Supporting Information

Recurrent supramolecular motifs in discrete complexes and coordination polymers based on mercury halides: prevalence of chelate ring stacking and substituent effects

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1. Table S1-S2

Table S1: Distances (Å) of the coordination bonds in compounds **1**–**5**

	1	**2**	**3**	**4**	**5**
Hg1-N1	2.378(6)	2.470(12)	2.427(4)	2.480(17)	2.478(5)
Hg1-N8	2.494(6)	2.267(12)	2.436(4)	2.642(14)	2.303(5)
Hg1-O10	2.628(6)	2.392(9)	2.805(4)	2.759(13)	2.393(4)
Hg1-Br1 (I1)	2.4409(11)	2.460(2)	2.6510(5)	2.6297(16)	2.6272(5)
Hg1-N13	2.420(7)	2.491(12)			2.471(5)
Hg1-Br2 (I2)	2.4829(9)		2.6642(5)	2.6483(15)	
Hg1-Br3	2.9168(11)				
Hg2-Br3	2.5206(10)				
Hg2-Br4	2.4962(9)				
N8-Hg1-Br1 (I1)		163.293)			
N1-Hg1-O10		137.294)			
Br1-Hg1-O10		123.2(3)			

Table S2 Geometric features of the H-bonds in compounds **1**-**5** (distances in Å and angles in degrees

D	H	A	D-H	H···A	D···A	D-H···A
1						
C3	H3	Br3^{i}	0.95	2.77	3.705(9)	168
C5	H5	Br4^{ii}	0.95	2.91	3.600(8)	131
C71	H71B	Br1^{iii}	0.98	3.09	3.683	121
C71	H71C	Br2^{iv}	0.98	2.91	3.865(9)	164
N9	H9	Br4^{v}	0.88	3.04	3.573(6)	121
2						
C15	H15	Br1^{vi}	0.93	2.94	3.694(19)	139
3						
N9	H9	N13^{vii}	0.86	2.25	2.875(6)	129
C3	H3	I2^{viii}	0.93	3.21	3.972(6)	142
C71	H71B	I2^{ix}	0.96	3.17	4.122	172
C14	H14	I1^{x}	0.93	3.26	3.938(6)	131
C15	H15	I1^{x}	0.93	3.28	3.928(5)	129
4						
N9	H9	O1A	0.86	2.21	2.829(18)	129
O1A	H1A	N13^{xi}	0.84	2.03	2.81(2)	155
C5	H5	I1^{xii}	0.93	3.30	4.18(2)	158
C14	H14	I2^{xi}	0.84	3.12	4.05(2)	177
5						
C2	H2	I1	0.95	3.28	3.918(7)	126
C15	H15	I1^{vi}	0.95	3.03	3.773(6)	136

Symmetry codes: ^{i} 1+x,y,1+z; ^{ii}3/2+x,3/2-y,1/2+z; ^{iii} 1/2-x,1/2+y,1/2-z; ^{iv} 1+x,y,z; ^{v} ½-x,-1/2+y,1/2-z; ^{vi} x,y,-1+z; ^{vii} x,3/2-y,-1/2+z; ^{viii} 1-x,2-y,1-z; ^{ix} 2-x,2-y,1-z; ^{x} 1+x,3/2-y,1/2+z;

2. Figures S1 to S8

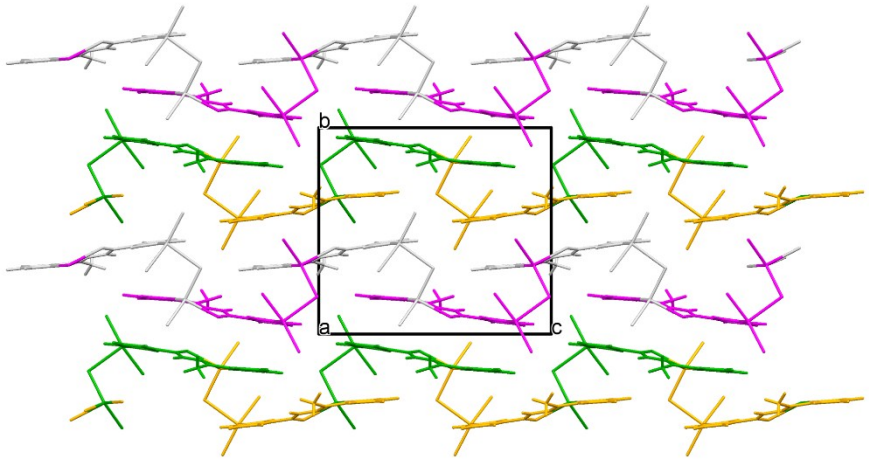
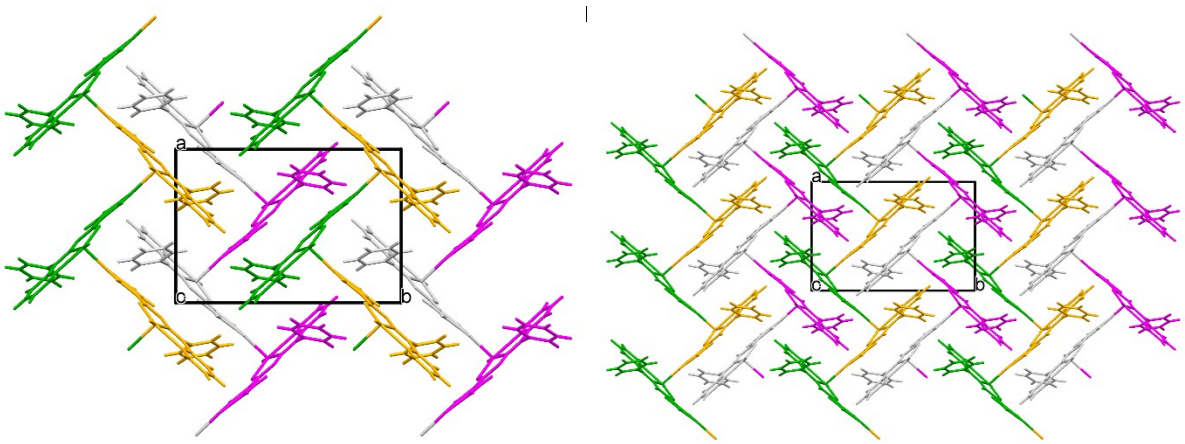


Figure S1. 3D Crystal packing of compound **1**



(a) **(b)**

Figure S2. 3D Crystal packing of compound **2** (la) and **5** (b)

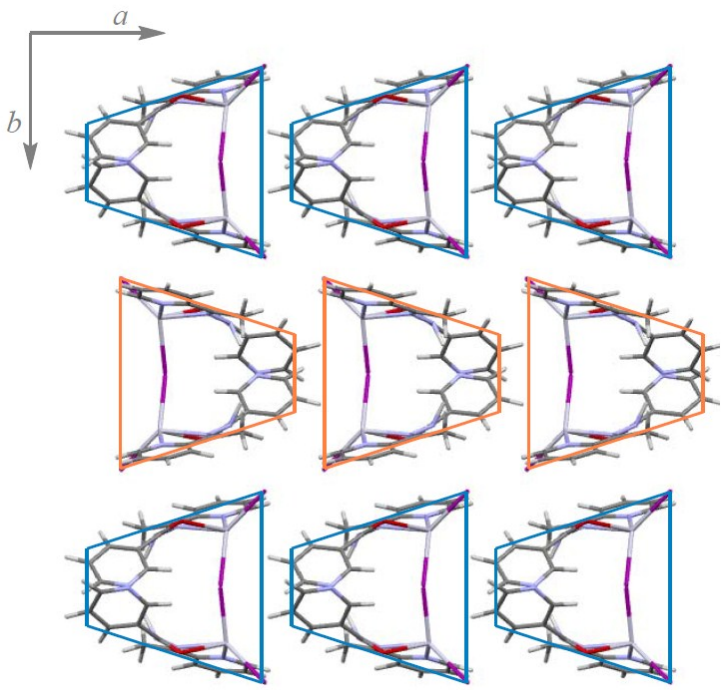


Figure S3. 3D architecture of compound **3** parallel stacking of trapezoidal prisms

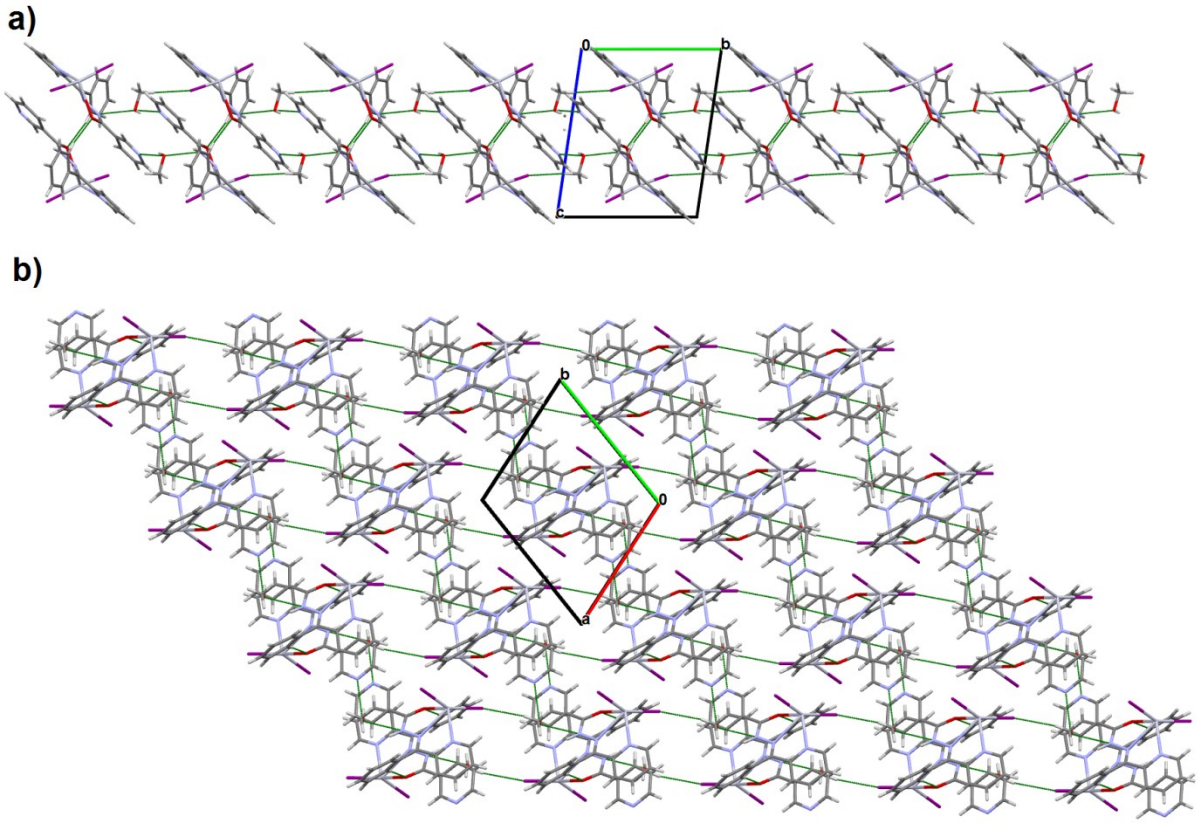


Figure S4. 2D-dimensional network generated by means of C -H···O hydrogen bonds. a) a projection along *a* axis, c) a projection along *c* axis.

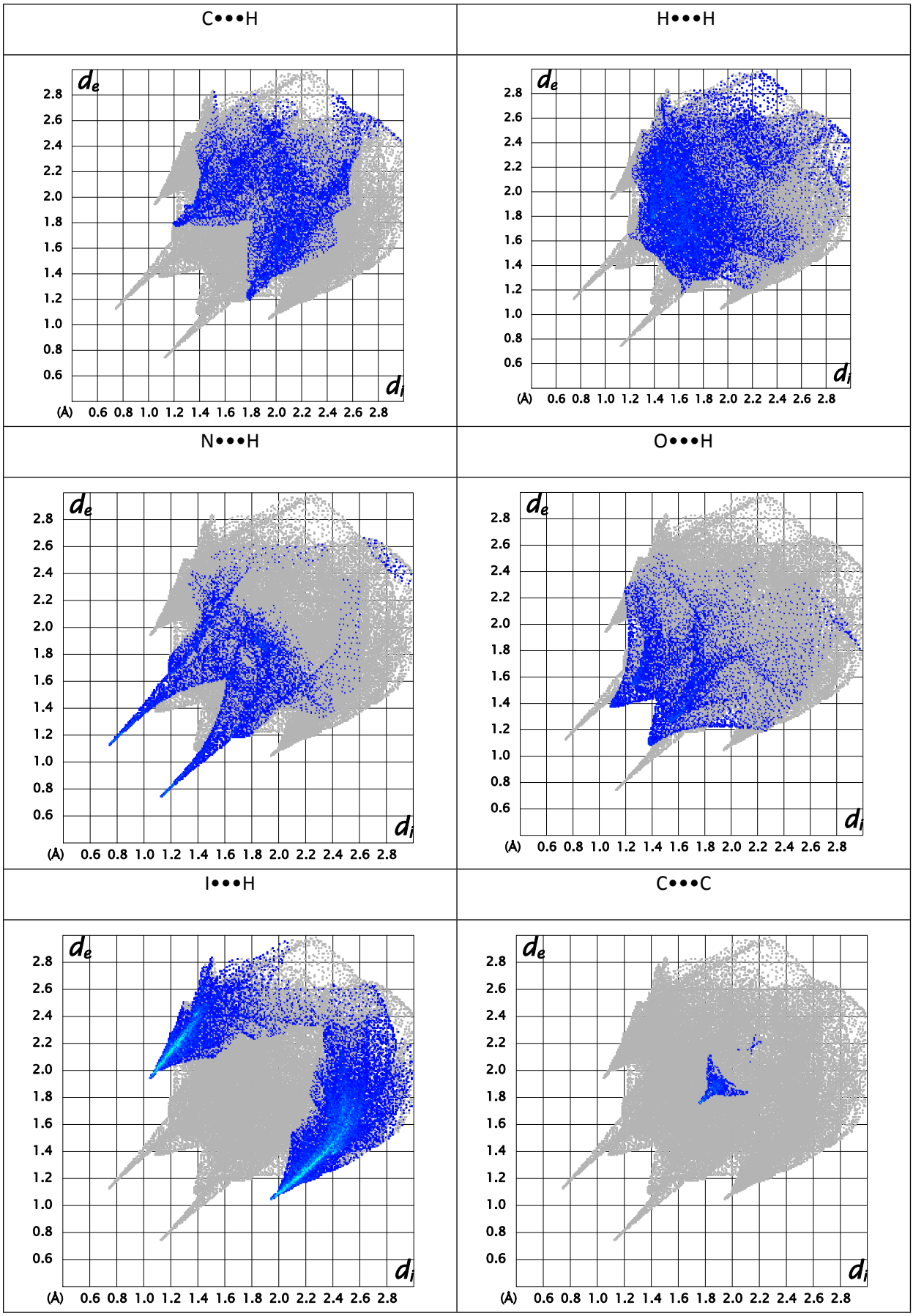


Figure S5. Decomposed fingerprint plots of compound **3**

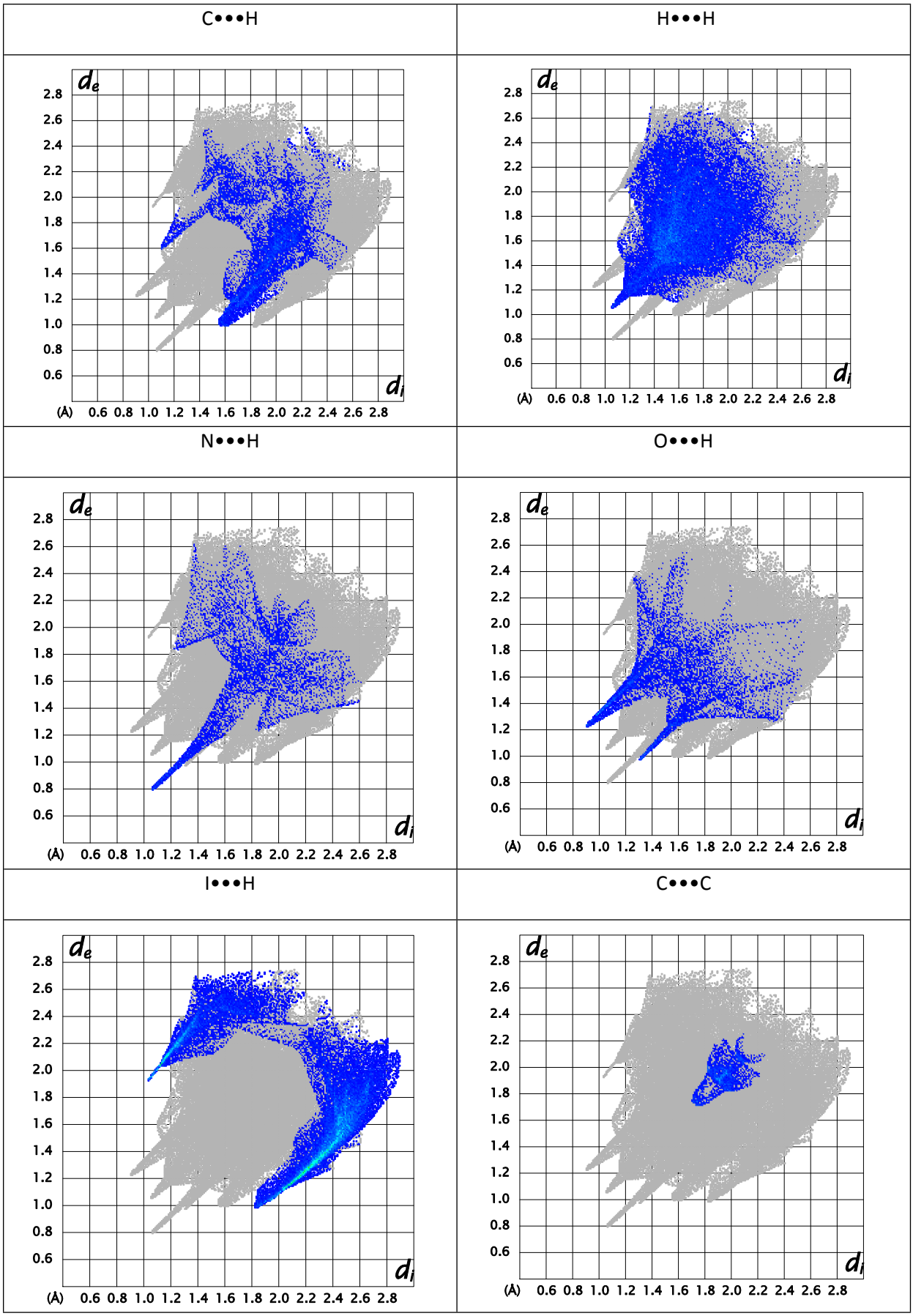


Figure S6. Decomposed fingerprint plots of compound **4**

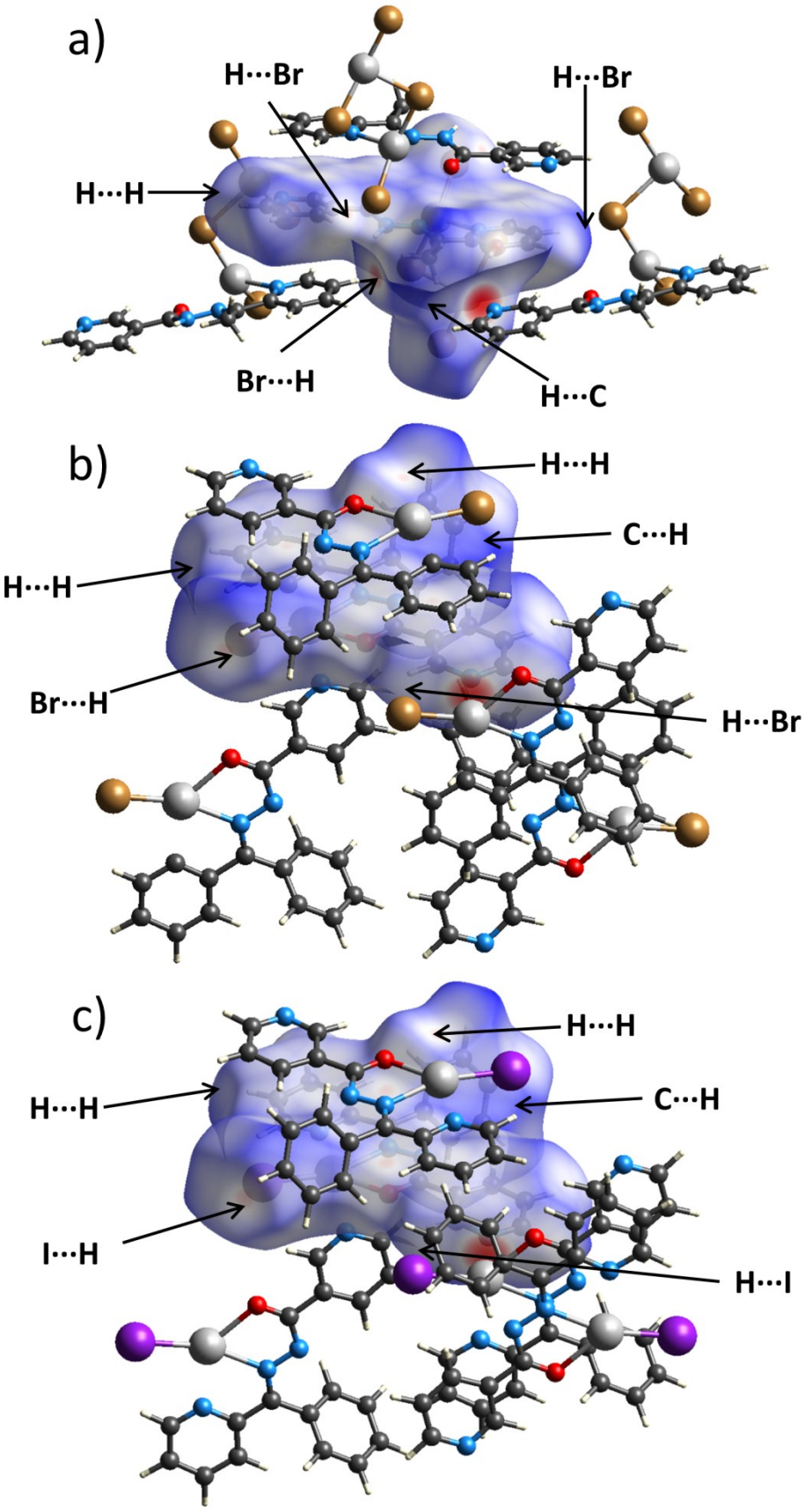


Figure S7. d_{norm}-mapped Hirshfeld surfaces for fragments of coordination polymers a) **1**, b) **2**, and c) **5** with indicated contact sites

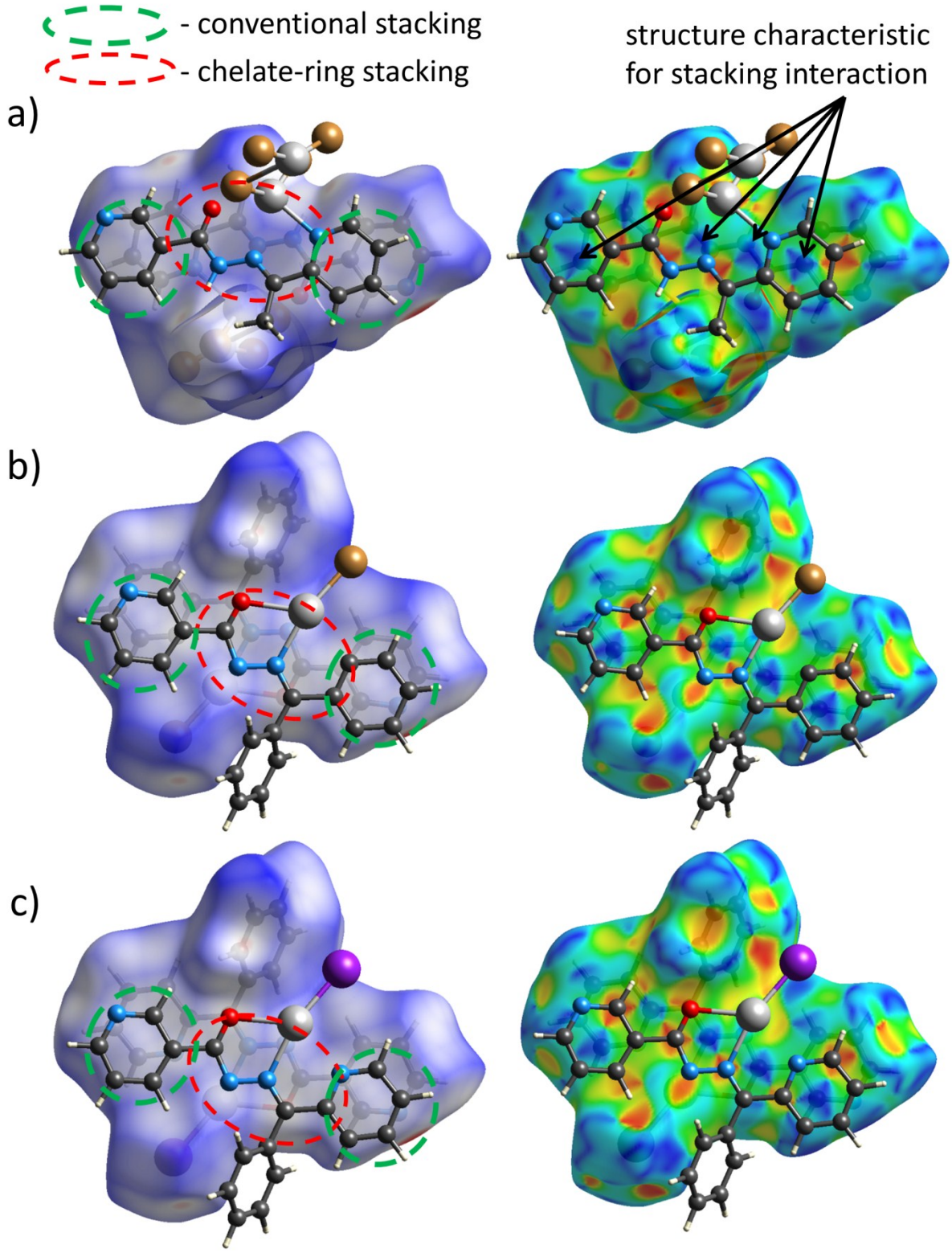


Figure S8. d_{norm}-mapped (left) and shape-index-mapped (right) Hirshfeld surfaces for fragments of coordination polymers a) **1**, b) **2**, and c) **5**.