Electronic Supporting Information

Supramolecular architecture of molecular crystals possessing shearing mechanical properties: columns versus layers

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Table S1. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **1**. Molecules belonging to the basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	x,-1+y,z	-2.00	4.2	8.842	0.620	C-Cl…Cl	3.651	167.3
2	x,-1+y,1+z	-2.06	4.3	8.826	0.637	C-Cl…Cl	3.594	129.4
3	x,y,-1+z	-1.35	2.8	8.880	0.420	C-Cl…Cl	3.662	128.8
4	x,y,1+z	-1.35	2.8	8.880	0.420	C-Cl…Cl	3.662	168.8
5	x,1+y,-1+z	-2.06	4.3	8.826	0.637	C-Cl…Cl	3.594	170.2
6	x,1+y,z	-2.00	4.2	8.842	0.620	C-Cl…Cl	3.651	128.0
7	-x,-1-y,1-z	-.071	1.5	9.327	0.233			
8	**-x,-y,-z**	**-12.53**	**26.3**	**3.944**	**1.731**	***Stacking***	**3.612**	**0**
9	-x,-y,1-z	-2.05	4.3	8.177	0.586			
10	-x,1-y,-z	-2.39	5.0	8.523	0.714			
11	1-x,-1-y,-z	-1.95	4.1	8.591	0.585			
12	1-x,-y,-1-z	-2.93	6.1	8.126	0.832			
13	**1-x,-y,-z**	**-14.28**	**30.0**	**3.796**	**1.898**	C-H…Cl ***Stacking***	2.992 **3.600**	171 **0**

Table S2. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **2**. Molecules belonging to basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	x,-1+y,-1+z	-1.89	3.6	9.094	0.560	C-Br…Br	3.658	168.8
2	x,-1+y,z	-1.69	3.2	9.062	0.500	C-Br…Br C-H…Br	3.596 3.007	124.6 155
3	x,y,-1+z	-1.84	3.5	9.081	0.544	C-Br…Br	3.626	127.9
4	x,y,1+z	-1.84	3.5	9.081	0.544	C-Br…Br	3.626	170.7
5	x,1+y,z	-1.69	3.2	9.062	0.500	C-Br…Br Br…H-C	3.596 3.007	174.6 155
6	x,1+y,1+z	-1.89	3.6	9.094	0.560	C-Br…Br	3.658	124.4
7	*-x,1-y,-1-z*	-2.10	4.0	8.740	0.597			
8	*-x,2-y,-1-z*	-2.85	5.4	8.184	0.760			
9	***-x,2-y,-z***	**-14.96**	**28.2**	**3.942**	**1.921**	***Stacking***	**3.619**	**0**
10	*-x,3-y,-z*	-0.88	1.7	9.406	0.270			
11	***1-x,2-y,-z***	**-15.35**	**29.0**	**3.944**	**1.972**	***Stacking***	**3.610**	**0**
12	*1-x,2-y,1-z*	-1.19	2.3	9.408	0.365			
13	*1-x,3-y,-z*	-1.98	3.7	8.725	0.562			
14	*1-x,3-y,1-z*	-2.84	5.4	8.198	0.757			

Table S3. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **3**. Molecules belonging to basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	x,-1+y,z	-2.25	3.8	9.611	0.673	C-I…I	3.888	173.4
2	x,-1+y,1+z	-2.01	3.4	9.641	0.604	C-H…I C-I…I	3.165 3.931	150 119.6
3	x,y,-1+z	-2.32	4.0	9.620	0.697	C-I…I	3.967	118.6
4	x,y,1+z	-2.32	4.0	9.620	0.697	C-I…I	3.967	165.1
5	x,1+y,-1+z	-2.01	3.4	9.641	0.604	Cl-I…I I…H-C	3.931 3.165	172.7 150
6	x,1+y,z	-2.25	3.8	9.610	0.673	Cl-I…I	3.888	120.1
7	-x,-1-y,-z	-1.17	2.0	9.810	0.359			
8	-x,-1-y,1-z	-3.07	5.2	8.528	0.816			
9	**-x,-y,-z**	**-16.02**	**27.4**	**4.168**	**2.084**	***Stacking***	**3.764**	**0**
10	-x,-y,1-z	-2.44	4.2	9.264	0.706			
11	1-x,-1-y,-z	-2.46	4.2	9.141	0.702			
12	1-x,-y,-1-z	-3.24	5.5	8.530	0.864			
13	**1-x,-y,-z**	**-15.56**	**26.6**	**4.149**	**2.015**	***Stacking***	**3.797**	**0**
14	1-x,1-y,-1-z	-1.40	2.4	9.959	0.434			

Table S4. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **4**. Molecules belonging to basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	x,-1+y,z	-1.92	3.5	9.427	0.612	C-I…I C-Cl…I	3.798 3.729	116.1 129.8
2	x,-1+y,1+z	-2.01	3.7	9.459	0.644	C-I…Cl C-I…I	3.715 3.825	131.2 173.7
3	x,y,-1+z	-2.04	3.7	9.430	0.650	C-I…I	3.865	164.3
4	x,y,1+z	-2.04	3.7	9.430	0.650	C-I…I	3.865	114.8
5	x,1+y,-1+z	-2.01	3.7	9.459	0.644	C-I…I C-Cl…I	3.825 3.715	115.9 131.0
6	x,1+y,z	-1.92	3.5	9.427	0.612	C-I…Cl C-I…I	3.729 3.798	129.7 170.3
7	1-x,-1-y,2-z	-1.22	2.2	9.695	0.398			
8	**1-x,-y,1-z**	**-14.43**	**26.4**	**3.972**	**1.937**	***Stacking***	**3.598**	**0**
9	1-x,-y,2-z	-2.89	5.3	8.284	0.809			
10	1-x,1-y,1-z	-2.62	4.8	8.934	0.789			
11	2-x,-y,-z	-2.62	4.8	9.067	0.801			
12	**2-x,-y,1-z**	**-14.80**	**27.0**	**4.014**	**2.007**	C-I…C ***Stacking***	3.651 **3.582**	84.6 **0**
13	2-x,1-y,-z	-2.82	5.2	8.316	0.793			
14	2-x,1-y,1-z	-1.42	2.6	9.559	0.459			

Table S5. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **5**. Molecules belonging to basic structural motif are highlighted in bold.

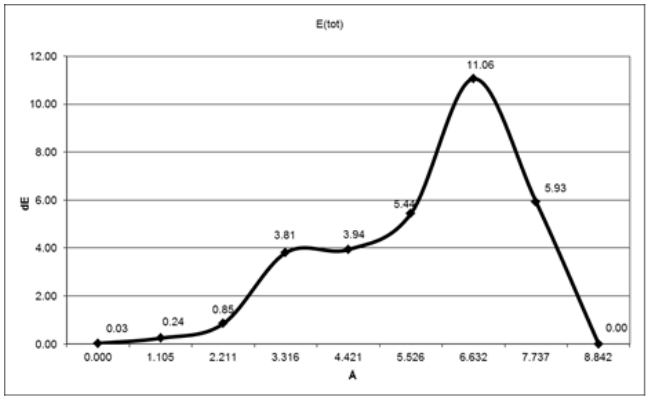
Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	x,-1+y,z	-2.25	3.4	9.496	0.656	C-I…I C-Br…I	3.755 3.782	119.7 125.6
2	x,-1+y,1+z	-4.68	7.0	9.524	1.368	C-I…Br C-I…I	3.795 3.776	126.4 176.6
3	x,y,-1+z	-2.41	3.6	9.512	0.703	C-I…Br C-I…I	3.791 3.798	125.9 170.1
4	x,y,1+z	-2.36	3.5	9.512	0.688	C-I…I C-Br…I	3.798 3.791	119.1 126.0
5	x,1+y,-1+z	-4.70	7.0	9.524	1.372	C-I…I C-Br…I	3.776 3.795	119.7 125.8
6	x,1+y,z	-2.25	3.4	9.496	0.656	C-I…Br C-I…I	3.782 3.755	125.8 174.2
7	1-x,-1-y,2-z	-1.75	2.6	9.764	0.525			
8	**1-x,-y,1-z**	**-16.08**	**24.0**	**4.087**	**2.015**	***Stacking***	**3.658**	**0**
9	1-x,-y,2-z	-3.27	4.9	8.387	0.841			
10	1-x,1-y,1-z	-2.93	4.4	9.061	0.813			
11	2-x,-y,-z	-2.94	4.4	9.123	0.822			
12	**2-x,-y,1-z**	**-16.31**	**24.4**	**4.112**	**2.056**	***Stacking***	**3.663**	**0**
13	2-x,1-y,-z	-3.25	4.9	8.396	0.838			
14	2-x,1-y,1-z	-1.72	2.6	9.701	0.510			

Table S6. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **6**. Molecules belonging to basic structural motif are highlighted in bold.

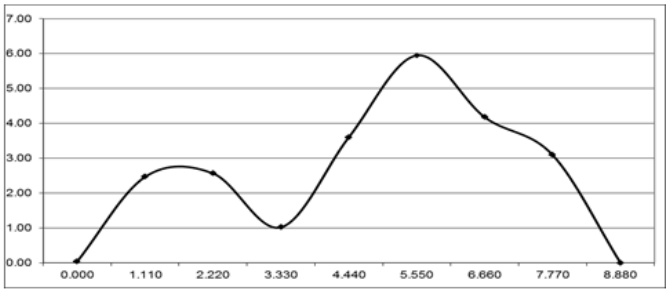
Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	-1+x,y,z	-1.62	3.8	7.967	0.529			
2	-1+x,1+y,z	-1.75	4.1	8.810	0.634			
3	**x,-1+y,z**	**-12.18**	**28.7**	**3.761**	**1.881**	***Stacking***	**3.447**	**0**
4	**x,1+y,z**	**-12.18**	**28.7**	**3.761**	**1.881**	***Stacking***	**3.447**	**0**
5	1+x,-1+y,z	-1.75	4.1	8.810	0.634			
6	1+x,y,z	-1.62	3.8	7.967	0.529			
7	-0.5-x,-0.5+y,-0.5-z	-1.59	3.7	8.408	0.549	C-Cl…Cl	3.444	174.6
8	-0.5-x,-0.5+y,0.5-z	-1.26	3.0	8.701	0.451	C-Cl…Cl	3.470	174.6
9	-0.5-x,0.5+y,-0.5-z	-1.59	3.7	8.408	0.549	C-Cl…Cl	3.444	175.0
10	-0.5-x,0.5+y,0.5-z	-1.26	3.0	8.701	0.451	C-Cl…Cl	3.470	124.4
11	0.5-x,-0.5+y,-0.5-z	-1.26	3.0	8.701	0.451	C-Cl…Cl	3.470	124.4
12	0.5-x,-0.5+y,0.5-z	-1.59	3.7	8.408	0.549	C-Cl…Cl	3.444	175.0
13	0.5-x,0.5+y,-0.5-z	-1.26	3.0	8.701	0.451	C-Cl…Cl	3.470	116.9
14	0.5-x,0.5+y,0.5-z	-1.59	3.7	8.408	0.549	C-Cl…Cl	3.444	116.9

Table S7. Symmetry codes of neighboring molecules for basic molecule located in asymmetric part of unit cell, energy of interaction of basic molecule with neighboring molecule (E_i) and its contribution into total energy of interactions of basic molecule with all molecules belonging to its first coordination sphere (EN_i), distance to geometrical center of basic molecule (R_i) and length of segment of line for visualization of interaction between molecules (L_i) for crystal structure **7**. Molecules belonging to basic structural motif are are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å	Contact	Dist., Å	Angle, deg
1	-1+x,y,-1+z	-2.58	4.6	10.078	2.312	C-Cl…N	3.031	177.5
2	**-1+x,y,z**	**-3.54**	**6.3**	**7.413**	**2.337**			
3	x,y,-1+z	-5.14	9.1	6.827	3.122			
4	x,y,1+z	-5.14	9.1	6.827	3.122			
5	**1+x,y,z**	**-3.54**	**6.3**	**7.413**	**2.337**			
6	1+x,y,1+z	-2.58	4.6	10.078	2.312	C-N…Cl	3.031	176.9
7	**-0.5+x,0.5-y,1-z**	**-5.61**	**10.0**	**6.487**	**3.244**	**C-N…π(C3)**	**3.137**	**141.3**
8	-0.5+x,0.5-y,2-z	-3.22	5.7	8.771	2.516			
9	**0.5+x,0.5-y,1-z**	**-5.61**	**10.0**	**6.487**	**3.244**	**C-N…π(C3)**	**3.137**	**141.3**
10	0.5+x,0.5-y,2-z	-3.22	5.7	8.771	2.516			
11	0.5-x,1-y,-0.5+z	-5.02	8.9	6.426	2.874	C-N…C C-N…C	3.111 3.232	134.2 142.0
12	0.5-x,1-y,0.5+z	-5.02	8.9	6.426	2.874	C…N-C C…N-C	3.111 3.232	134.2 142.0
13	1.5-x,1-y,-0.5+z	-3.02	5.4	8.657	2.331			
14	1.5-x,1-y,0.5+z	-3.02	5.4	8.657	2.331			



Shift along [0 1 0] direction



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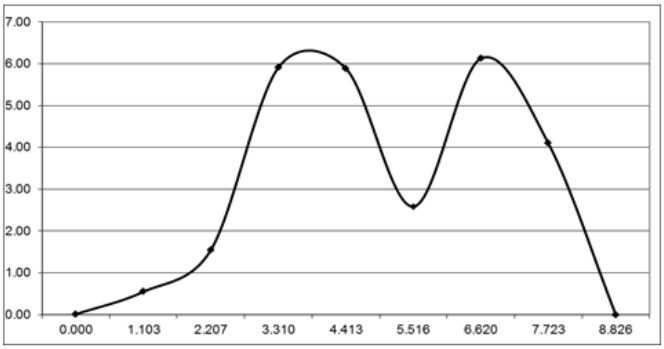

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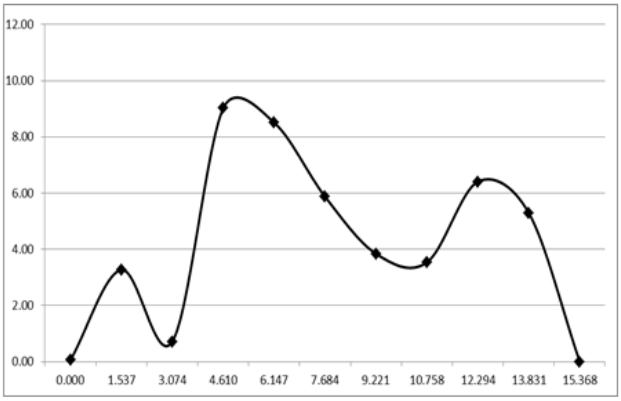

Shift along [0 -1 1] direction

Fig. S1 Change of energy during shift of molecule **2** towards different directions within [1 0 0] crystallographic plane.