STRUCTURAL CHEMISTRY

Volume 74 (2018)

Supporting information for article:

Comparison of computationally cheap methods for providing insight into the crystal packing of highly bromomethylated azobenzenes

Christophe M. L. Vande Velde, Matthias Zeller and Vladimir A. Azov

Table S1 Details of lattice energy calculations with CrystalExplorer and CLP-PIXEL (kJ/mol). For packing of molecules with different symmetry elements according to the color codes in the table, see Figures S1-S5.

5		CE/B3LYP 6-311(d,p)					CLP/MP2 6-311(d,p)					CLP/B3LYP 6-311(d,p)				
N	Symop	ele	pol	disp	rep	total	ele	pol	disp	rep	total	ele	pol	disp	rep	total
2	2-x, y+/-1/2, -z+3/2	-25.1	-2.1	-46.3	34.4	-39.0	-26.2	-9.2	-56.1	59.2	-32.2	-25.9	-9.2	-55.9	57.9	-33.1
2	1-x, y+/-1/2, -z+3/2	-30.3	-1.0	-47.4	40.2	-38.5	-30.2	-10.6	-58.9	70.3	-29.4	-29.5	-10.5	-58.7	68.7	-30.1
2	x, y +/-1, z	-16.4	-1.9	-36.8	21.9	-33.1	-17.4	-5.9	-41.9	31.9	-33.3	-17.5	-5.9	-41.7	31.1	-34.0
2	x, 2.5-y, z+/-1/2	-8.5	-1.3	-12.3	8.8	-13.2	-7.0	-1.9	-14.1	15.8	-7.3	-7.1	-1.9	-14.1	15.4	-7.8
1	2-x, 3-y, 2-z	-1.4	-0.2	-6.4	3.5	-4.6	-2.0	-0.6	-6.9	5.5	-4.1	-1.9	-0.6	-6.9	5.3	-4.0
6																
N	Symop	ele	pol	disp	rep	total	ele	pol	disp	rep	total	ele	pol	disp	rep	total
2	x, y+/-1, z;1-x,1-y+/-1;1-z	-26.3	-0.7	-33.3	35.2	-25.1	-27.3	-7.5	-43.0	57.3	-20.5	-27.3	-7.5	-43.0	57.3	-20.5
4	x, y+/-1, z+/-1/2	-14.4	-1.4	-24.6	18.5	-21.8	-13.6	-5.5	-30.2	26.8	-22.4	-13.6	-5.5	-30.2	26.8	-22.4
2	x+/-1/2, y-/+3/2,1-z	-11.8	-1.0	-18.4	11.4	-19.8	-11.6	-3.1	-21.7	16.3	-20.0	-11.6	-3.1	-21.7	16.3	-20.0
2	1-x, y, -z+/-3/2	-1.4	-0.3	-20.0	5.1	-16.6	-1.6	-1.2	-21.0	7.6	-16.3	-1.6	-1.2	-21.0	7.6	-16.3
2	x+/-1/2, y-/+2.5, -z	-7.8	-0.4	-13.2	9.7	-11.7	-6.0	-1.6	-14.4	16.3	-5.7	-6.0	-1.6	-14.4	16.3	-5.7
4	-x+/-1/2, y+/-1/2, -z+/-1/2	-6.4	-0.3	-19.1	15.2	-10.6	-6.7	-2.9	-20.8	24.7	-5.7	-6.7	-2.9	-20.8	24.7	-5.7
7																
N	Symop	ele	pol	disp	rep	total	ele	pol	disp	rep	total	ele	pol	disp	rep	total
1	1-x, 1-y, 1-z	-21.1	-0.1	-64.9	39.9	-46.2	-22.4	-9.4	-66.9	67.5	-31.2	-21.6	-9.3	-66.7	65.1	-32.5
1	1-x, 1-y, -z	-15.3	-0.9	-33.9	19.3	-30.8	-15.5	-4.2	-36.0	32.0	-23.7	-15.8	-4.2	-35.9	31.0	-24.8
2	x, 1/2-y, z+/-1/2	-9.2	-1.7	-26.0	12.5	-24.4	-9.3	-3.9	-29.5	20.6	-22.1	-9.6	-3.9	-29.4	20.2	-22.7
1	2-x, 1-y, 1-z	-23.8	-0.8	-30.2	34.4	-20.5	-25.7	-7.7	-39.6	60.1	-12.9	-24.6	-7.5	-39.6	58.2	-13.5
2	1-x, y+/-1/2, -z+1/2	-11.1	-0.1	-21.2	14.2	-18.2	-11.4	-4.9	-24.6	22.3	-18.6	-11.2	-4.9	-24.5	21.7	-18.9
1	2-x, 1-y, -z	-15.0	-1.0	-14.7	14.7	-16.1	-9.6	-2.8	-17.0	17.6	-11.8	-9.8	-2.9	-16.9	16.9	-12.7
2	x+/-1, y, z	-5.3	-0.7	-21.4	11.4	-16.0	-5.8	-2.9	-25.1	16.7	-17.1	-5.7	-3.0	-25.0	16.5	-17.2
2	x+/-1, -y+1/2, z+/-1/2	-3.9	-0.4	-7.5	5.9	-5.8	-3.7	-1.4	-9.0	9.0	-5.1	-3.7	-1.4	-9.0	8.9	-5.3
8																
N	Symop	ele	pol	disp	rep	total	ele	pol	disp	rep	total	ele	pol	disp	rep	total
2	x-1, y, z; 1-x,y,1-z	-31.7	-1.2	-82.0	55.2	-59.8	-32.7	-12.6	-89.6	88.0	-46.9	-31.4	-12.3	-89.3	84.9	-48.1
2	x, y+/-1, z	-15.7	-1.4	-22.7	18.7	-21.2	-15.5	-4.4	-28.5	26.9	-21.5	-15.7	-4.4	-28.4	26.5	-22
2	-x-/+1, -y, -z	-15.2	-0.3	-24.8	19.4	-20.9	-15.7	-6.7	-32.3	30.6	-24.2	-15.6	-6.8	-32.2	29.9	-24.8
2	-x, -y, -z	-3.3	-2.3	-15.9	8.3	-13.2	-2.8	-1.6	-15.7	11.8	-8.2	-2.9	-1.6	-15.7	11.5	-8.6
2	x+/-1, y+/-1, z	-5.1	-0.1	-18.2	11.1	-12.4	-5.9	-2.4	-20.9	15.8	-13.5	-5.7	-2.5	-20.9	15.6	-13.5
2	x-/+1, y-/+1, z+/-1	-0.5	-0.1	-5.9	1.8	-4.8	0.0	-0.3	-6.0	2.8	-3.4	0.1	-0.4	-5.9	2.8	-3.5

9

N	Symop	ele	pol	disp	rep	total	ele	pol	disp	rep	total	ele	pol	disp	rep	total
1	2-x, 1-y, 1-z	-24.6	-1.3	-71.9	39.6	-58.2	-24.8	-7.4	-74.7	64.5	-42.5	-24.7	-7.2	-74.5	62.3	-44.2
1	1-x, 1-y, 1-z	-21.6	-0.9	-66.1	34.1	-54.4	-21.5	-6.2	-67.5	59.2	-36.0	-21.2	-6.0	-67.3	56.9	-37.6
1	2-x, 2-y, 1-z	-37.9	-0.8	-46.4	48.8	-36.4	-39.4	-12.0	-61.3	82.1	-30.5	-38.4	-11.6	-61.1	79.3	-31.9
1	1-x, 2-y, 1-z	-38.1	-0.4	-45.1	49.3	-34.3	-38.9	-10.1	-59.0	86.0	-22.0	-37.9	-9.7	-58.9	82.9	-23.6
1	2-x, 1-y, 2-z	-11.9	-0.1	-20.7	14.0	-18.8	-11.3	-3.6	-26.0	19.3	-21.7	-11.6	-3.7	-26.0	18.9	-22.3
2	x, y+/-1, z	-6.4	-0.6	-20.3	13.8	-13.5	-6.8	-3.6	-25.1	20.6	-14.9	-6.7	-3.6	-25.0	20.3	-15.0
1	-x, 1-y, 1-z	-6.0	-0.1	-12.5	6.9	-11.6	-4.0	-1.2	-13.2	11.8	-6.6	-4.0	-1.2	-13.2	11.5	-6.9
2	x+/-1, y, z+/-1	0.1	-0.1	-11.4	6.1	-5.3	-	-	-	-	-	0.0	-1.0	-11.7	9.6	-3.0

Table S2 Details of intermolecular contacts (< VdW radius + 0.2Å) correlated to the calculated intermolecular energies for compound **5**

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, -1/2+y, 3/2-z			-39.0	-32.2	-33.1
A-X···Y-B	**In Fig.1**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br2···Br3-C17	A	3.5707(8)	149.48(10)	76.9(1)	
C7-Br2···C17-C14		3.668(3)	121.31(11)	109.3(2)	
C7-Br2···H17B-C17	B	3.00	112	126	
C11-N2···H16-C16		2.88	118	160	
C4-C3···H15-C15		3.02	86.47	151	
Br3-C17···Br2-C7		3.738(3)	135.55(14)	112.75(11)	
C17-H17B···Br2-C7		3.23	114	102	
Cg(2)···Cg(1)		5.053(2)			73.25(16)
Cg(1)···Cg(2)		4.976(2)			73.25(16)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, -1/2+y, 3/2-z			-38.5	-29.4	-30.1
A-X···Y-B	**In Fig.1**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br1···Br3-C17		3.8719(9)	73.1(1)	147.80(10)	
C17-Br3···Br1-C7	C	3.4764(8)	80.79(11)	156.01(10)	
C12-C13···Br1-C7		3.738(3)	128.1(2)	93.30(11)	
H17B-C17···Br1-C7		3.713(4)	156	125.09(11)	
C5-H5···C13-C12		3.07	147	85	
C6-H6···N1-C1		2.89	161	122	
C6-H6···C11-C16		3.06	131	114	
C6-H6···C12-C13		3.07	131	113	
C7-H7···Br3-C17	D	3.01	136	120	

C13-H13···Br1-C7		3.16	121	83	
C17-H17A···Br1-C7		3.24	111	115	
Cg(1)···Cg(2)		5.066(2)			73.25(16)
Cg(2)···Cg(1)		4.989(2)			73.25(16)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, -1+y, z			-33.1	-33.3	-34.0
A-X···Y-B	**In Fig.1**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-H7···Br1-C7	E	2.95	152	134	
C17-H17A···Br3-C17		3.11	170	119	
Cg(1)···Cg(1)		5.283(2)			0.02(16)
Cg(2)···Cg(2)		5.283(2)			0.02(16)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, 5/2-y, -1/2+z			-13.2	-7.3	-7.8
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C17-Br3···Br1-C7		3.7194(10)	146.50(10)	140.91(10)	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x,3-y,2-z			-4.6	-4.1	-4.0
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, 2-y, 1-z			>-4.0		
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C17-Br3···Br3-C17		3.7334(10)	132.98(10)	132.98(10)	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 1-y, 2-z			>-4.0		

A-X···Y-B	**In Fig.1**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br2···Br2-C7	F	3.6306(10)	125.68(10)	125.68(10)	

Cg(1): 0.695880(16), 0.7507(3), 0.84298(4); Cg(2): 0.80638(16), 0.7645(3), 0.69903(4)

Table S3 Details of intermolecular contacts (< VdW radius + 0.2Å) correlated to the calculated intermolecular energies for compound **6**

Symm code	**In Fig. 2.**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, y-1, z; 1-x, 1-y, 1-z			-25.1	-20.5	-20.5
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7- Br2···N1-C1	A	3.201(2)	166.40(9)	104.62(14)	
C7- Br2···C6-C5		3.7160(19)	153.97(9)	136.78(17)	
C7-Br2···H6-C6		3.21	147	115	
C7-Br2···C2-C1		3.662(3)	121.73(8)	100.67(16)	
C7-Br2···H2-C2	B	3.01	123	127	
Cg(1)···Cg(1)		5.6621(16)			0.03(11)
Symm code	**In Fig 2.**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, 1-y, -1/2+z			-21.8	-22.4	-22.4
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br1···H5-C5		3.11	92	158	
C7-Br1···H7-C7	C	3.03	108	169	
C1-C2···Br2-C7		3.705(3)	127.89(14)	97.63(8)	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1/2-x, 3/2-y, 1-z			-19.8	-20.0	-20.0
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br1···H6-C6		3.17	102	129	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, y, 3/2-z			-16.6	-16.3	-16.3

A-X···Y-B	**D(X···Y) (Å)**			**Interplane angle (°)**
Cg(1)···Cg(1)	4.8661(16)			49.90(11)

Symm code	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1/2-x, 5/2-y, 1-z		-11.7	-5.7	-5.7

Symm code	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1/2-x, -1/2+y, 1/2-z		-10.6	-5.7	-5.7

A-X···Y-B	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**A-X···π (°)**
C7-Br1···C1-N1	3.572(2)	159.36(8)	103.16(11)	
C7-Br1···C2-H2	3.728(3)	138.01(8)	110	
C7-Br1···C6-H6	3.613(3)	166.28(7)	106	
C7-Br1···Br1-C7	3.8090(7)	113.00(8)	132.34(5)	
C7-Br1···Cg(1)	3.4931(11)	147.35(6)		65.29

Cg(1): 0.39966(5), 0.72502(8), 0.50313(11)

Table S4 Details of intermolecular contacts (< VdW radius + 0.2Å) correlated to the calculated intermolecular energies for compound **7**

Symm code	**In Fig. 3**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, 1-y, 1-z			-46.2	-31.2	-32.5
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7- Br1···C17-Br3		3.686(4)	92.3(2)	109.56(17)	
C7- Br1···H17A-C17	A	2.99	94	128	
C2-C1···C12-H12		3.575(4)	100.0(2)	104	
C6-C5···C14-C15		3.518(5)	94.46(22)	91.75(22)	
C5-C6···C12-C13		3.547(4)	97.70(22)	84.57(20)	
Cg(1) ···Cg(2)		3.942(2)			6.79(15)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, 1-y, -z			-30.8	-23.7	-24.8
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C4···C6		3.565(4)			
Cg(1)···Cg(1)		3.8138(18)			0.03(14)
Symm code	**In Fig. 3**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, 1/2-y, -1/2+z			-24.4	-22.1	-22.7
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C1-N1···H14-C14		2.91	113	130	
N1-N2···C15-C16		3.415(4)	92.54(19)	155.6(3)	
C11-N2···H15-C15	B	2.71	106	131	
C3-C2···H15-C15		3.10	129	142	
C16-C11···H14-C14		2.98	115	130	

C13-C12···H14-C14		3.10	119	130	
Cg(1)···Cg(2)		5.745(2)			83.23(15)
Cg(2)···Cg(2)		5.3955(19)			84.74(15)
Symm code	**In Fig. 3**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 1-y, 1-z			-20.5	-12.9	-13.5
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C7-Br1···N2-N1	C	3.122(3)	165.86(11)	120.9(2)	
C7-Br1···C16-C15		3.714(4)	127.32(11)	138.7(2)	
C7-Br1···H2-C2		3.23	147	118	
C7-Br1···H16-C16		3.24	122	113	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, -1/2+y, 1/2-z			-18.2	-18.6	-18.9
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C17-Br3···H7-C7		3.22	118	134	
C15-C14···H4-C4		2.90	95	144	
C14-C15···H5-C5		2.93	105	135	
C11-C16···H5-C5		2.97	106	153	
Cg(2)···Cg(1)		5.091(2)			83.23(15)
Symm code	**In Fig. 3**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 1-y, -z			-16.1	-11.8	-12.7
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br2···H7-C7	D	2.91	103	145	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1+x, y, z			-16.0	-17.1	-17.2

A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br1···H12-C12		3.18	106	157	
Symm code	**In Fig. 3**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
-1+x, 1/2-y, -1/2+z			-5.8	-5.1	-5.3
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C17-Br3···C16-C11		3.714(3)	151.37(13)	145.8(2)	
C17-Br3···H16-C16		3.15	154	120	
C17-Br3···Br2-C7	E	3.5193(7)	97.34(9)	160.33(9)	

Cg(1): 0.60752(16), 0.53632(8), 0.18618(12), Cg(2): 0.46735(17), 0.29448(8), 0.58415(12)

Table S5 Details of intermolecular contacts (< VdW radius + 0.2Å) correlated to the calculated intermolecular energies for compound **8**

Symm code	**In Fig. 4**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x-1, y, z / 1-x, y, 1-z			-59.8	-46.9	-48.1
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7- Br2···H7-C7	A	2.91	112	152	
C5-N1···C2-C1		3.419(4)	77.49(15)	97.95(16)	
C5-N1···C3-C2		3.280(4)	90.86(16)	83.55(17)	
C4-C5···C2-C1		3.408(4)	108.00(19)	108.65(19)	
C6-C5···C3-C4		3.597(4)	108.33(19)	115.32(19)	
C1-C6···C2-C3		3.578(4)	115.37(19)	109.0(2)	
C3-C4···C6-C1		3.596(4)	109.6(2)	109.55(19)	
N1-C5…C5-N1	B	3.369(4)	91.66(17)	91.66(17)	
C6-C5···C6-H6		3.581(4)	109.98(18)	102	
Cg(1) ···Cg(1)		4.899(3)			0.03(14)
Cg(1) ···Cg(1)		4.263(2)			0.03(14)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, -1+y, z			-21.2	-21.5	-22
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C2-C3···Br1-C7		3.747(4)	145.5(2)	103.19(10)	
C3-H3···Br1-C7		3.12	125	94	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, -y, -z			-20.9	-24.2	-24.8

A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C7-Br2···H3-C3		3.14	91	130	
C3-C2···H2-C2		2.99	122	129	
C2-H2···H2-C2		2.50	112	112	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
-x, -y, -z			-13.2	-8.2	-8.6
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C7-Br2···C3-C2		3.687(3)	142.74(11)	99.53(17)	
Cg(1)···Cg(1)		5.941(3)			0.03(14)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
-1+x, -1+y, z			-12.4	-13.5	-13.5
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C4-H4···Br1-C7		3.19	145	122	
Symm code	**In Fig. 4**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
-1+x, -1+y, 1+z			-4.8	-3.4	-3.5
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 1-y, -z			>-4.0		
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C7-Br1···Br1-C7	C	3.5936(15)	141.66(9)	141.66(9)	

Symm code	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
-x, 1-y, -z		>-4.0		
A-X···Y-B	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C7-Br2···Br2-C7	3.7057(16)	151.92(10)	151.92(10)	

Table S6 Details of intermolecular contacts (< VdW radius + 0.2Å) correlated to the calculated intermolecular energies for compound 9

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 1-y, 1-z			-58.2	-42.5	-44.2
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C6-C4···C7-C8		3.430(8)	91.94(34)	92.88(35)	
Cg(2)···Cg(1)		3.778(3)			3.3(3)
Cg(1) ···Cg(2)		3.777(3)			3.3(3)
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, 1-y, 1-z			-54.4	-36.0	-37.6
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	**Interplane angle (°)**
C10-Br4···H6-C6		3.19	91	136	
C4-C6···C14-H14		3.581(8)	105.4(4)	103	
C6-C9···C11-C15		3.542(8)	86.58(33)	99.13(33)	
Cg(1)···Cg(2)		3.724(3)			3.3(3)
Cg(2)···Cg(1)		3.724(3)			3.3(3)
Symm code	**In Fig. 5**	**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 2-y, 1-z			-36.4	-30.5	-31.9
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C3-Br1···N1-N2	A	3.123(5)	162.65(18)	124.1(3)	
C3-Br1···C5-C16		3.622(6)	145.61(19)	139.5(4)	
C3-Br1···C14-C11		3.661(6)	127.81(18)	100.2(3)	
C3-Br1···H5-C5		3.06	143	119	
C3-Br1···H14-C14	B	3.00	131	128	

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1-x, 2-y, 1-z			-34.3	-22.0	-23.6
A-X···Y-B	**In Fig. 5**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C3-Br2···N1-N2	C	3.223(5)	160.56(18)	128.3(3)	
C3-Br2···C5-C16		3.581(6)	148.58(19)	138.0(4)	
C3-Br2···C14-C11		3.720(6)	124.23(18)	105.7(4)	
C3-Br2···H5-C5	D	2.96	146	124	
C3-Br2···H14-C14	E	2.93	126	141	

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
2-x, 1-y, 2-z			-18.8	-21.7	-22.3
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C10-Br5···H8-C8		3.14	92	141	

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
x, 1+y, z			-13.5	-14.9	-15.0
A-X···Y-B	**In Fig. 5**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C3-Br1···H9-C9	F	3.01	87	147	
C10-Br2···H9-C9	G	3.03	87	145	

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
-x, 1-y, 1-z			-11.6	-6.6	-6.9

Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1+x, y, 1+z			-5.3	-	-3.0
A-X···Y-B	**In Fig. 5**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	

C10-Br5···Br3-C3	H	3.6804(12)	161.3(2)	131.29(16)	
Symm code		**Interaction energy (kJ/mol)**	**CE/B3LYP 6-311(d,p)**	**CLP/MP2 6-311(d,p)**	**CLP/B3LYP 6-311(d,p)**
1+x, y, z			>-4.0		
A-X···Y-B		**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C3-Br1···Br2-C3		3.8782(10)	142.33(16)	143.89(16)	
x, y, z-1			>-4.0		
A-X···Y-B	**In Fig. 5**	**D(X···Y) (Å)**	**A(A-X···Y) (°)**	**A(X···Y-B) (°)**	
C3-Br3···Br4-C10	I	3.6593(11)	129.65(16)	136.0(2)	

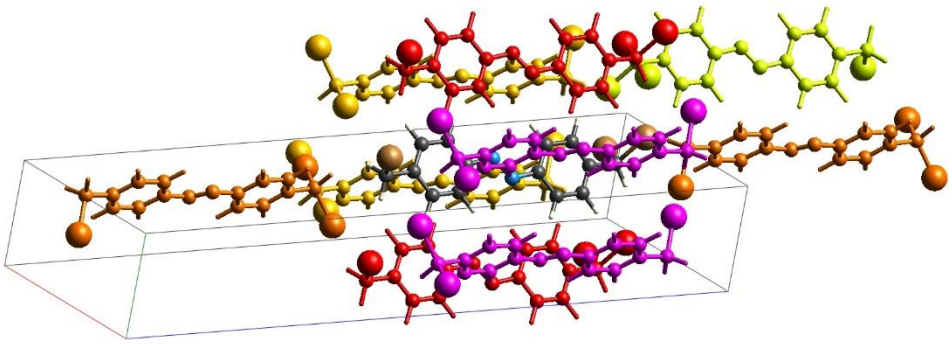

Figure S1 Compound **5**, cluster of molecules with interaction energies over 4.0 kJ/mol in the CE results.

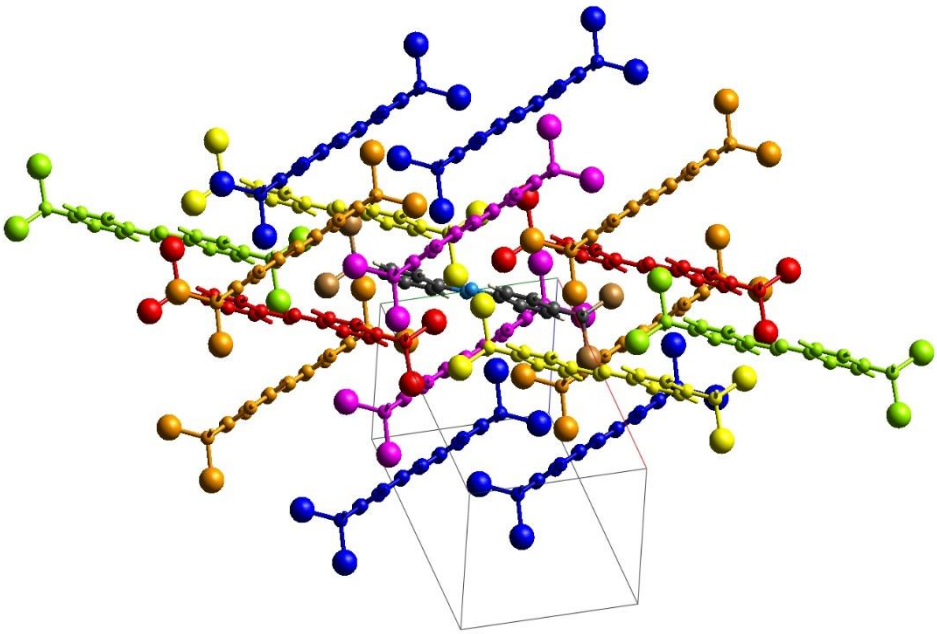

Figure S2 Compound **6**, cluster of molecules with interaction energies over 4.0 kJ/mol in the CE results.

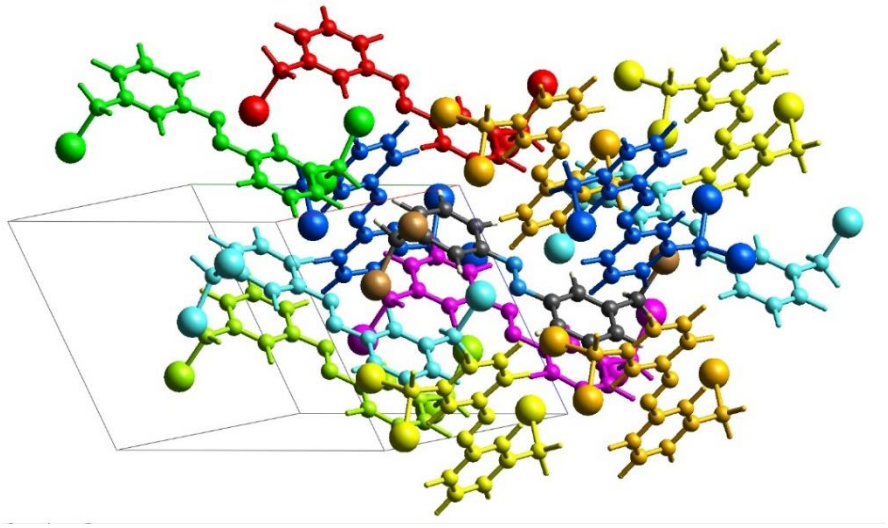

Figure S3 Compound **7**, cluster of molecules with interaction energies over 4.0 kJ/mol in the CE results.

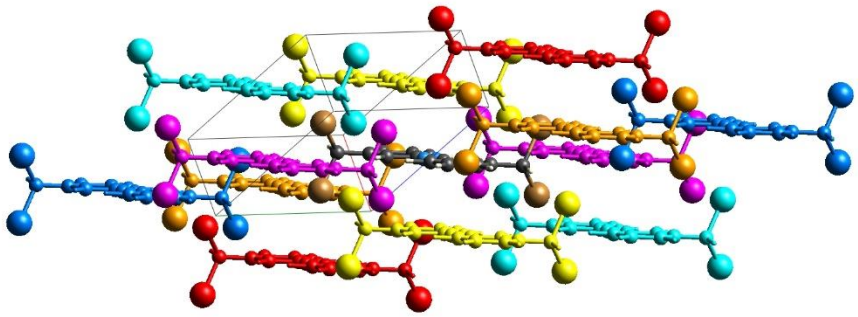

Figure S4 Compound **8**, cluster of molecules with interaction energies over 4.0 kJ/mol in the CE results.

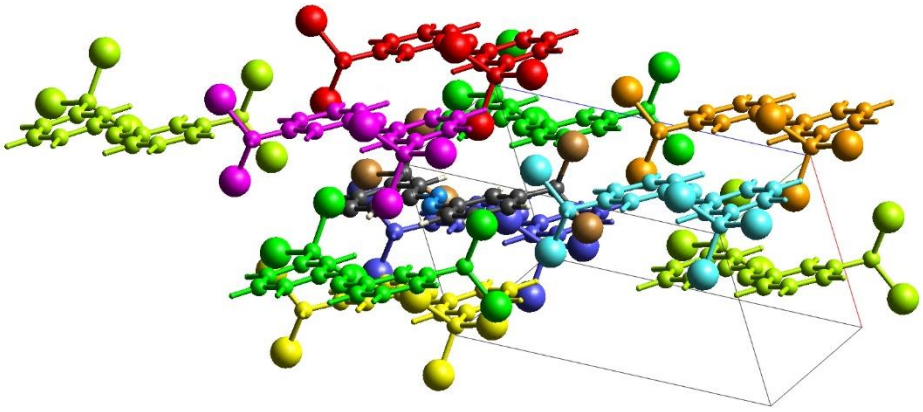

Figure S5 Compound **9**, cluster of molecules with interaction energies over 4.0 kJ/mol in the CE results.

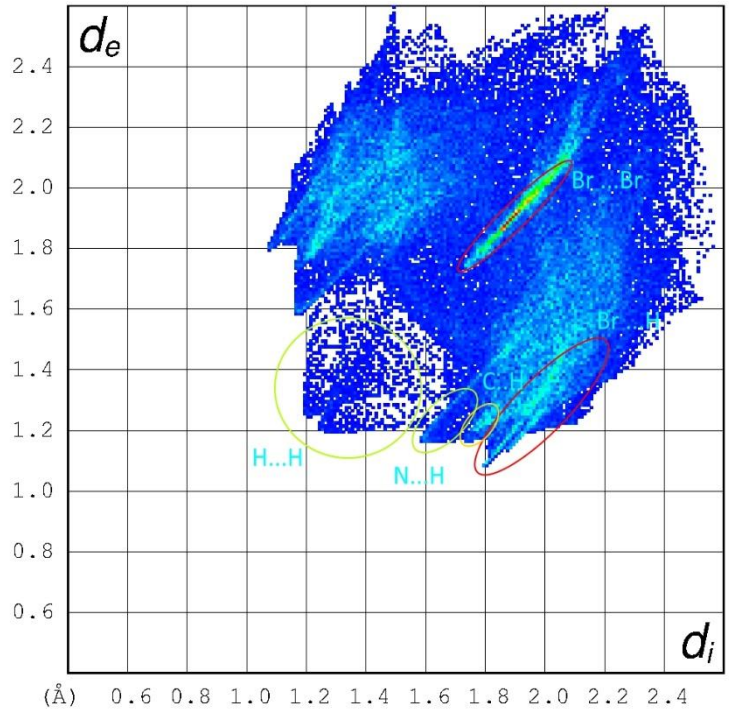

Figure S6 Fingerprint plot for compound **5**. Characteristic regions for specific contacts are designated with ovals.

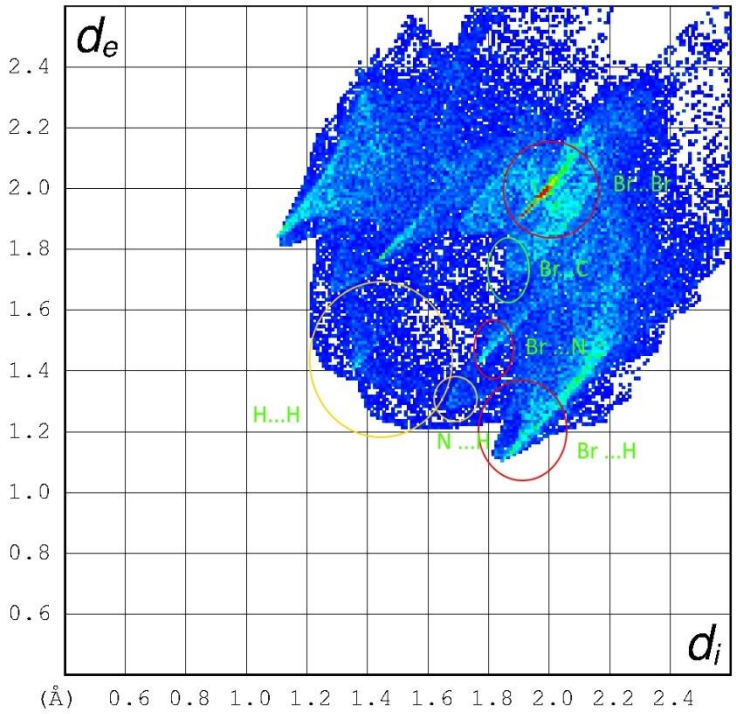

Figure S7 Fingerprint plot for compound 6. Characteristic regions for specific contacts are designated with ovals.

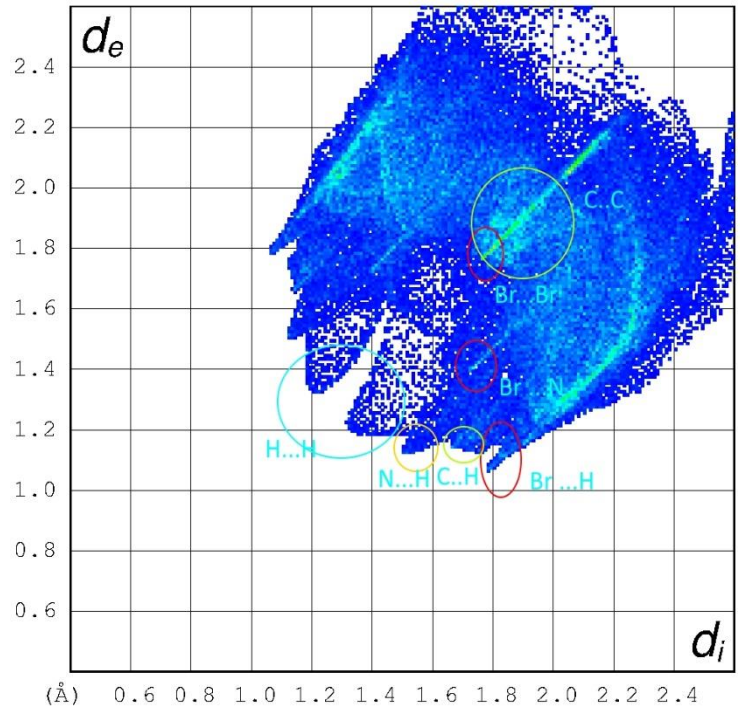

Figure S8 Fingerprint plot for compound **7**. Characteristic regions for specific contacts are designated with ovals.

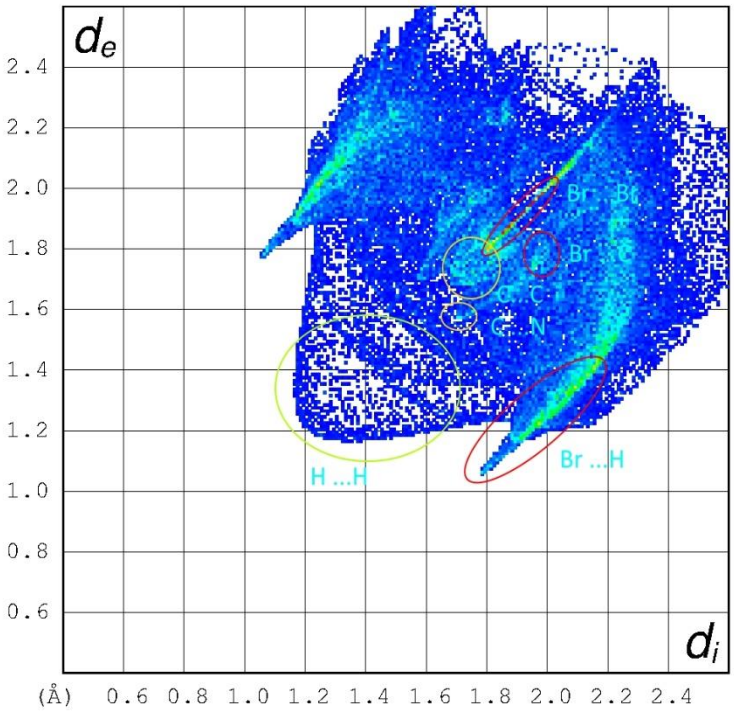

Figure S9 Fingerprint plot for compound **8**. Characteristic regions for specific contacts are designated with ovals.

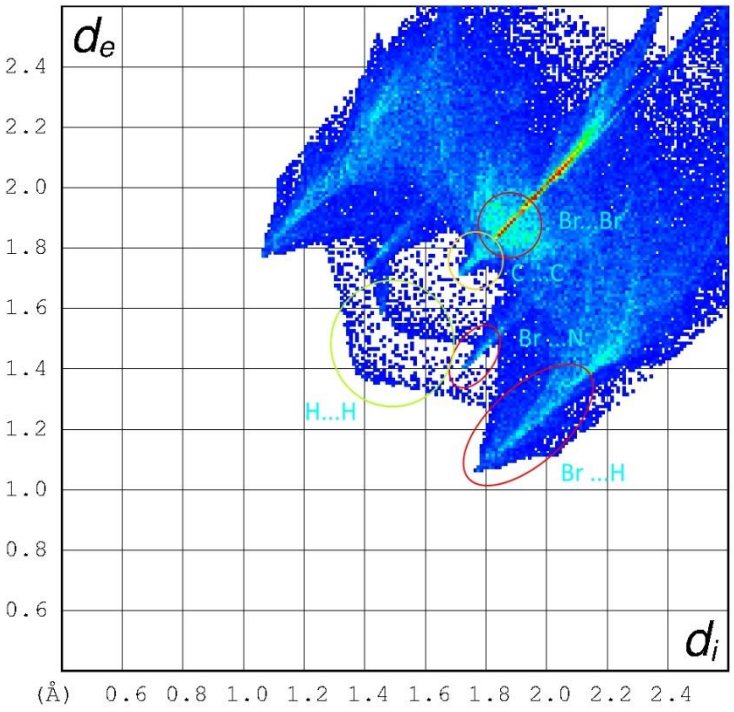

Figure S10 Fingerprint plot for compound **9**. Characteristic regions for specific contacts are designated with ovals.

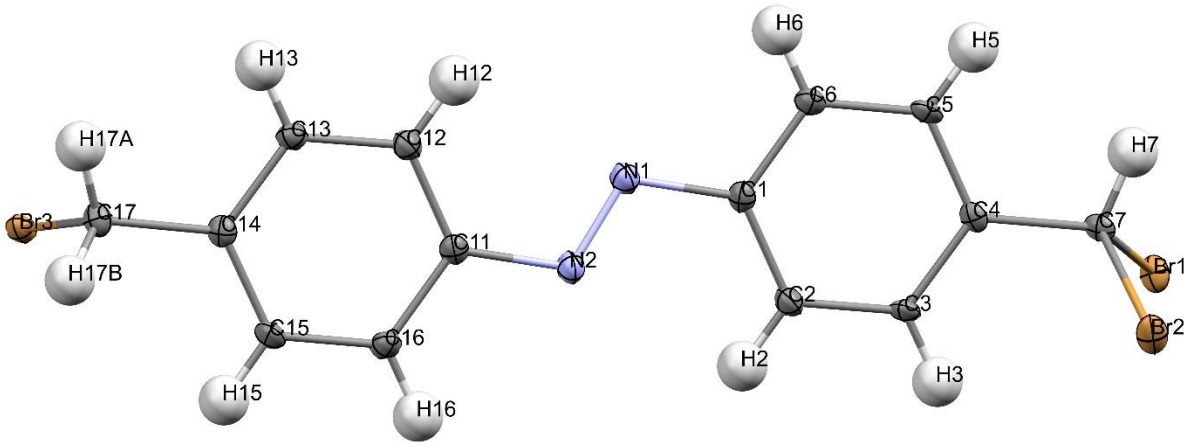

Figure S11 ORTEP plot of **5**, with displacements at the 50% probability level. H atoms are represented by spheres of arbitrary radius.

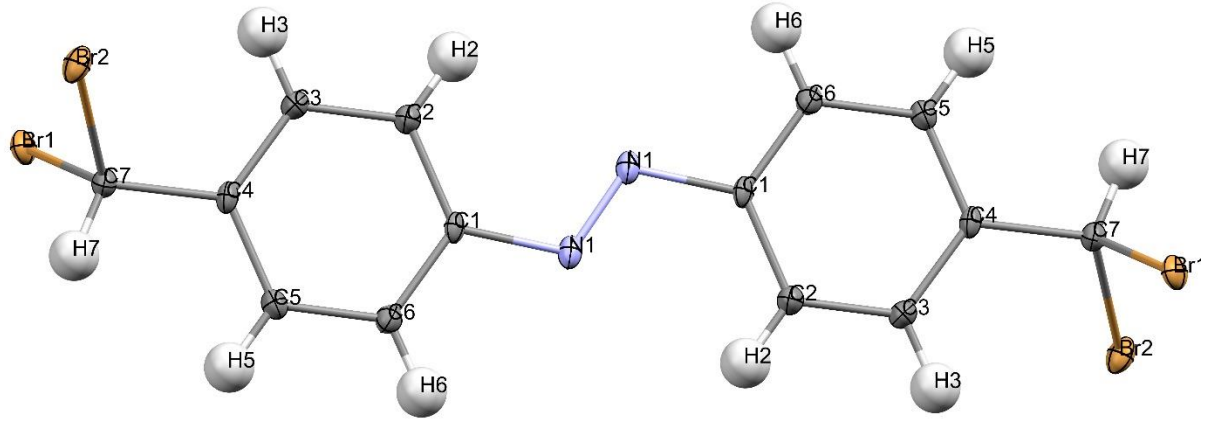

Figure S12 ORTEP plot of **6**, with displacements at the 50% probability level. H atoms are represented by spheres of arbitrary radius.

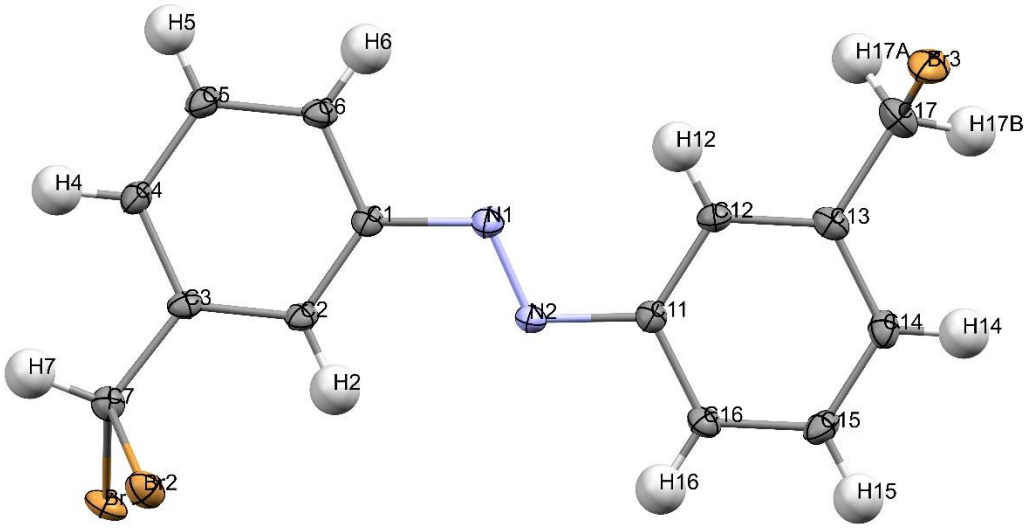

Figure S13 ORTEP plot of **7**, with displacements at the 50% probability level. H atoms are represented by spheres of arbitrary radius.

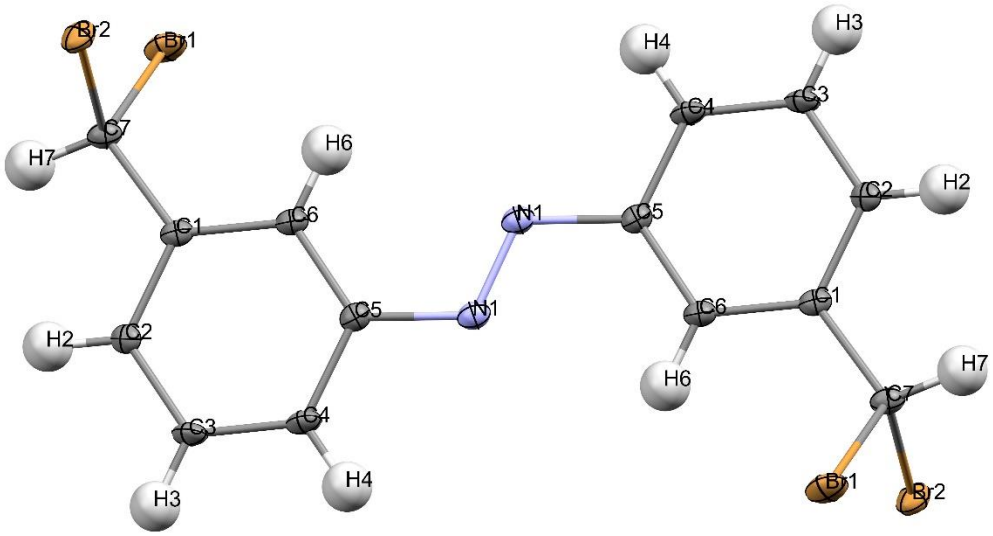

Figure S14 ORTEP plot of **8**, with displacements at the 50% probability level. H atoms are represented by spheres of arbitrary radius.

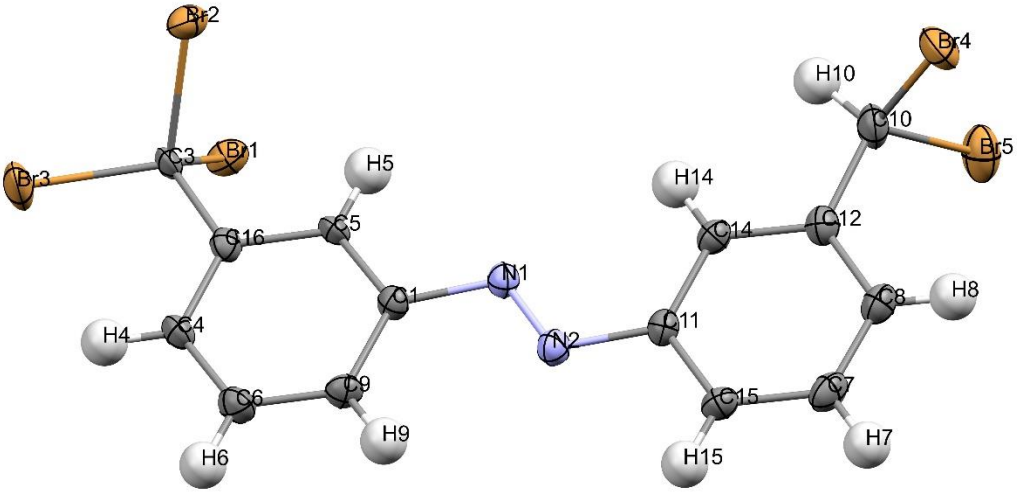

Figure S15 ORTEP plot of **9**, with displacements at the 50% probability level. H atoms are represented by spheres of arbitrary radius.