Electronic Supplementary Information

Supramolecular architecture of crystals of saturated fused hydrocarbons based on topology of intermolecular interactions

Viktoriya V. Dyakonenko[1], Andrey V. Maleev[2], Oleg V. Shishkin[1,3*,]

[1] STC "Institute for Single Crystals" National Academy of Science of Ukraine, 60 Lenina ave., Kharkiv, 61001, Ukraine

[2] Vladimir State University, 87 Gorky str., Vladimir, 600000, Russian Federation

[3] Department of Inorganic Chemistry, V. N. Karazin Kharkiv National University, 4 Svobody sq., Kharkiv 61077, Ukraine

*. E-mail: shishkin@xray.isc.kharkov.com

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
1	1-x, -y, 1-z	-2,74	10.6	5.905	2.715
2	**-1+x, y, z**	**-2,98**	**11.5**	**5.511**	**2.756**
3	**1+x, y, z**	**-2,98**	**11.5**	**5.511**	**2.756**
4	2-x, -y, 2-z	-2,39	9.3	6.089	2.442
5	0.5+x, 0.5-y, 0.5+z	-2,29	8.9	5.948	2.285
6	-0.5+x, 0.5-y, -0.5+z	-2,29	8.9	5.948	2.285
7	-0.5+x, 0.5-y, 0.5+z	-1.74	6.7	6.718	1.961
8	0.5+x, 0.5-y, -0.5+z	-1.74	6.7	6.718	1.961
9	x, y, -1+z	-2.14	8.3	6.799	2.441
10	x, y, 1+z	-2.14	8.3	6.799	2.441
11	1-x, -y, 2-z	-1.48	5.7	6.432	1.597
12	2-x, -y, 1-z	-0.90	3.5	7.076	1.069

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 the basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å
1	**1-x, -0.5+y, 0.5-z**	**-2.74**	**12.2**	**5.256**	**1.967**
2	**1-x, 0.5+y, 0.5-z**	**-2.74**	**12.2**	**5.256**	**1.967**
3	**2-x, -y, 1-z**	**-3.66**	**16.3**	**4.739**	**2.370**
4	x, -0.5-y, -0.5+z	-1.14	5.1	5.973	0.930
5	x, -0.5-y, 0.5+z	-1.14	5.1	5.973	0.930
6	2-x, -0.5+y, 0.5-z	-1.97	8.8	5.675	1.527
7	2-x, 0.5+y, 0.5-z	-1.97	8.8	5.675	1.527
8	x, 0.5-y, -0.5+z	-1.14	5.1	5.615	0.874
9	x, 0.5-y, 0.5+z	-1.14	5.1	5.615	0.874
10	**x, -1+y, z**	**-1.79**	**8.0**	**5.956**	**1.456**
11	**x, 1+y, z**	**-1.79**	**8.0**	**5.956**	**1.456**
12	1-x, -y, 1-z	-0.84	3.7	6.192	0.711
13	**2-x, -1-y, 1-z**	**-0.40**	**1.8**	**7.061**	**0.386**

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 the basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å
1	-x, -0.5+y, 1.5-z	-2.31	9.0	5.442	1.871
2	-x, 0.5+y, 1.5-z	-2.31	9.0	5.442	1.871
3	**1-x, -y, 2-z**	**-3.36**	**13.1**	**6.082**	**3.041**
4	**1-x, -0.5+y, 1.5-z**	**-3.32**	**12.9**	**5.501**	**2.718**
5	**1-x, 0.5+y, 1.5-z**	**-3.32**	**12.9**	**5.501**	**2.718**
6	**x, -1+y, z**	**-2.37**	**9.2**	**5.940**	**2.095**
7	**x, 1+y, z**	**-2.37**	**9.2**	**5.940**	**2.095**
8	-x, -y, 1-z	-0.98	3.8	6.575	0.959
9	**x, 0.5-y, -0.5+z**	**-1.53**	**5.9**	**6.391**	**1.455**
10	**x, 0.5-y, 0.5+z**	**-1.53**	**5.9**	**6.391**	**1.455**
11	**x, -0.5-y, -0.5+z**	**-0.99**	**3.8**	**6.541**	**0.964**
12	**x, -0.5-y, 0.5+z**	**-0.99**	**3.8**	**6.541**	**0.964**
13	1-x, 1-y, 2-z	-0.36	1.4	8.386	0.449

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 the basic structural motif are highlighted in bold.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å
1	**-1+x, y, z**	**-6.70**	**16.5**	**5.990**	**2.995**
2	**1+x, y, z**	**-6.70**	**16.5**	**5.990**	**2.995**
3	1-x, 1-y, 1-z	-3.63	9.0	8.106	2.196
4	-x, 1-y, 1-z	-2.78	6.9	8.336	1.729
5	-x, -0.5+y, 0.5-z	-3.29	8.1	8.692	2.134
6	-x, 0.5+y, 0.5-z	-3.29	8.1	8.692	2.134
7	1-x, -0.5+y, 0.5-z	-2.72	6.7	9.155	1.858
8	1-x, 0.5+y, 0.5-z	-2.72	6.7	9.155	1.858
9	x, -1+y, z	-1.80	4.4	9.476	1.273
10	x, 1+y, z	-1.80	4.4	9.476	1.273
11	-1+x, 1+y, z	-1.65	4.1	11.211	1.380
12	-x, 2-y, 1-z	-1.79	4.4	11.298	1.509
13	1+x, -1+y, z	-1.65	4.1	11.211	1.380

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 primary and secondary basic structural motifs are highlighted in bold and italic, respectively.

Neighbor	Symmetry code	E_i, kcal/mol	EN_i, %	R_i, Å	L_i, Å
1	***x, 0.5-y, -0.5+z***	***-5.60***	***15.1***	***6.680***	***3.340***
2	***x, 0.5-y, 0.5+z***	***-5.60***	***15.1***	***6.680***	***3.340***
3	*-1-x, -0.5+y, 0.5-z*	*-3.99*	*10.8*	*8.081*	*2.879*
4	*-1-x, 0.5+y, 0.5-z*	*-3.99*	*10.8*	*8.081*	*2.879*
5	*-1-x, 1-y, 1-z*	*-3.28*	*8.9*	*7.516*	*2.201*
6	-x, 1-y, 1-z	-2.32	6.2	8.398	1.740
7	-1+x, y, z	-1.90	5.1	8.904	1.511
8	1+x, y, z	-1.90	5.1	8.904	1.511
9	*-1-x, 1-y, -z*	*-1.59*	*4.3*	*9.384*	*1.332*
10	-x, -0.5+y, 0.5-z	-1.54	4.2	10.482	1.441
11	-x, 0.5+y, 0.5-z	-1.54	4.2	10.482	1.441
12	-1+x, 0.5-y, -0.5+z	-1.47	4.0	9.664	1.268
13	1+x, 0.5-y, 0.5+z	-1.47	4.0	9.664	1.268
14	-x, -y, 1-z	-0.84	2.3	12.076	0.906