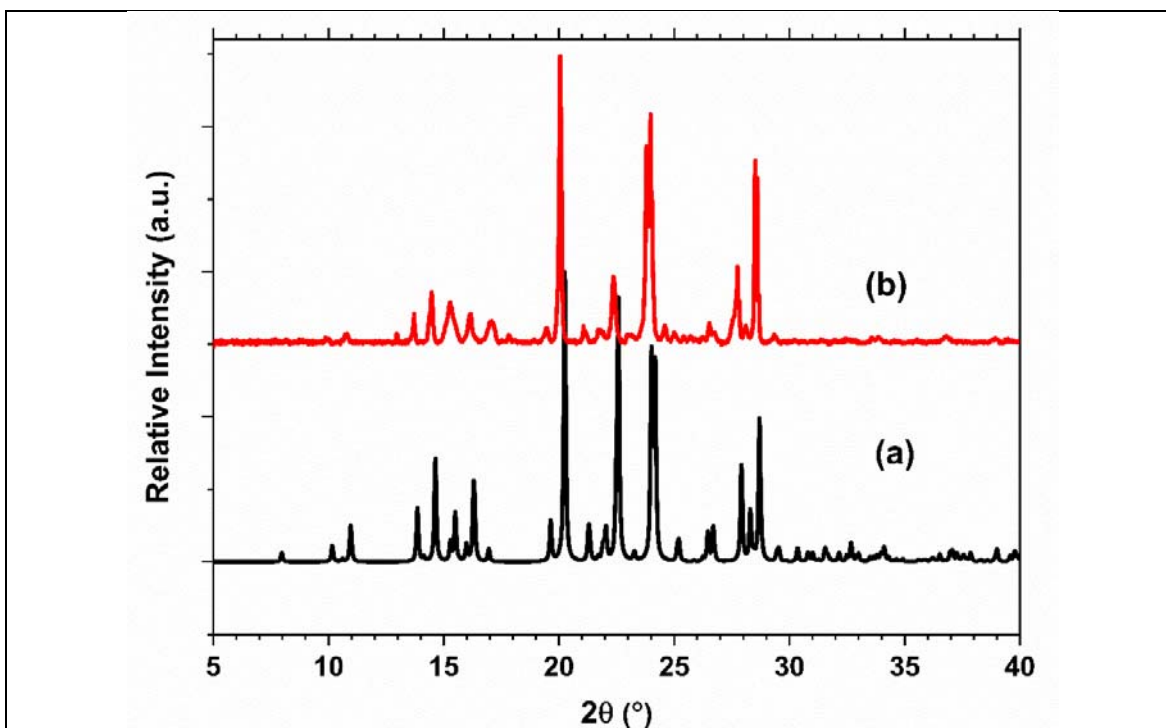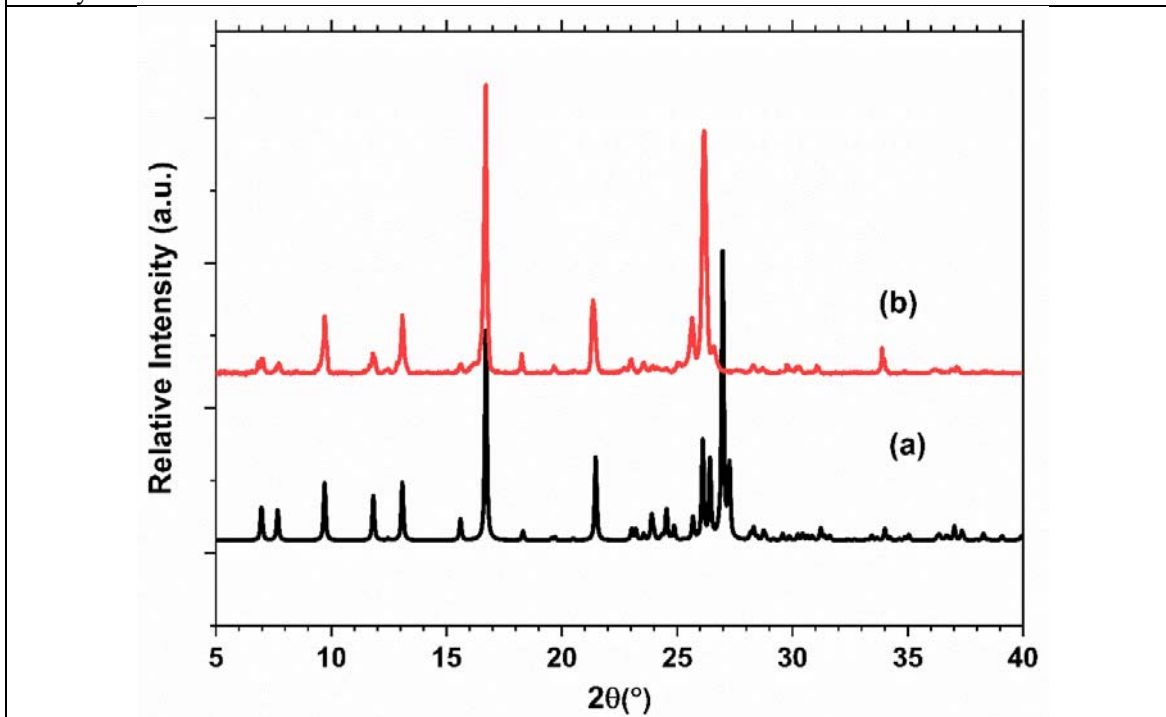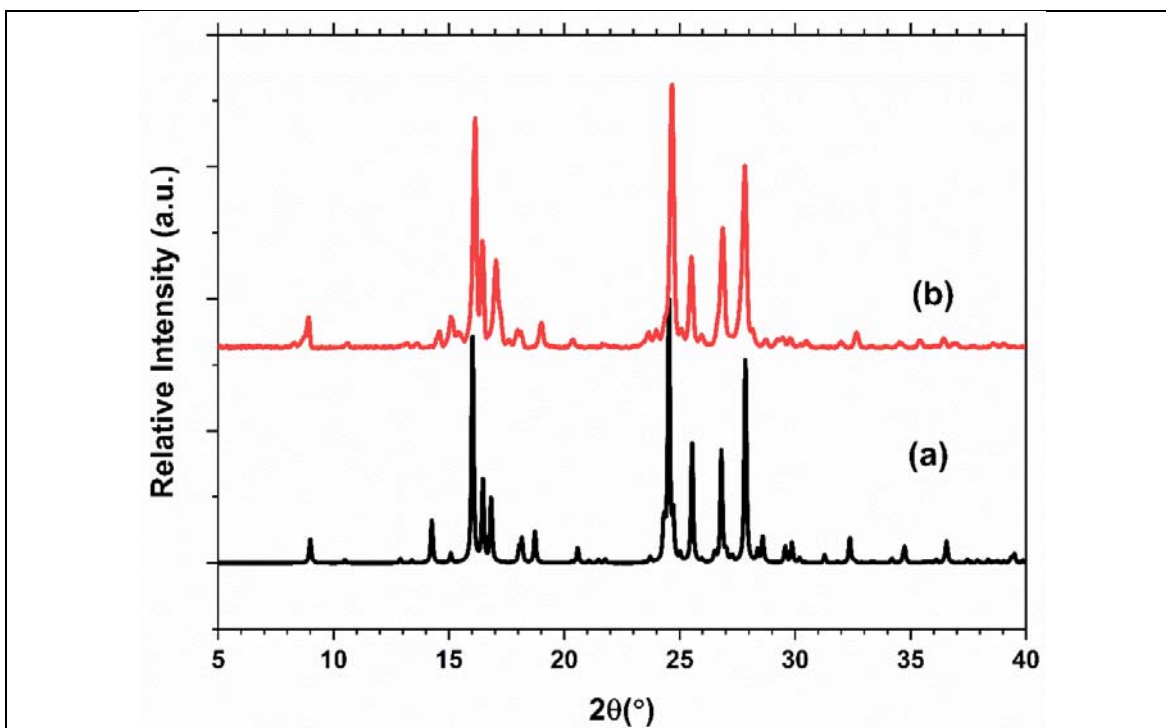

Figure S2h. Powder X-ray diffraction patterns of **7b** (a) Simulated patterns (b) Experimental ground co-crystals.
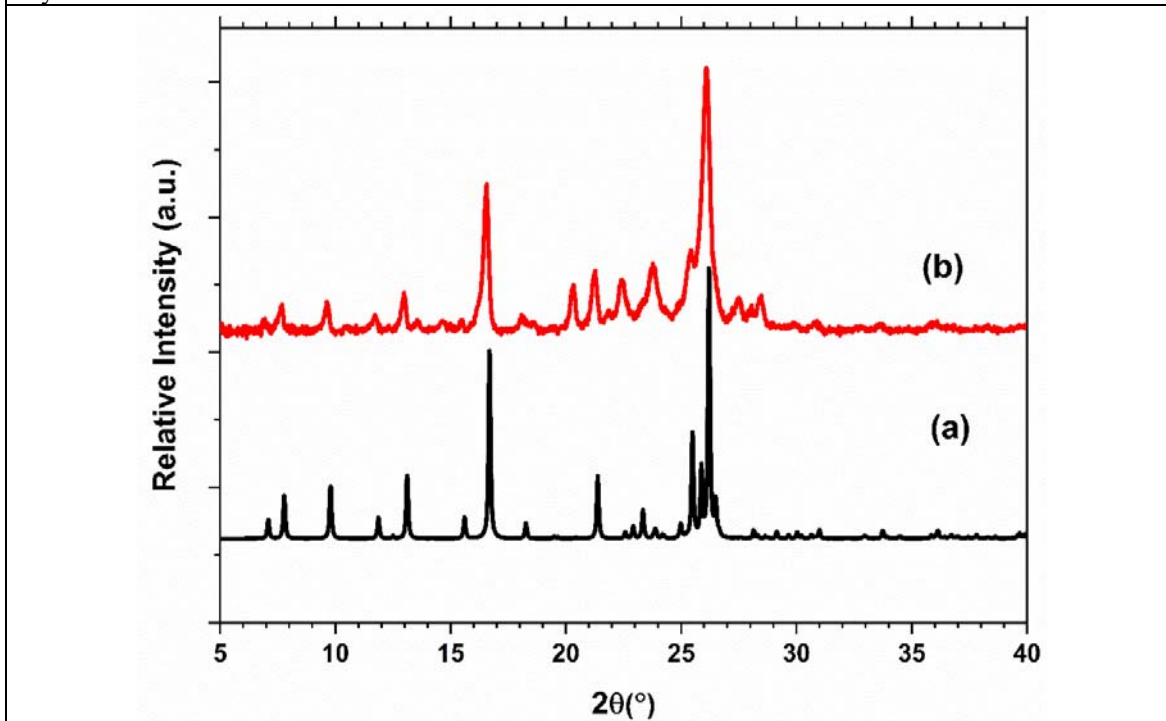
S4. Isostructurality

The iso-structurality index (Is) is calculated by using formula (1). Unit-cell similarity index $\prod$ was also calculated by the formula (2) which uses the unit-cell parameters of the two crystals,

$$(Is)_n = \left| \left[\sum \frac{(\Delta Ri)2}{n} \right]^{1/2} - 1 \right| \cdots\cdots\cdots (1)$$
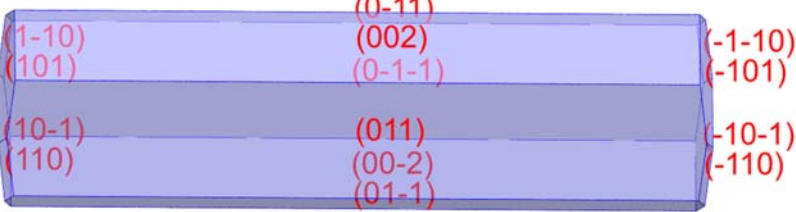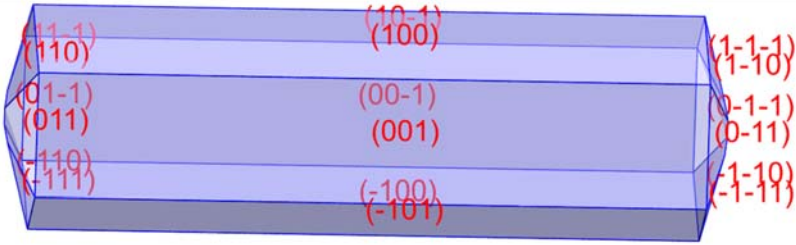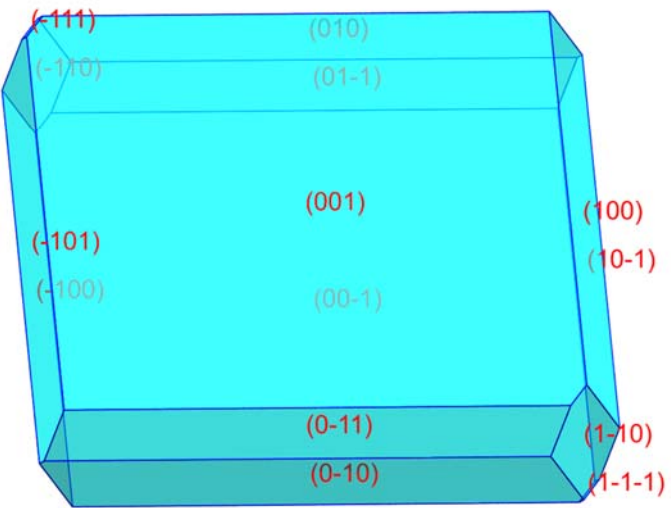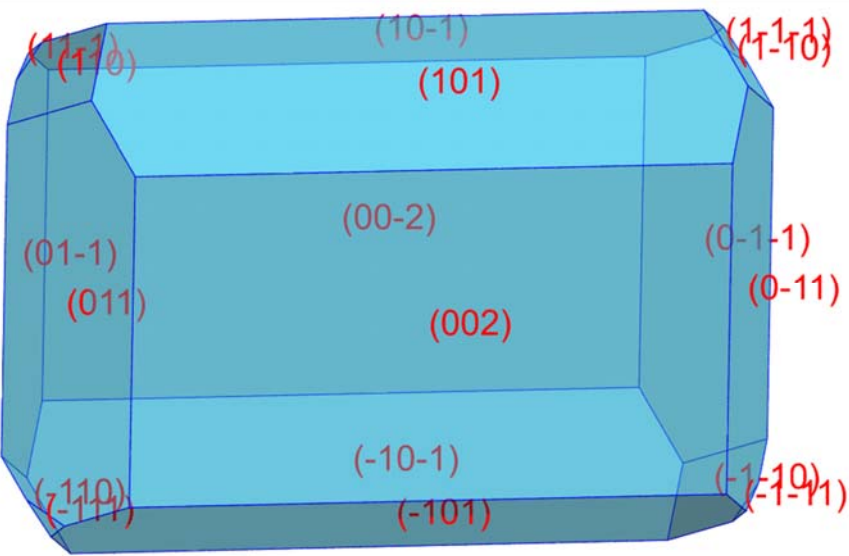
$$\prod = \frac{a+b+c}{a'+b'+c'} - 1 \cdots\cdots\cdots (2)$$
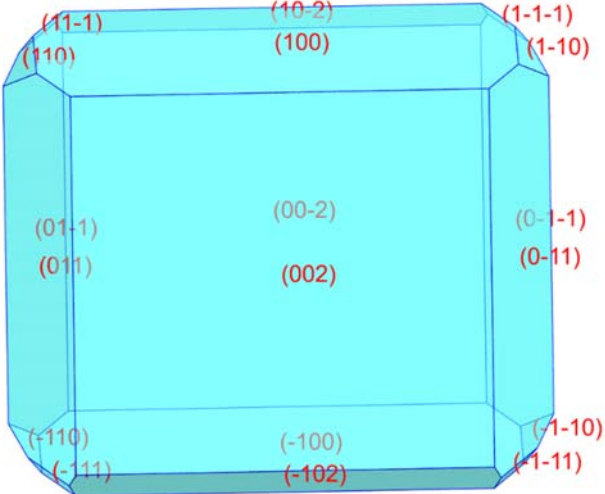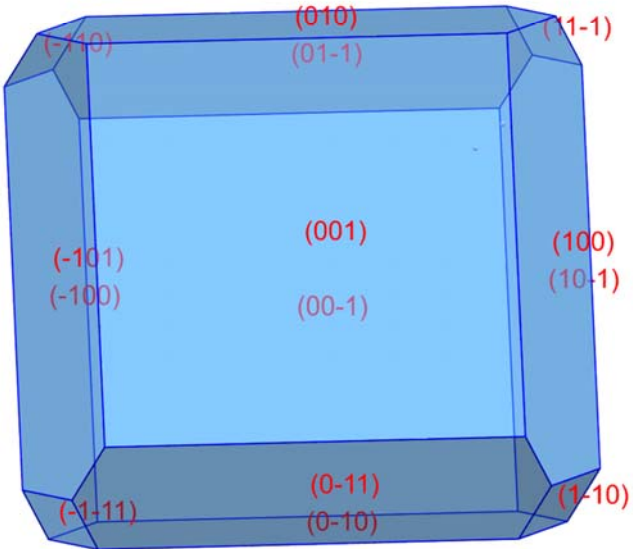
wherein n is the number of related non-hydrogen atoms, ΔR_i are the distance differences between their atomic coordinates. a, b, c and a', b', c' are the reduced unit cell axes of the comparable crystal structures, where, $a+b+c > a'+b'+c'$. Degree of isostructurality increases as Is value close to 100 and the value of $\prod$ tends to zero.

Table S2. Similarity index ($\prod$), Isostructurality Index (Is), root-mean-square deviation (RMSD) and PXRD similarity for all the pairs of structures **1 – 7**, **6a**, **6b**, **7a** and **7b**.
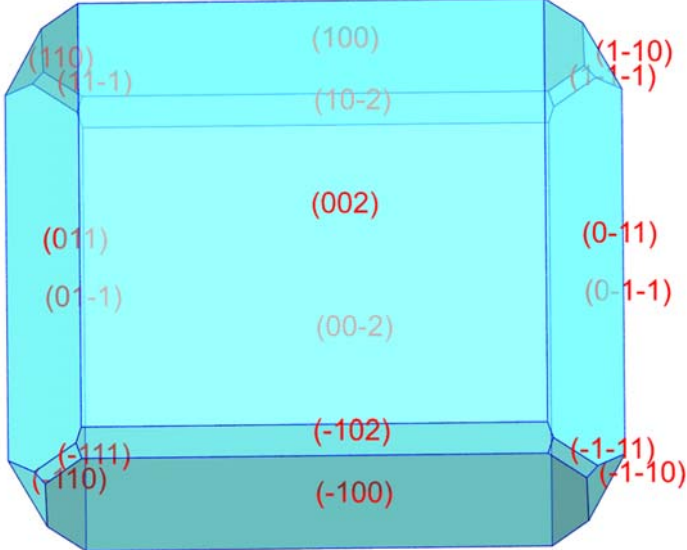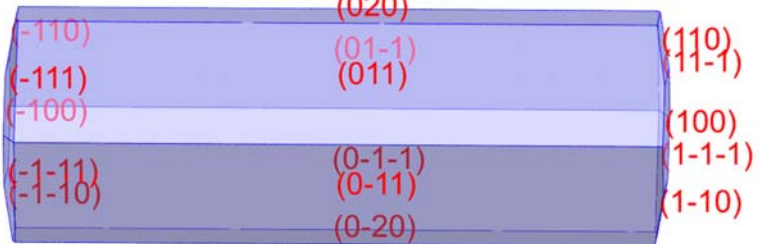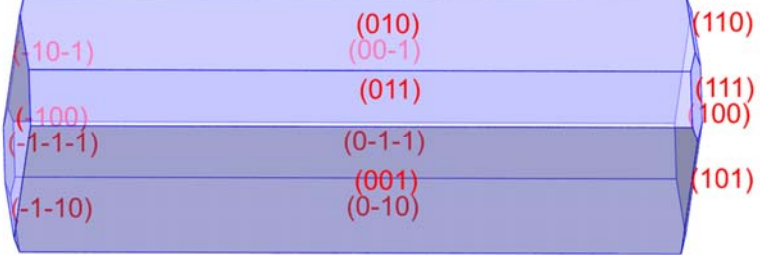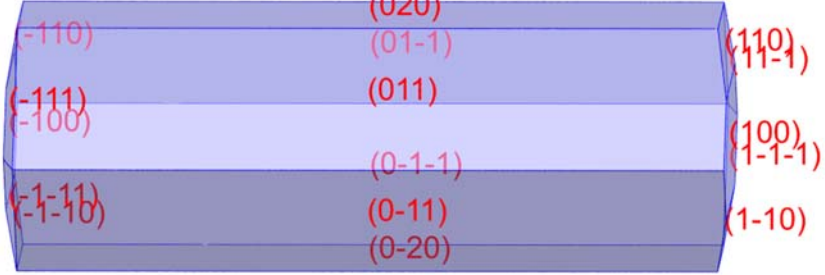
Co-crystals Pair	$\prod$	Is (%)	RMSD	PXRD	Co-crystal Pairs	$\prod$	Is (%)	RMSD	PXRD
1/2	0.380	-15.4	1.154	0.933	4/6	0.126	85.3	0.147	0.893
1/3	0.598	87.3	0.127	0.931	4/6a	0.309	-25	1.25	0.858
¼	0.196	24.8	0.752	0.895	4/6b	0.015	93.5	0.065	0.885
1/5	0.525	82.1	0.179	0.849	4/7	0.114	88.3	0.117	0.93
1/6	0.348	86.7	0.133	0.878	4/7a	0.266	84.3	0.157	0.892
1/6a	0.566	-58.9	1.589	0.879	4/7b	0.052	94.1	0.059	0.897
1/6b	0.154	92	0.08	0.933	5/6	0.131	14.8	0.852	0.771
1/7	0.333	95.5	0.045	0.904	5/6a	0.026	65.5	0.345	0.926
1/7a	0.515	94.6	0.054	0.928	5/6b	0.321	92.2	0.078	0.791
1/7b	0.137	93.9	0.061	0.909	5/7	0.144	14.6	0.854	0.826
2/3	0.157	91.1	0.089	0.879	5/7a	0.006	65.5	0.345	0.926
2/4	0.153	-27.7	1.277	0.791	5/7b	0.341	92.5	0.075	0.808
2/5	0.105	86.1	0.139	0.820	6/6a	0.161	28.2	0.718	0.773
2/6	0.024	94.6	0.054	0.823	6/6b	0.015	94.4	0.056	0.877
2/6a	0.134	-91.1	1.911	0.788	6/7	0.011	97.5	0.025	0.959
2/6b	0.195	90.8	0.092	0.904	6/7a	0.124	95.5	0.045	0.905
2/7	0.035	94.5	0.055	0.836	6/7b	0.185	95	0.05	0.857
2/7a	0.097	94.8	0.052	0.874	6a/6b	0.356	87.5	0.125	0.80
2/7b	0.214	93.8	0.062	0.904	6a/7	0.174	60.3	0.397	0.826
¾	0.336	-27.5	1.275	0.911	6a/7a	0.033	47.4	0.526	0.838
3/5	0.047	-81.0	1.81	0.847	6a/7b	0.377	74.9	0.251	0.775
3/6	0.185	94.2	0.058	0.905	6b/7	0.154	94.1	0.059	0.891
3/6a	0.020	-78.5	1.785	0.854	6b/7a	0.312	96.2	0.038	0.932
3/6b	0.384	81	0.190	0.898	6b/7b	0.015	97.0	0.03	0.932
3/7	0.198	94.3	0.057	0.936	7/7a	0.136	93.4	0.066	0.919
3/7a	0.054	91	0.090	0.929	7/7b	0.172	96.5	0.035	0.904
3/7b	0.405	86.9	0.131	0.913	7a/7b	0.332	96.5	0.035	0.904
4/5	0.275	86.6	0.134	0.838					

S5. BFDH Morphology and Attachment Energies

Co-crystals	BFDH Morphology
1	
2	
3	
4	

5	
6	
6a	

7	
6b	
7a	
7b	

Attachment Energy

The attachment energies were calculated by utilizing the coordinates from the single-crystal structures in BIOVIA Materials Studio 2020 (version 20.1.0.5).
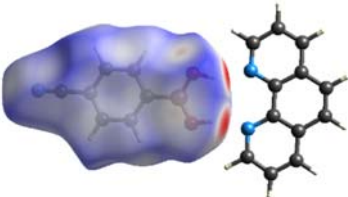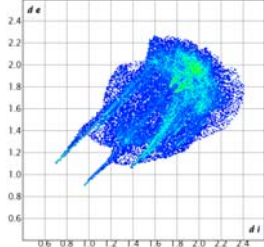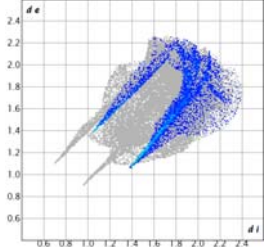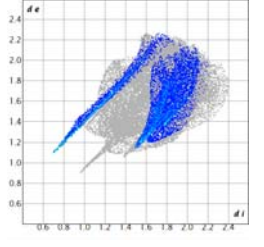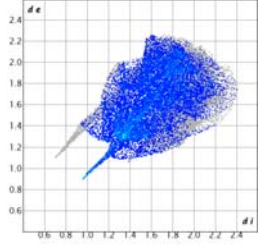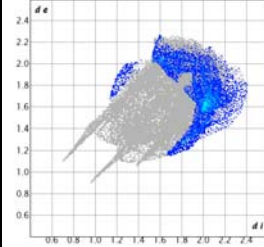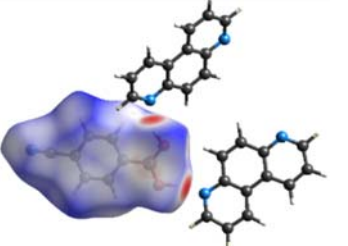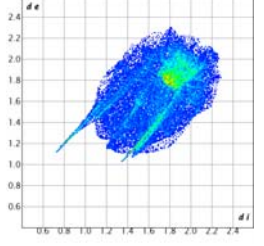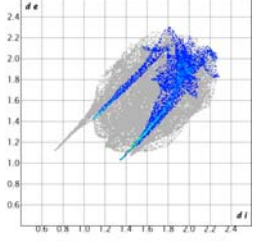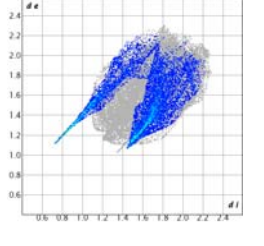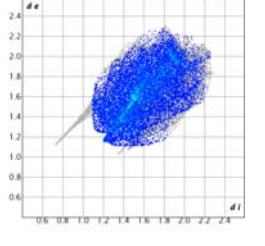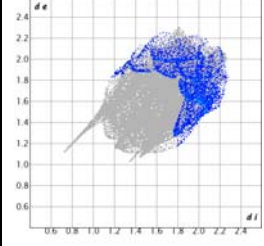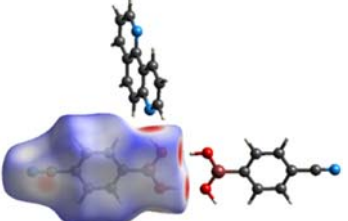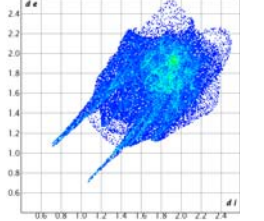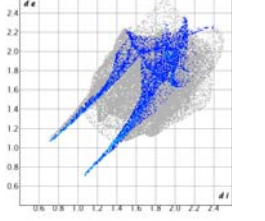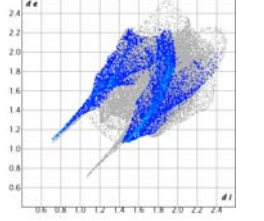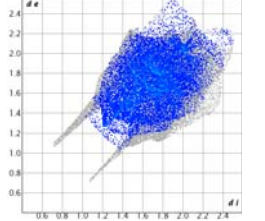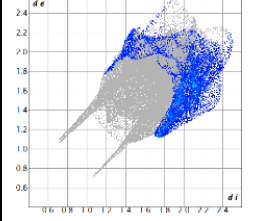
Table S3. Attachment Energies of complexes **1 – 7**, **6a**, **6b**, **7a**, **7b**.

Complexes	hkl	d_{hkl} (Å)	Surface area	E_{att}(Total) (kcal/mol)	Distance	% Total facet area
1	(011)	14.40	123.20	-22.99	22.99	55.81
	(002)	13.09	67.75	-19.54	19.54	35.96
	(111)	3.79	468.12	-139.14	139.14	3.75
	(020)	8.62	102.90	-27.34	27.33	0.71
2	(001)	14.01	57.68	-19.38	19.37	38.91
	(10-1)	12.80	63.14	-23.02	23.02	27.48
	(100)	13.45	60.06	-25.87	25.87	21.87
	(011)	3.73	216.26	-88.55	88.55	3.35
	(0-11)	3.73	216.26	-88.55	88.55	3.35
	(1-1-1)	3.71	217.78	-89.58	89.58	1.59
	(1 -1-1)	3.71	217.78	-89.58	89.58	1.59
	(110)	3.72	216.90	-90.57	90.57	0.91
	(1-10)	3.72	216.90	-90.57	90.57	0.91
3	(001)	13.44	62.27	-21.31	21.31	46.48
	(010)	8.63	97.02	-33.29	33.28	27.69
	(100)	7.05	118.68	-50.99	50.99	17.03
	(01-1)	7.76	107.83	-39.17	39.17	4.29
	(10-1)	6.62	126.38	-55.18	55.18	3.29
	(1-10)	5.78	144.70	-62.05	62.05	0.89
	(1-1-1)	5.27	158.56	-62.33	62.33	0.26
4	(10-1)	10.38	163.02	-56.55	56.55	34.01
	(002)	10.41	81.25	-60.27	60.27	31.69
	(011)	6.91	244.77	-116.56	117.88	15.12
	(110)	6.091	244.77	-116.56	116.56	10.04
	(101)	9.12	185.59	-80.60	80.60	9.11
5	(001)	11.26	83.84	-35.42	35.42	32.32
	(010)	10.76	87.70	-39.56	39.56	27.38
	(100)	6.98	135.18	-57.19	57.19	24.76
	(01-1)	8.96	135.18	-43.49	43.49	14.76
	(10-1)	6.94	137.53	-76.76	76.76	0.50
	(1-10)	6.97	136.02	-82.28	82.44	0.02
6	(002)	9.79	58.84	-45.373	45.373	40.40
	(100)	8.24	139.84	-58.99	58.99	27.13
	(011)	6.68	172.51	-79.65	79.65	18.53
	(110)	5.38	214.13	-83.18	83.18	9.01
	(11-1)	5.27	218.68	-86.65	88.59	4.024
	(111)	5.11	225.41	-88.65	88.65	0.87
6a	(001)	11.08	80.55	-26.30	26.30	32.87

	(010)	8.70	102.60	-33.90	33.90	21.43
	(100)	8.34	107.00	-38.86	38.86	19.98
	(01-1)	8.06	110.68	-36.60	36.60	13.62
	(10-1)	8.11	110.04	-45.67	45.67	8.23
	(1-10)	6.38	139.77	-47.20	47.20	3.84
6b	(0 1 1)	12.28	101.89	-34.45	34.45	65.89
	(0 2 0)	11.19	55.90	-40.00	40.00	20.35
	(1 0 0)	3.79	329.93	-112.89	112.89	11.80
	(1 1 0)	3.74	334.63	-116.52	116.52	1.94
7	(002)	9.82	61.81	-51.46	51.46	41.18
	(100)	8.42	144.11	-67.33	67.33	29.22
	(011)	6.85	177.03	-96.03	96.03	19.66
	(110)	5.52	219.74	-102.45	102.45	7.33
	(11-1)	5.37	225.81	-107.75	107.75	1.84
	(111)	5.26	230.70	-108.16	108.16	0.75
7a	(001)	15.41	44.43	-10.77	10.77	52.75
	(010)	11.21	61.07	-15.35	15.35	36.99
	(101)	3.78	181.01	-55.39	55.439	10.25
7b	(011)	12.45	107.03	-32.85	32.85	71.49
	(020)	11.34	58.75	-42.12	42.12	16.52
	(100)	3.93	338.78	-127.04	127.04	11.98
	(010)	10.76	87.70	-39.56	39.56	27.38
	(100)	6.98	135.18	-57.19	57.19	24.76
	(01-1)	8.96	135.18	-43.49	43.49	14.76
	(10-1)	6.94	137.53	-76.76	76.76	0.50
	(1-10)	6.97	136.02	-82.28	82.44	0.02

S6. Hirshfeld Surface Analysis

Table S4. The 3D d_{norm} Surface and Overall 2D Fingerprint Plots Considering the **CB** Surface for the Co-crystals **1** - **7**, **6a**, **6b**, **7a** and **7b**.

Complexes	3D d_{norm} surface	2D finger print (full)	O···H/H···O	N···H/H···N	H···H	C···H/H···C
1						
2						
3						
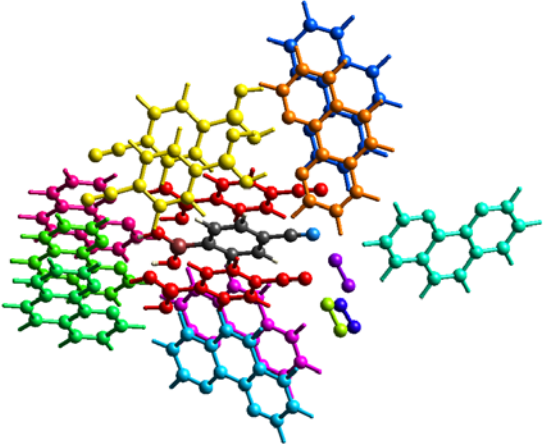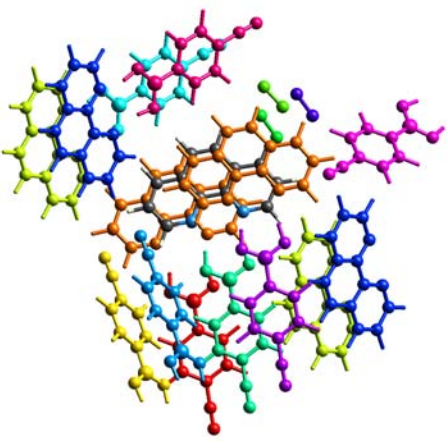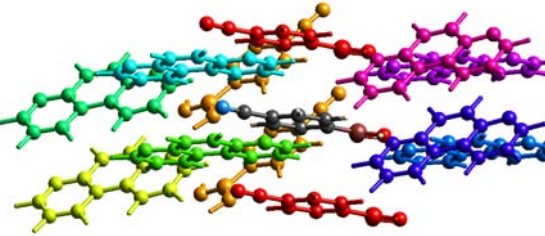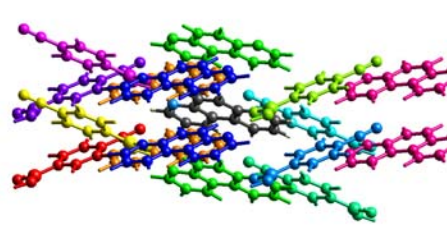
Table S5. Contribution of Different Intermolecular Interactions in Hirshfeld Surface.

Co-crystals	O···H/ H···O	N···H/ H···N	C···H/ H···C	H···H	C···C	H···B	C···O	B···C	B···O	N···C
1	12.5	19.9	15.8	34.8	8.3	1.5	0.2	0.5	2.7	1.2
2	13.7	21.2	9.7	34.7	10.6	1.2	1.7	2.4	1.2	1.8
3	14.2	21.4	15.6	33.9	0.7	0	6.2	4	0	2.6
4	15.1	23.1	18	33.8	0.9	1.4	3.5	2.5	0	1.1
5	20.6	21.5	23.9	28	0.5	2.7	1.5	0.1	0	1
6	14.1	24.1	11.6	30.6	8.4	1	2.7	2.6	0	3.5
6a	14.1	19.3	21.1	30.8	1.6	1.4	3.2	2.7	0	2.6
6b	10.7	21.4	9.1	40.1	10.9	0.7	0.3	2	1.6	2.7
7	14.3	22.6	11.9	33.1	9.6	0.7	2.4	3.4	0	1.4
7a	23.6	19	12	27.2	10	1.6	0.3	1.7	1.2	1.8
7b	10.9	20.7	8.5	42	10.3	0.9	0.3	2	1.4	2.5

S7. Interaction Energy Calculation

Complete details of computational procedure. The Crystal Explorer software (version 21.5) was utilized to perform the interaction energy by using B3LYP/6-31G(d,p) method. As the co-crystals comprised of multiple molecules within their asymmetric units, the energy contribution from each molecule in the crystal structure was considered individually. To accurately represent the energy contribution from each molecule, a cluster with a radius 3.8 Å was generated around each individual molecule, and the energy calculation was performed accordingly. The resulting clusters of molecules were symmetrically color-coded with respect to each co-former, as shown in Table S6. The scale factor for calculating energy frameworks in Crystal Explorer is given in Table S7. The overall energy profiles of each co-crystal are given below in the following Table S8.

Table S6. Cluster of molecules with symmetrically coloured coded in Energy Frameworks calculation.

Co-crystals	Residue 1 (4-cyanophenylboronic acid)	Residue 1 (*N*-donor compound)
1		
2		

3		
4		
5		
6		

6a		
6b		
7		
7a		

7b	
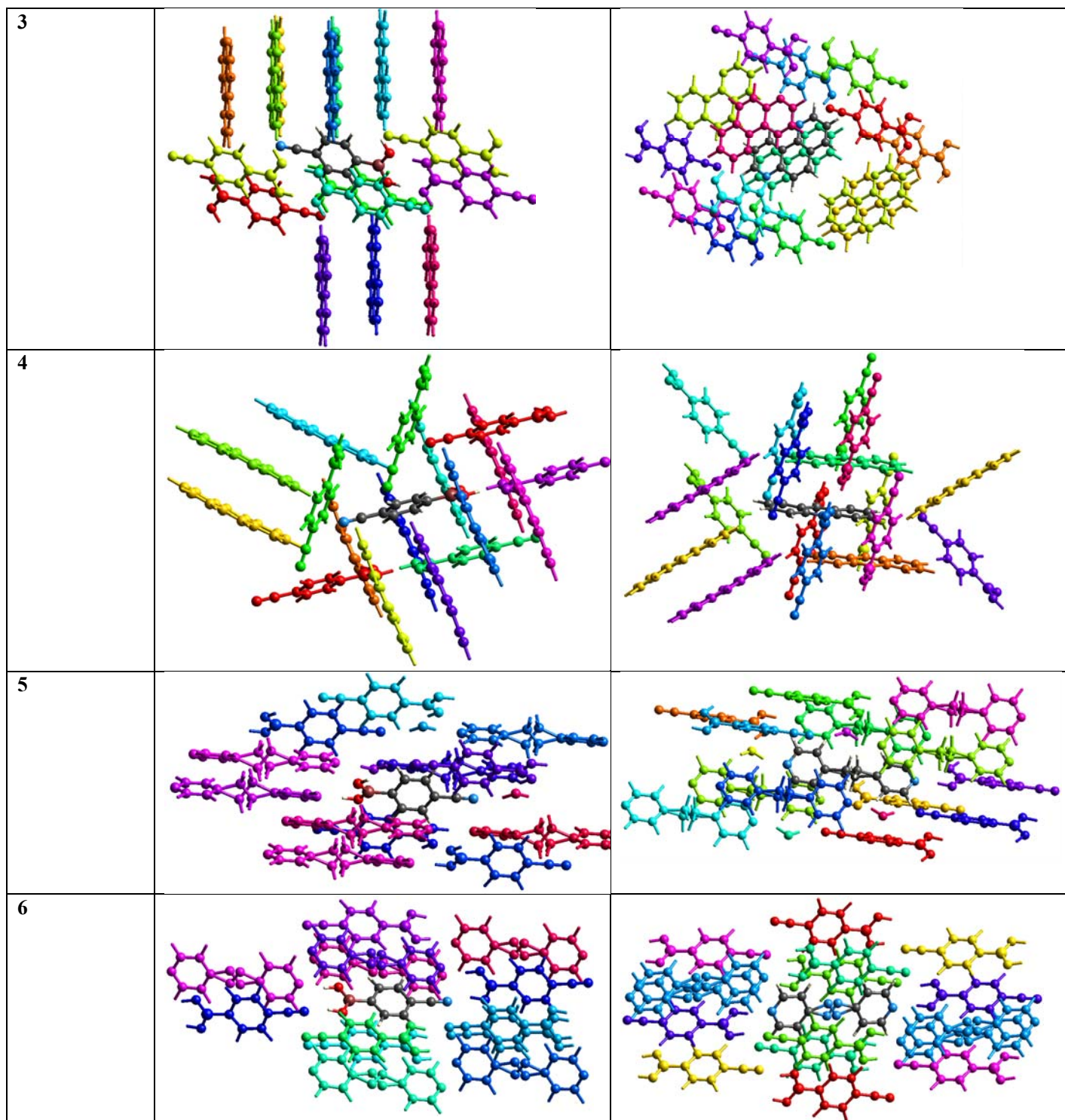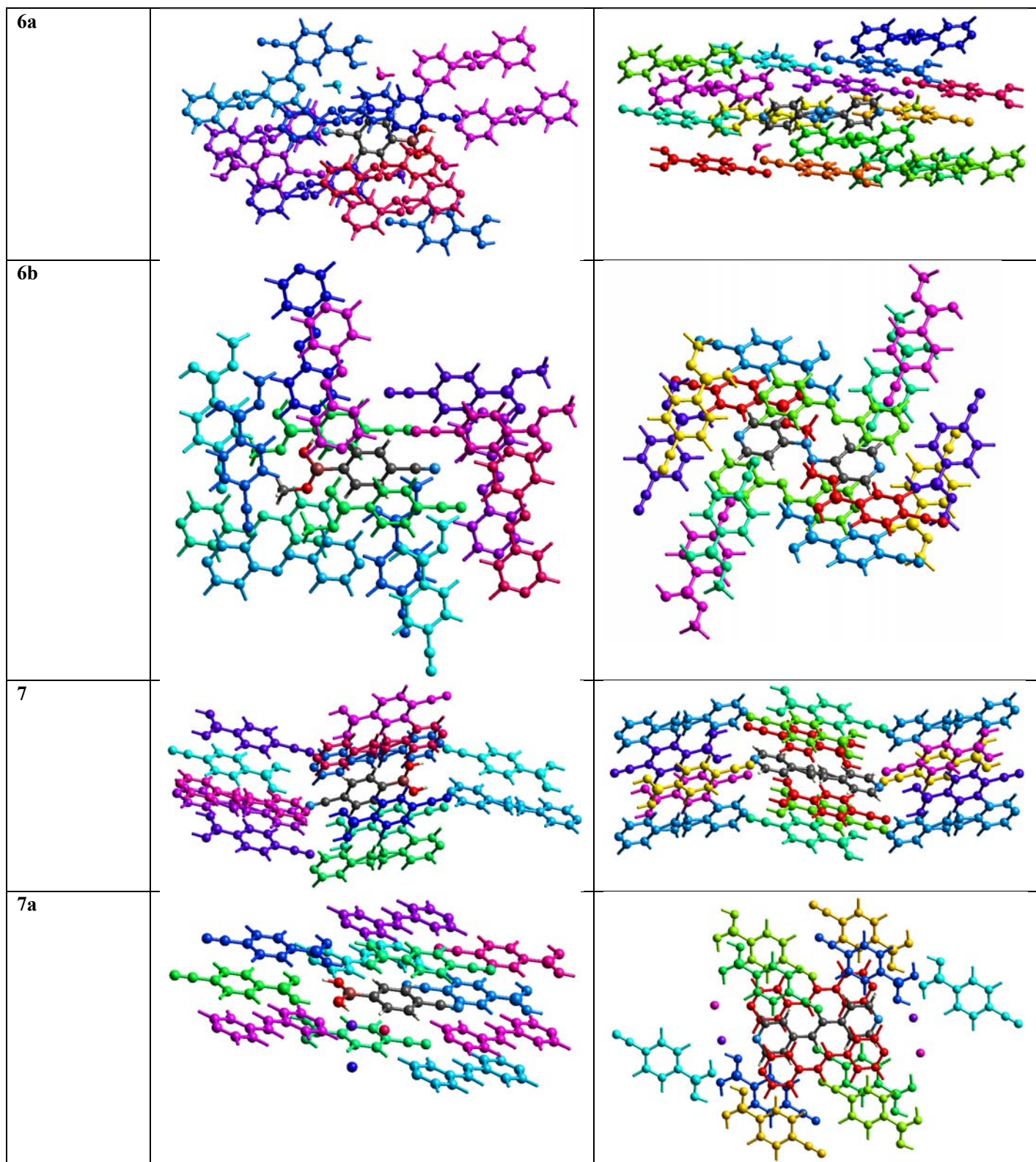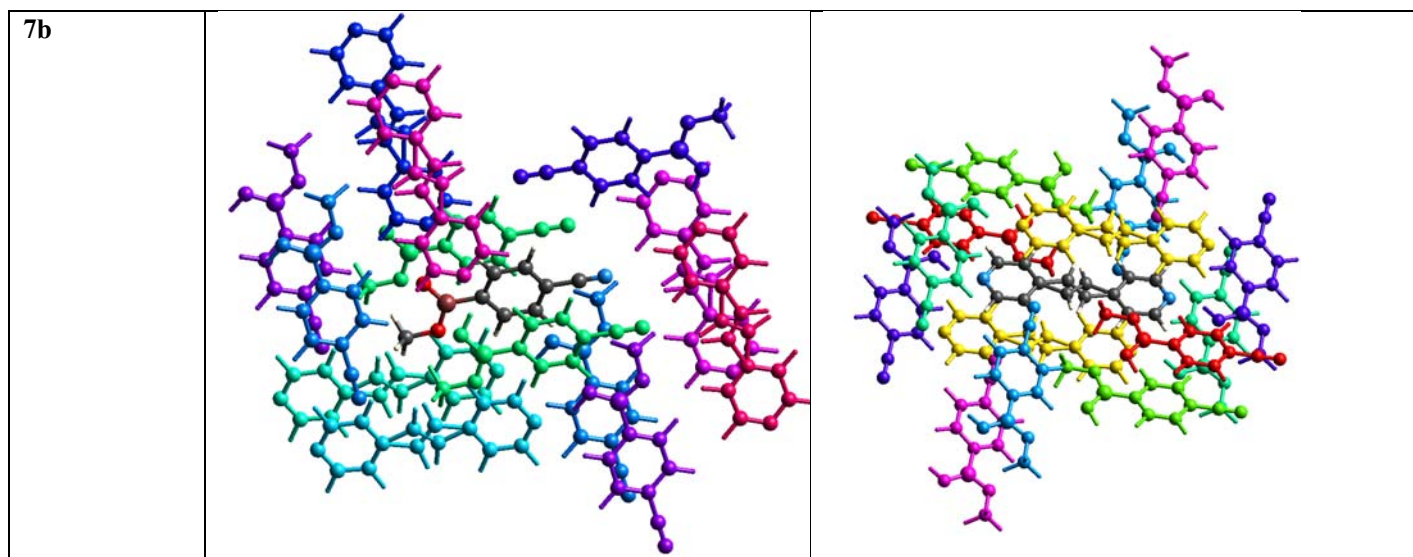
Table S7. Pictorial Representation of all Energy Frameworks for Crystal Structures **1 – 7**, **6a**, **6b**, **7a** and **7b**.

Co-crystals	Electrostatic term	Dispersion term	Total interaction energy
1			
2			
3			

4			
5			
6			
6a			
6b			
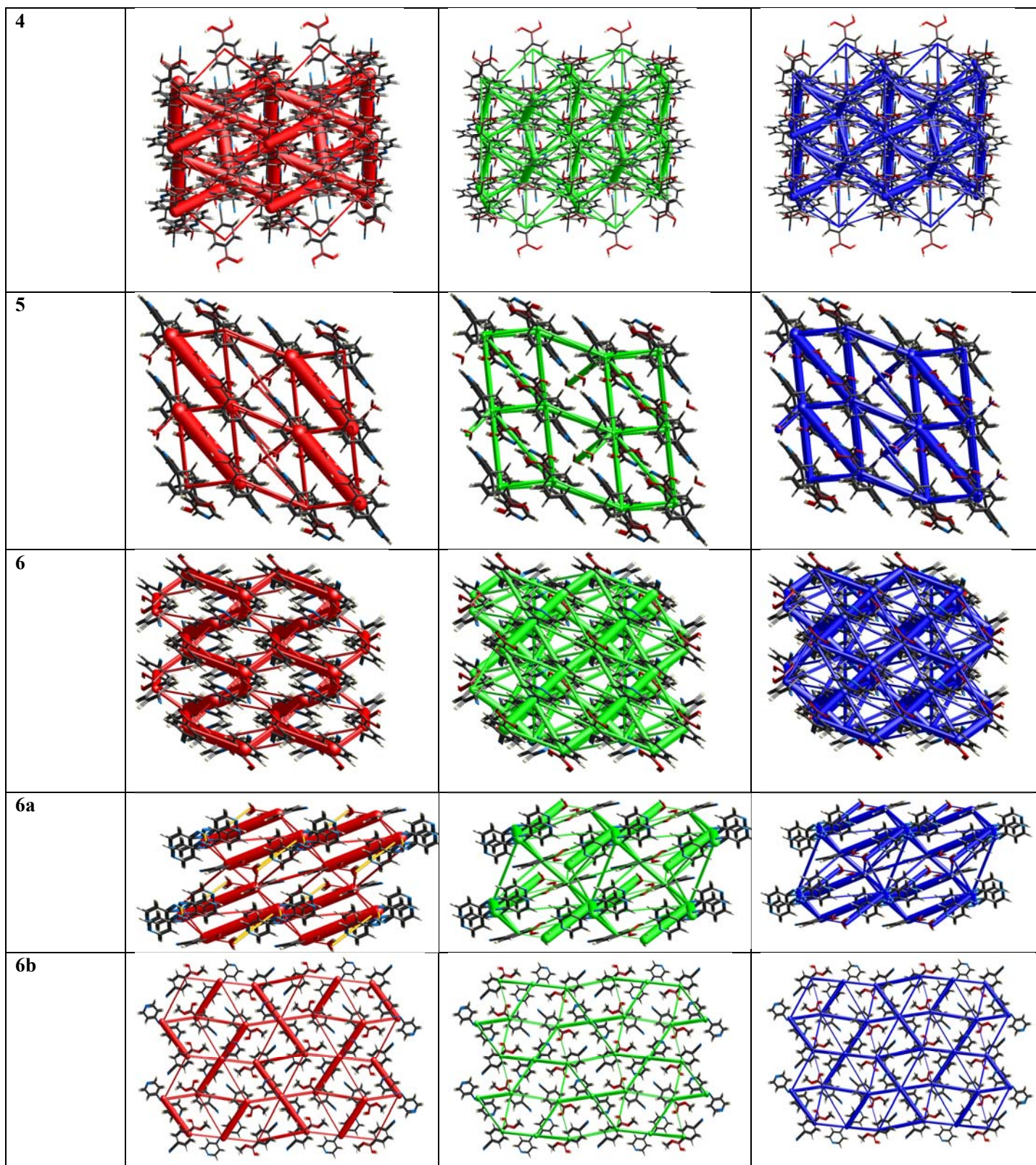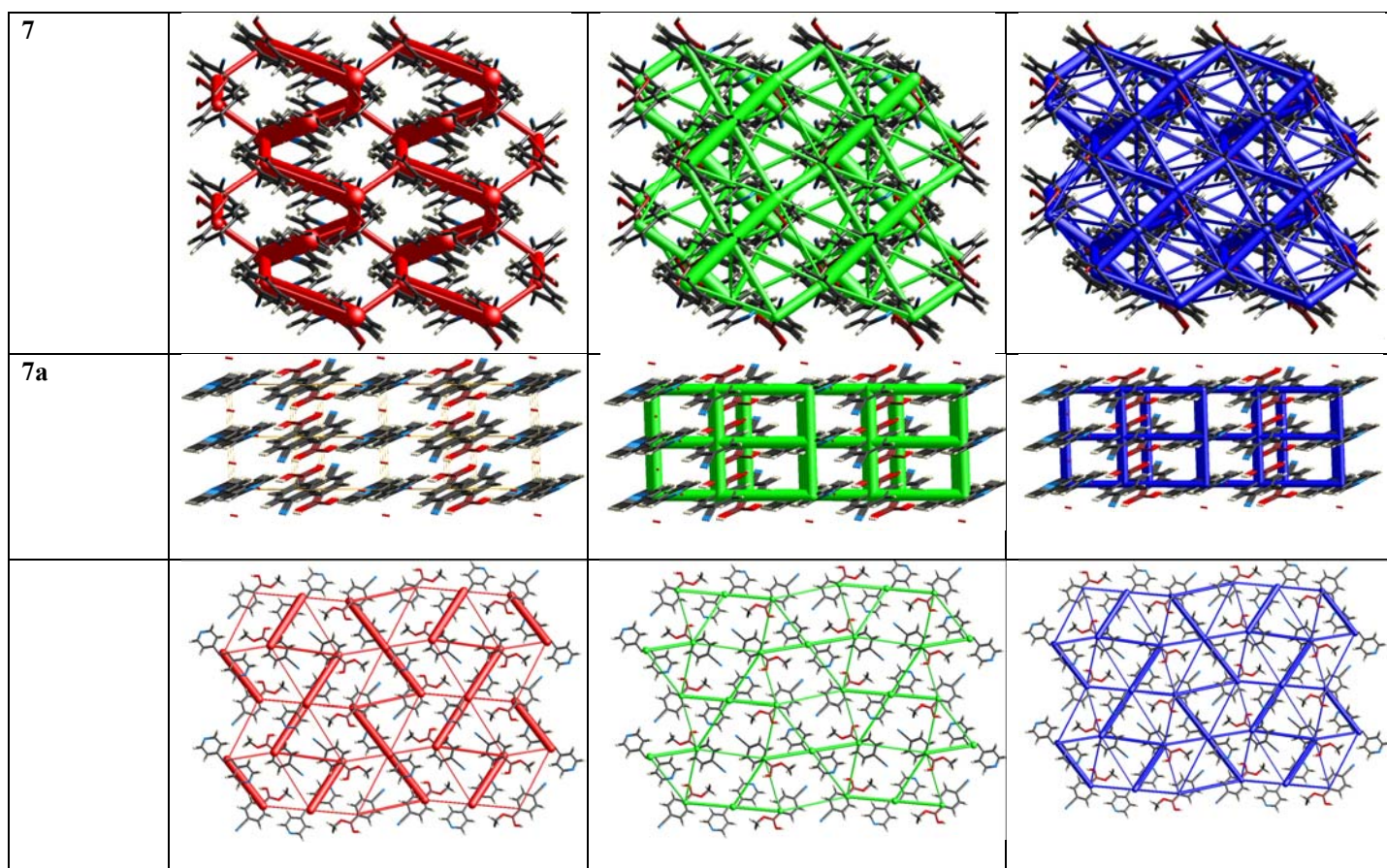
Table S8. Scale factors for benchmarked energy models

Energy Model	E_{ele}	E_{pol}	E_{dis}	E_{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

Table S9. Overall Energy Profile for Co-crystal 1.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	8.73	B3LYP/6-31G(d,p)	-4.7	-1.2	-2.7	0.1	-8.2
	0	x, y, z	3.93	B3LYP/6-31G(d,p)	2.3	-2.5	-59.3	32.1	-31.2
	0	-	8.82	B3LYP/6-31G(d,p)	-6.2	-1.6	-7.0	5.4	-10.6
	0	-x, y+1/2, -z+1/2	8.98	B3LYP/6-31G(d,p)	-2.6	-0.6	-8.3	4.1	-7.9
	0	-	6.40	B3LYP/6-31G(d,p)	-0.2	-0.1	-0.5	0.0	-0.8
	0	-	6.13	B3LYP/6-31G(d,p)	0.0	-0.2	0.0	0.0	-0.2
	0	-	7.39	B3LYP/6-31G(d,p)	-121.0	-34.6	-21.4	127.9	-93.1

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	6.63	B3LYP/6-31G(d,p)	-5.1	-0.9	-14.5	12.7	-10.7
	0	-	8.47	B3LYP/6-31G(d,p)	-2.4	-1.7	-6.0	2.9	-7.3
	0	-x, y+1/2, -z+1/2	8.91	B3LYP/6-31G(d,p)	-1.7	-0.4	-8.9	5.5	-6.5
	0	-	6.70	B3LYP/6-31G(d,p)	0.3	-0.0	-0.3	0.0	0.1
	0	-	8.00	B3LYP/6-31G(d,p)	-4.0	-1.7	-4.5	0.3	-9.3
	0	-	10.67	B3LYP/6-31G(d,p)	-5.4	-2.2	-3.8	5.2	-7.5
	0	-	6.99	B3LYP/6-31G(d,p)	-0.3	-0.4	-10.2	5.1	-6.3
	2	x, y, z	3.93	B3LYP/6-31G(d,p)	9.6	-1.2	-31.7	13.1	-10.3
	1	-	8.47	B3LYP/6-31G(d,p)	-2.4	-1.7	-6.0	2.9	-7.3
	2	x+1/2, -y+1/2, -z	5.68	B3LYP/6-31G(d,p)	-11.5	-0.8	-15.1	12.7	-18.0
	1	-	6.22	B3LYP/6-31G(d,p)	-5.1	-0.9	-14.5	12.7	-10.7
	1	-	7.39	B3LYP/6-31G(d,p)	-121.0	-34.6	-21.4	127.9	-93.1
	1	-	8.00	B3LYP/6-31G(d,p)	-4.0	-1.7	-4.5	0.3	-9.3
	1	-	10.67	B3LYP/6-31G(d,p)	-5.4	-2.2	-3.8	5.2	-7.5
	1	-	6.63	B3LYP/6-31G(d,p)	-5.1	-0.9	-14.5	12.7	-10.7
	1	-	8.82	B3LYP/6-31G(d,p)	-6.2	-1.6	-7.0	5.4	-10.6
	1	-	6.91	B3LYP/6-31G(d,p)	-5.4	-2.2	-3.8	5.2	-7.5
	1	-	6.02	B3LYP/6-31G(d,p)	-0.3	-0.4	-10.2	5.1	-6.3
	1	-	6.99	B3LYP/6-31G(d,p)	-0.3	-0.4	-10.2	5.1	-6.3
	1	-	8.73	B3LYP/6-31G(d,p)	-4.7	-1.2	-2.7	0.1	-8.2

Table S10. Overall Energy Profile for Co-crystal 2**.**

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	9.65	B3LYP/6-31G(d,p)	-8.7	-2.2	-7.8	9.5	-11.7
	0	-x, y+1/2, -z	8.94	B3LYP/6-31G(d,p)	0.8	-0.5	-7.2	3.0	-4.0
	0	-	7.93	B3LYP/6-31G(d,p)	-1.2	-0.7	-7.9	1.7	-7.6
	0	-	7.42	B3LYP/6-31G(d,p)	-47.2	-11.3	-18.0	50.1	-43.0
	0	x, y, z	3.88	B3LYP/6-31G(d,p)	0.2	-1.5	-53.1	26.2	-30.9
	0	-	8.57	B3LYP/6-31G(d,p)	-11.0	-3.3	-8.8	11.0	-14.9
	0	-	7.33	B3LYP/6-31G(d,p)	-1.3	-2.4	-14.1	8.4	-10.3

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	7.73	B3LYP/6-31G(d,p)	-1.4	-1.0	-9.5	6.2	-6.7
	0	-x, y+1/2, -z	7.94	B3LYP/6-31G(d,p)	1.0	-0.1	-5.0	0.7	-3.0
	0	-	9.41	B3LYP/6-31G(d,p)	-0.8	-0.4	-4.1	0.8	-4.2
	0	-	8.56	B3LYP/6-31G(d,p)	-57.7	-12.6	-13.8	66.4	-41.3
	0	-x, y+1/2, -z	10.94	B3LYP/6-31G(d,p)	0.4	-0.2	-2.5	0.3	-1.7
	2	x, y, z	3.88	B3LYP/6-31G(d,p)	3.5	-1.2	-38.1	21.3	-17.1
	2	-x, y+1/2, -z	6.02	B3LYP/6-31G(d,p)	-6.8	-0.8	-12.3	10.3	-12.2
	1	-	9.41	B3LYP/6-31G(d,p)	-0.8	-0.4	-4.1	0.8	-4.2
	1	-	7.33	B3LYP/6-31G(d,p)	-1.3	-2.4	-14.1	8.4	-10.3
	1	-	9.65	B3LYP/6-31G(d,p)	-8.7	-2.2	-7.8	9.5	-11.7
	1	-	8.57	B3LYP/6-31G(d,p)	-11.0	-3.3	-8.8	11.0	-14.9
	1	-	8.56	B3LYP/6-31G(d,p)	-57.7	-12.6	-13.8	66.4	-41.3
	1	-	7.42	B3LYP/6-31G(d,p)	-47.2	-11.3	-18.0	50.1	-43.0
	1	-	7.93	B3LYP/6-31G(d,p)	-1.2	-0.7	-7.9	1.7	-7.6
	1	-	7.73	B3LYP/6-31G(d,p)	-1.4	-1.0	-9.5	6.2	-6.7

Table S11. Overall Energy Profile for Co-crystal 3.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	7.36	B3LYP/6-31G(d,p)	0.0	-0.6	-13.2	7.3	-7.4
	0	-	10.06	B3LYP/6-31G(d,p)	-1.8	-1.2	-2.6	0.7	-4.7
	0	-x, -y, -z	7.43	B3LYP/6-31G(d,p)	-3.1	-0.7	-13.6	6.3	-11.7
	0	x, y, z	8.75	B3LYP/6-31G(d,p)	-0.4	-0.4	-6.5	4.1	-3.9
	0	-	8.10	B3LYP/6-31G(d,p)	-6.6	-1.0	-9.9	13.6	-7.9
	0	-	6.52	B3LYP/6-31G(d,p)	-61.4	-15.9	-19.0	76.1	-46.3
	0	-x, -y, -z	3.95	B3LYP/6-31G(d,p)	0.2	-1.0	-49.9	20.2	-31.5
	0	-	7.13	B3LYP/6-31G(d,p)	-5.8	-1.6	-9.9	7.7	-11.3
	0	-	6.62	B3LYP/6-31G(d,p)	-6.7	-1.5	-13.0	8.2	-14.4
	0	-	8.52	B3LYP/6-31G(d,p)	0.6	-0.1	-2.7	0.2	-1.7
	0	-	9.29	B3LYP/6-31G(d,p)	-5.1	-1.7	-7.2	9.0	-7.3
	0	-	9.34	B3LYP/6-31G(d,p)	-1.0	-0.1	-1.5	0.0	-2.4
	0	-	9.61	B3LYP/6-31G(d,p)	-3.7	-0.3	-2.1	0.1	-5.9
	0	-x, -y, -z	4.05	B3LYP/6-31G(d,p)	-1.5	-1.0	-47.9	20.6	-31.3

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	1	-x, -y, -z	7.80	B3LYP/6-31G(d,p)	-8.4	-2.4	-10.5	8.9	-14.3
	1	-	10.06	B3LYP/6-31G(d,p)	-1.8	-1.2	-2.6	0.7	-4.7
	1	-	9.29	B3LYP/6-31G(d,p)	-5.1	-1.7	-7.2	9.0	-7.3
	2	x, y, z	7.15	B3LYP/6-31G(d,p)	-2.1	-1.5	-15.1	7.9	-11.7
	1	-	7.13	B3LYP/6-31G(d,p)	-5.8	-1.6	-9.9	7.7	-11.3
	1	-x, -y, -z	5.74	B3LYP/6-31G(d,p)	-2.5	-0.2	-9.3	1.7	-9.8
	1	-	7.36	B3LYP/6-31G(d,p)	0.0	-0.6	-13.2	7.3	-7.4
	1	-x, -y, -z	4.68	B3LYP/6-31G(d,p)	-2.0	-0.5	-25.0	7.3	-19.8
	1	-	6.52	B3LYP/6-31G(d,p)	-61.4	-15.9	-19.0	76.1	-46.3
	1	-	6.62	B3LYP/6-31G(d,p)	-6.7	-1.5	-13.0	8.2	-14.4
	1	-	8.10	B3LYP/6-31G(d,p)	-6.6	-1.0	-9.9	13.6	-7.9
	1	-	8.52	B3LYP/6-31G(d,p)	0.6	-0.1	-2.7	0.2	-1.7
	1	-x, -y, -z	9.19	B3LYP/6-31G(d,p)	-70.1	-14.2	-13.3	85.1	-43.6
	1	-	9.34	B3LYP/6-31G(d,p)	-1.0	-0.1	-1.5	0.0	-2.4
	1	-	9.61	B3LYP/6-31G(d,p)	-3.7	-0.3	-2.1	0.1	-5.9

Table S12. Overall Energy Profile for Co-crystal 4.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	6.58	B3LYP/6-31G(d,p)	-6.4	-1.2	-10.5	10.0	-10.6
	0	-x, -y, -z	5.30	B3LYP/6-31G(d,p)	-4.4	-1.4	-43.8	25.3	-28.1
	0	x+1/2, -y+1/2, z+1/2	11.15	B3LYP/6-31G(d,p)	0.2	-0.2	-4.6	2.6	-2.3
	0	-	7.52	B3LYP/6-31G(d,p)	-1.0	-1.0	-11.5	8.3	-6.6
	0	-	7.16	B3LYP/6-31G(d,p)	-0.1	-0.6	-16.5	8.9	-9.4
	0	-	8.97	B3LYP/6-31G(d,p)	-0.9	-0.1	-1.9	0.0	-2.7
	0	-x, -y, -z	4.02	B3LYP/6-31G(d,p)	-7.6	-1.7	-59.5	35.3	-39.3
	0	-	11.09	B3LYP/6-31G(d,p)	-1.2	-0.7	-1.7	0.2	-3.1
	0	-	7.83	B3LYP/6-31G(d,p)	-0.7	-0.2	-2.8	0.1	-3.3
	0	-	5.75	B3LYP/6-31G(d,p)	-65.1	-17.5	-22.7	85.2	-48.9
	0	-	7.15	B3LYP/6-31G(d,p)	-5.2	-1.6	-11.0	7.0	-11.9
	0	-	10.95	B3LYP/6-31G(d,p)	-3.4	-1.2	-3.3	3.1	-5.4

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-x+1/2, y+1/2, -z+1/2	9.07	B3LYP/6-31G(d,p)	-1.7	-0.3	-8.8	2.7	-8.0
	0	-	6.49	B3LYP/6-31G(d,p)	-0.3	-0.3	-11.7	6.2	-6.9
	0	-	8.12	B3LYP/6-31G(d,p)	-3.1	-0.4	-3.3	0.2	-6.4
	2	x, y, z	7.33	B3LYP/6-31G(d,p)	-1.8	-1.4	-12.0	4.2	-10.9
	1	-	7.15	B3LYP/6-31G(d,p)	-5.2	-1.6	-11.0	7.0	-11.9
	1	-	11.09	B3LYP/6-31G(d,p)	-1.2	-0.7	-1.7	0.2	-3.1
	1	-	7.83	B3LYP/6-31G(d,p)	-0.7	-0.2	-2.8	0.1	-3.3
	1	-	10.95	B3LYP/6-31G(d,p)	-3.4	-1.2	-3.3	3.1	-5.4
	2	-x+1/2, y+1/2, -z+1/2	7.59	B3LYP/6-31G(d,p)	-6.1	-1.8	-6.6	8.0	-8.6
	1	-x, -y, -z	4.92	B3LYP/6-31G(d,p)	-3.9	-0.6	-23.6	9.1	-19.5
	1	-	5.75	B3LYP/6-31G(d,p)	-65.1	-17.5	-22.7	85.2	-48.9
	1	-	7.16	B3LYP/6-31G(d,p)	-0.1	-0.6	-16.5	8.9	-9.4
	1	-	6.58	B3LYP/6-31G(d,p)	-6.4	-1.2	-10.5	10.0	-10.6
	1	-	7.52	B3LYP/6-31G(d,p)	-1.0	-1.0	-11.5	8.3	-6.6
	1	-	6.49	B3LYP/6-31G(d,p)	-0.3	-0.3	-11.7	6.2	-6.9
	1	-x, -y, -z	9.15	B3LYP/6-31G(d,p)	-74.9	-14.4	-13.4	95.2	-42.8
	1	-	8.12	B3LYP/6-31G(d,p)	-3.1	-0.4	-3.3	0.2	-6.4
	1	-	8.97	B3LYP/6-31G(d,p)	-0.9	-0.1	-1.9	0.0	-2.7

Table S13. Overall Energy Profile for Co-crystal 5.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	5.52	B3LYP/6-31G(d,p)	-6.3	-2.7	-29.1	19.2	-22.1
	0	-	10.75	B3LYP/6-31G(d,p)	-4.9	-0.4	-3.6	1.0	-8.0
	0	-	6.17	B3LYP/6-31G(d,p)	-3.4	-2.2	-25.5	12.3	-19.9
	0	-	7.35	B3LYP/6-31G(d,p)	-0.1	-1.0	0.0	0.0	-1.1
	0	x, y, z	7.55	B3LYP/6-31G(d,p)	-16.1	-5.1	-27.6	9.0	-39.3
	0	-	6.01	B3LYP/6-31G(d,p)	1.9	-1.3	-20.9	10.7	-10.6
	0	-x, -y, -z	5.74	B3LYP/6-31G(d,p)	-1.5	-0.8	-26.9	14.1	-16.9
	0	-	6.64	B3LYP/6-31G(d,p)	-7.6	-0.8	-4.8	0.0	-12.8
	0	-x, -y, -z	12.23	B3LYP/6-31G(d,p)	-7.6	-0.8	-4.8	0.0	-12.8

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	9.14	B3LYP/6-31G(d,p)	-4.9	-1.6	-7.5	1.6	-11.9
	0	-x, -y, -z	6.89	B3LYP/6-31G(d,p)	-12.1	-5.2	-32.2	26.8	-28.1
	0	-	10.52	B3LYP/6-31G(d,p)	-5.7	-1.2	-4.8	3.1	-9.3
	0	-	10.60	B3LYP/6-31G(d,p)	-67.4	-17.0	-11.4	73.6	-48.4
	0	-	4.05	B3LYP/6-31G(d,p)	-16.1	-5.1	-27.6	9.0	-39.3
	0	-x, -y, -z	9.20	B3LYP/6-31G(d,p)	-4.7	-0.5	-11.4	6.4	-11.3
	0	-	6.06	B3LYP/6-31G(d,p)	-12.1	-5.2	-32.2	26.8	-28.1
	1	-x, -y, -z	7.49	B3LYP/6-31G(d,p)	3.2	-0.7	-3.0	0.2	0.4
	1	-	4.63	B3LYP/6-31G(d,p)	-4.9	-1.6	-7.5	1.6	-11.9
	1	-	9.14	B3LYP/6-31G(d,p)	-4.9	-1.6	-7.5	1.6	-11.9
	2	x, y, z	7.55	B3LYP/6-31G(d,p)	-2.3	-1.4	-10.3	3.5	-10.2
	1	-x, -y, -z	5.76	B3LYP/6-31G(d,p)	-10.0	-1.1	-14.5	10.0	-17.9
	1	-	5.52	B3LYP/6-31G(d,p)	-6.3	-2.7	-29.1	19.2	-22.1
	1	-x, -y, -z	6.71	B3LYP/6-31G(d,p)	-14.7	-2.5	-14.7	7.9	-25.4
	1	-	4.46	B3LYP/6-31G(d,p)	-4.9	-0.4	-3.6	1.0	-8.0
	1	-	10.60	B3LYP/6-31G(d,p)	-67.4	-17.0	-11.4	73.6	-48.4
	1	-	10.75	B3LYP/6-31G(d,p)	-4.9	-0.4	-3.6	1.0	-8.0
	1	-	6.17	B3LYP/6-31G(d,p)	-3.4	-2.2	-25.5	12.3	-19.9
	1	-	6.01	B3LYP/6-31G(d,p)	1.9	-1.3	-20.9	10.7	-10.6
	1	-	7.22	B3LYP/6-31G(d,p)	4.3	-0.2	-0.3	0.0	4.1
	1	-	10.52	B3LYP/6-31G(d,p)	-5.7	-1.2	-4.8	3.1	-9.3

Table S14. Overall Energy Profile for Co-crystal 6.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	6.19	B3LYP/6-31G(d,p)	-1.0	-1.6	-14.3	8.1	-9.6
	0	-	10.43	B3LYP/6-31G(d,p)	-4.9	-1.6	-5.8	8.7	-6.1
	0	-	3.77	B3LYP/6-31G(d,p)	-5.5	-6.0	-52.5	29.5	-37.8
	0	-	5.27	B3LYP/6-31G(d,p)	-1.1	-2.3	-25.3	15.0	-15.6
	0	-x, y+1/2, -z+1/2	10.46	B3LYP/6-31G(d,p)	-3.0	-1.1	-7.7	4.9	-7.7
	0	-	10.52	B3LYP/6-31G(d,p)	-57.8	-15.6	-9.0	57.3	-45.1
	0	-	9.98	B3LYP/6-31G(d,p)	-3.6	-1.5	-4.6	2.3	-7.6
	1	-x, -y, -z	6.05	B3LYP/6-31G(d,p)	-4.6	-0.8	-14.8	9.0	-12.9

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	1	-	6.19	B3LYP/6-31G(d,p)	-1.0	-1.6	-14.3	8.1	-9.6
	1	-x, -y, -z	3.64	B3LYP/6-31G(d,p)	-17.1	-1.5	-40.8	25.6	-38.9
	2	-x, y+1/2, -z+1/2	9.65	B3LYP/6-31G(d,p)	-2.1	-1.8	-3.4	1.4	-5.6
	1	-	10.43	B3LYP/6-31G(d,p)	-4.9	-1.6	-5.8	8.7	-6.1
	2	x, -y+1/2, z+1/2	9.97	B3LYP/6-31G(d,p)	-33.9	-8.2	-5.3	30.6	-27.6
	1	-	3.77	B3LYP/6-31G(d,p)	-5.5	-6.0	-52.5	29.5	-37.8
	1	-x, -y, -z	5.79	B3LYP/6-31G(d,p)	-12.8	-0.7	-18.0	16.5	-19.5
	1	-	10.52	B3LYP/6-31G(d,p)	-57.8	-15.6	-9.0	57.3	-45.1
	1	-	5.27	B3LYP/6-31G(d,p)	-1.1	-2.3	-25.3	15.0	-15.6
	1	-	9.98	B3LYP/6-31G(d,p)	-3.6	-1.5	-4.6	2.3	-7.6

Table S15. Overall Energy Profile for Co-crystal 6a.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	9.17	B3LYP/6-31G(d,p)	0.0	-1.2	0.0	0.0	-0.9
	0	-	4.73	B3LYP/6-31G(d,p)	-7.3	-2.2	-27.2	15.0	-23.7
	0	-	9.30	B3LYP/6-31G(d,p)	-0.1	-0.5	-5.8	2.3	-4.2
	0	-x, -y, -z	5.34	B3LYP/6-31G(d,p)	0.1	-3.4	-32.5	13.7	-22.2
	0	-	7.20	B3LYP/6-31G(d,p)	0.0	-0.2	-0.3	0.0	-0.5
	0	x, y, z	12.22	B3LYP/6-31G(d,p)	0.0	0.0	0.0	0.0	0.0
	0	-x, -y, -z	3.86	B3LYP/6-31G(d,p)	12.5	-8.0	-64.3	25.5	-32.9
	0	-x, -y, -z	11.94	B3LYP/6-31G(d,p)	-1.0	-0.1	-0.9	0.0	-1.9
	0	-	10.57	B3LYP/6-31G(d,p)	-61.7	-16.7	-9.5	58.4	-49.8
	0	-	5.69	B3LYP/6-31G(d,p)	-7.4	-4.1	-24.3	12.4	-24.4
	0	-	6.48	B3LYP/6-31G(d,p)	-0.9	-0.4	-2.3	0.0	-3.2
	0	-	7.50	B3LYP/6-31G(d,p)	-2.6	-1.1	-10.0	3.0	-10.4
	0	-x, -y, -z	8.78	B3LYP/6-31G(d,p)	-3.6	-0.5	-7.7	2.2	-9.5
	0	-	5.52	B3LYP/6-31G(d,p)	-3.6	-0.5	-7.7	2.2	-9.5
	0	-	5.75	B3LYP/6-31G(d,p)	-2.6	-1.7	-16.4	10.7	-11.7
	0	-x, -y, -z	11.39	B3LYP/6-31G(d,p)	-4.7	-0.4	-5.9	7.7	-5.7
	0	-	6.93	B3LYP/6-31G(d,p)	12.5	-8.0	-64.3	25.5	-32.9
	0	-	10.87	B3LYP/6-31G(d,p)	-6.9	-1.9	-4.4	8.9	-7.1
	1	-	5.28	B3LYP/6-31G(d,p)	-6.9	-1.9	-4.4	8.9	-7.1
	1	-	10.87	B3LYP/6-31G(d,p)	-6.9	-1.9	-4.4	8.9	-7.1

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	2	x, y, z	8.87	B3LYP/6-31G(d,p)	0.6	-0.3	-2.0	0.1	-1.3
	1	-	5.69	B3LYP/6-31G(d,p)	-7.4	-4.1	-24.3	12.4	-24.4
	1	-x, -y, -z	4.32	B3LYP/6-31G(d,p)	-9.6	-2.5	-32.3	15.9	-30.3
	1	-	7.50	B3LYP/6-31G(d,p)	-2.6	-1.1	-10.0	3.0	-10.4
	1	-	4.60	B3LYP/6-31G(d,p)	-2.6	-1.1	-10.0	3.0	-10.4
	1	-	9.17	B3LYP/6-31G(d,p)	-2.0	-1.2	-8.8	5.0	-7.6
	1	-x, -y, -z	9.17	B3LYP/6-31G(d,p)	-11.7	-4.2	-8.9	10.2	-16.9
	1	-	10.57	B3LYP/6-31G(d,p)	-61.7	-16.7	-9.5	58.4	-49.8
	1	-	9.30	B3LYP/6-31G(d,p)	-0.1	-0.5	-5.8	2.3	-4.2
	1	-	4.76	B3LYP/6-31G(d,p)	-0.1	-0.5	-5.8	2.3	-4.2
	1	-	6.15	B3LYP/6-31G(d,p)	-6.7	-0.6	-0.9	0.0	-8.2
	1	-	5.75	B3LYP/6-31G(d,p)	-2.6	-1.7	-16.4	10.7	-11.7
	1	-	4.73	B3LYP/6-31G(d,p)	-7.3	-2.2	-27.2	15.0	-23.7

Table S16. Overall Energy Profile for Co-crystal 6b.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	7.62	B3LYP/6-31G(d,p)	-2.5	-0.5	-16.6	10.8	-10.7
	0	-	8.04	B3LYP/6-31G(d,p)	-2.0	-1.3	-12.1	7.0	-9.3
	0	x, y, z	3.80	B3LYP/6-31G(d,p)	-1.4	-0.8	-52.1	31.1	-28.3
	0	-	9.05	B3LYP/6-31G(d,p)	-1.4	-1.4	-4.8	2.2	-5.4
	0	-	6.98	B3LYP/6-31G(d,p)	-7.7	-1.5	-21.8	21.6	-14.8
	0	-	8.84	B3LYP/6-31G(d,p)	-55.6	-13.1	-15.8	65.2	-42.0
	0	-	10.27	B3LYP/6-31G(d,p)	-7.2	-2.4	-4.4	6.9	-9.0
	2	x, y, z	3.80	B3LYP/6-31G(d,p)	1.8	-1.7	-46.3	27.7	-22.6
	1	-	7.62	B3LYP/6-31G(d,p)	-2.5	-0.5	-16.6	10.8	-10.7
	2	x, -y+1/2, z+1/2	8.93	B3LYP/6-31G(d,p)	-3.5	-0.8	-6.2	1.8	-8.5
	1	-	6.98	B3LYP/6-31G(d,p)	-7.7	-1.5	-21.8	21.6	-14.8
	2	x, -y+1/2, z+1/2	7.83	B3LYP/6-31G(d,p)	-1.9	-0.7	-9.5	4.6	-7.9
	1	-	8.84	B3LYP/6-31G(d,p)	-55.6	-13.1	-15.8	65.2	-42.0
	1	-x, -y, -z	8.71	B3LYP/6-31G(d,p)	-12.6	-2.3	-8.5	4.8	-19.5
	1	-	9.05	B3LYP/6-31G(d,p)	-1.4	-1.4	-4.8	2.2	-5.4

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	1	-	8.04	B3LYP/6-31G(d,p)	-2.0	-1.3	-12.1	7.0	-9.3
	1	-x, -y, -z	10.02	B3LYP/6-31G(d,p)	-6.2	-0.7	-2.3	0.1	-9.0
	1	-	10.27	B3LYP/6-31G(d,p)	-7.2	-2.4	-4.4	6.9	-9.0

Table S17. Overall Energy Profile for Co-crystal 7.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	6.34	B3LYP/6-31G(d,p)	0.3	-1.1	-12.9	4.8	-8.8
	0	-	10.56	B3LYP/6-31G(d,p)	-4.7	-1.6	-5.6	6.8	-6.8
	0	-	3.90	B3LYP/6-31G(d,p)	-2.3	-2.5	-52.6	25.1	-34.6
	0	-	5.41	B3LYP/6-31G(d,p)	-2.1	-1.5	-24.1	11.6	-17.2
	0	-x, y+1/2, -z+1/2	10.50	B3LYP/6-31G(d,p)	-3.7	-0.8	-8.9	6.4	-8.3
	0	-	10.69	B3LYP/6-31G(d,p)	-59.6	-15.7	-9.1	64.3	-42.9
	0	-	9.85	B3LYP/6-31G(d,p)	-3.8	-1.5	-5.1	1.8	-8.4
	1	-	5.41	B3LYP/6-31G(d,p)	-2.1	-1.5	-24.1	11.6	-17.2
	1	-x, -y, -z	5.94	B3LYP/6-31G(d,p)	-9.3	-0.5	-13.8	9.3	-16.5
	2	x, -y+1/2, z+1/2	10.00	B3LYP/6-31G(d,p)	-33.2	-7.9	-5.1	26.1	-29.2
	1	-	10.69	B3LYP/6-31G(d,p)	-59.5	-15.7	-9.1	64.3	-42.8
	1	-	3.90	B3LYP/6-31G(d,p)	-2.3	-2.5	-52.6	25.1	-34.5
	1	-x, -y, -z	3.72	B3LYP/6-31G(d,p)	-15.9	-1.6	-36.7	18.3	-38.7
	2	-x, y+1/2, -z+1/2	9.63	B3LYP/6-31G(d,p)	-2.2	-1.6	-3.2	1.3	-5.6
	1	-	9.85	B3LYP/6-31G(d,p)	-3.8	-1.5	-5.1	1.8	-8.4
	1	-x, -y, -z	6.28	B3LYP/6-31G(d,p)	-4.1	-0.7	-11.9	5.1	-12.1
	1	-	10.56	B3LYP/6-31G(d,p)	-4.7	-1.6	-5.6	6.8	-6.8
	1	-	6.34	B3LYP/6-31G(d,p)	0.3	-1.1	-12.9	4.8	-8.8

Table S18. Overall Energy Profile for Co-crystal 7a.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	x, y, z	3.87	B3LYP/6-31G(d,p)	1.3	-1.2	-47.9	21.8	-27.7
	0	-	8.09	B3LYP/6-31G(d,p)	0.0	-0.7	0.0	0.0	-0.7
	0	-	7.59	B3LYP/6-31G(d,p)	0.0	0.0	0.0	0.0	0.0
	0	-	6.79	B3LYP/6-31G(d,p)	0.6	-0.0	-0.2	0.0	0.4
	0	-	11.70	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	7.13	B3LYP/6-31G(d,p)	1.3	-1.2	-47.9	21.8	-27.7
	0	-	7.38	B3LYP/6-31G(d,p)	0.0	0.00	0.0	0.0	0.0
	0	-	8.04	B3LYP/6-31G(d,p)	0.0	-1.3	0.0	0.0	-1.3
	1	-x, -y, -z	9.19	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3
	2	x, y, z	3.87	B3LYP/6-31G(d,p)	1.3	-1.2	-47.9	21.8	-27.7
	1	-	7.59	B3LYP/6-31G(d,p)	0.0	0.0	0.0	0.0	0.0
	1	-	8.09	B3LYP/6-31G(d,p)	0.0	0.0	0.0	0.0	0.0
	1	-	6.79	B3LYP/6-31G(d,p)	0.6	-0.0	-0.2	0.0	0.4
	1	-x, -y, -z	7.84	B3LYP/6-31G(d,p)	0.2	-0.0	-0.1	0.0	0.2
	1	-x, -y, -z	8.54	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.0	0.0	-0.2
	1	-	5.72	B3LYP/6-31G(d,p)	0.6	-0.0	-0.2	0.0	0.4
	1	-	4.58	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3
	1	-	7.13	B3LYP/6-31G(d,p)	1.3	-1.2	-47.9	21.8	-27.7
	1	-	11.70	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.1	0.0	-0.3
	1	-	7.59	B3LYP/6-31G(d,p)	0.2	-0.0	-0.1	0.0	0.2
	1	-x, -y, -z	8.57	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.1
	1	-	5.71	B3LYP/6-31G(d,p)	0.2	-0.0	-0.1	0.0	0.2

Table S19. Overall Energy Profile for Co-crystal 7b.

	N	Symop	R	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	0	-	7.62	B3LYP/6-31G(d,p)	-1.5	-0.6	-16.8	10.7	-10.0
	0	-	8.04	B3LYP/6-31G(d,p)	-2.2	-1.4	-12.1	7.0	-9.6
	0	x, y, z	3.80	B3LYP/6-31G(d,p)	0.2	-1.4	-54.7	35.1	-26.8
	0	-	9.05	B3LYP/6-31G(d,p)	-1.5	-1.5	-4.8	2.2	-5.6
	0	-	6.98	B3LYP/6-31G(d,p)	-6.9	-1.7	-22.3	22.5	-14.1
	0	-	8.84	B3LYP/6-31G(d,p)	-56.6	-13.7	-15.8	64.8	-43.7
	0	-	10.27	B3LYP/6-31G(d,p)	-7.4	-2.4	-4.4	7.1	-9.1
	2	x, y, z	3.80	B3LYP/6-31G(d,p)	1.7	-1.8	-46.5	28.1	-22.7
	1	-	7.62	B3LYP/6-31G(d,p)	-1.5	-0.6	-16.8	10.7	-10.0
	2	x, -y+1/2, z+1/2	8.93	B3LYP/6-31G(d,p)	-3.4	-0.8	-6.1	1.8	-8.4
	1	-	6.98	B3LYP/6-31G(d,p)	-6.9	-1.7	-22.3	22.5	-14.1

	2	x, -y+1/2, z+1/2	7.83	B3LYP/6-31G(d,p)	-1.9	-0.7	-9.5	4.8	-7.9
	1	-	8.84	B3LYP/6-31G(d,p)	-56.6	-13.7	-15.8	64.8	-43.7
	1	-x, -y, -z	8.71	B3LYP/6-31G(d,p)	-12.6	-2.3	-8.5	4.7	-19.5
	1	-	9.05	B3LYP/6-31G(d,p)	-1.5	-1.5	-4.8	2.2	-5.6
	1	-	8.04	B3LYP/6-31G(d,p)	-2.2	-1.4	-12.1	7.0	-9.6
	1	-x, -y, -z	10.02	B3LYP/6-31G(d,p)	-6.1	-0.7	-2.3	0.1	-8.9
	1	-	10.27	B3LYP/6-31G(d,p)	-7.4	-2.4	-4.4	7.1	-9.1