Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supporting Information

Role of Different Molecular Fragments in Formation of the Supramolecular Architecture of the Crystal of 1,1-Dioxo-tetrahydro-1λ^6-thiopyran-3-one

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Table S1. Energy of interactions of basic molecule **1** with molecules belonging to its first coordination sphere. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry code	$E_{int.}$, kcal/mol
1-1	-1+x,-1+y,z	-1.93
1-2	-1+x,y,z	-3.85
1-3	**x,-1+y,z**	**-5.79**
1-4	**x,1+y,z**	**-5.79**
1-5	1+x,y,z	-3.85
1-6	1+x,1+y,z	-1.93
1-7	-x,-y,1-z	-6.93
1-8	**1-x,-y,1-z**	**-14.35**
1-9	**1-x,-y,2-z**	**-0.54**
1-10	**1-x,1-y,1-z**	**-7.63**
1-11	**1-x,1-y,2-z**	**-7.57**
1-12	2-x,1-y,2-z	-4.47
1-13	2-x,2-y,2-z	0.61

Table S2. Energy of interactions of basic molecule **2** with molecules belonging to its first coordination sphere. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry code	$E_{int.}$, kcal/mol
2-1	1.5-x,-0.5+y,-z	-2.84
2-2	**1.5-x,-0.5+y,1-z**	**-4.53**
2-3	1.5-x,0.5+y,-z	-2.84
2-4	**1.5-x,0.5+y,1-z**	**-4.53**
2-5	1-x,1-y,-z	-1.81
2-6	**1-x,1-y,1-z**	**-12.29**
2-7	2-x,1-y,-z	-4.00
2-8	**2-x,1-y,1-z**	**-1.72**
2-9	**-0.5+x,0.5-y,z**	**-8.90**
2-10	**-0.5+x,1.5-y,z**	**-1.24**
2-11	**0.5+x,0.5-y,z**	**-8.90**
1-12	**0.5+x,1.5-y,z**	**-1.24**

Table S3. Energy of interactions of basic molecule **3** with molecules belonging to its first coordination sphere. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry code	$E_{int.}$, kcal/mol
3-1	**x,y,-1+z**	**0.73**
3-2	**x,y,1+z**	**0.73**
3-3	-0.5+x,-0.5+y,z	-4.98
3-4	-0.5+x,0.5+y,z	-4.98
3-5	0.5+x,-0.5+y,z	-4.98
3-6	0.5+x,0.5+y,z	-4.98
3-7	1-x,-y,-0.5+z	0.79
3-8	1-x,-y,0.5+z	0.79
3-9	**1-x,1-y,-0.5+z**	**-7.85**
3-10	**1-x,1-y,0.5+z**	**-7.85**
3-11	0.5-x,0.5-y,-0.5+z	-5.73
3-12	0.5-x,0.5-y,0.5+z	-5.73
3-13	1.5-x,0.5-y,-0.5+z	-5.73
3-14	1.5-x,0.5-y,0.5+z	-5.73

Table S4. Energy of interactions of basic molecule **4** with molecules belonging to its first coordination sphere. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry code	$E_{int.}$, kcal/mol
4-1	**-1+x,y,z**	**-3.03**
4-2	x,-1+y,z	-1.96
4-3	x,1+y,z	-1.96
4-4	**1+x,y,z**	**-3.03**
4-5	-0.5+x,-0.5-y,-z	-1.92
4-6	**-0.5+x,0.5-y,-z**	**-4.96**
4-7	0.5+x,-0.5-y,-z	-1.92
4-8	**0.5+x,0.5-y,-z**	**-4.96**
4-9	-x,-0.5+y,0.5-z	-1.19
4-10	-x,0.5+y,0.5-z	-1.19
4-11	1-x,-0.5+y,0.5-z	-3.26
4-12	1-x,0.5+y,0.5-z	-3.26

Table S5. Energy of interactions of basic molecule **5** with molecules belonging to its first coordination sphere. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry code	$E_{int.}$, kcal/mol
5-1	-1+x,y,-1+z	-1.24
5-2	-1+x,y,z	-5.94
5-3	**x,y,-1+z**	**-3.28**
5-4	**x,y,1+z**	**-3.28**
5-5	1+x,y,z	-5.94
5-6	1+x,y,1+z	-1.24
5-7	-x,1-y,-z	-0.23
5-8	**1-x,-y,-z**	**-13.66**
5-9	**1-x,-y,1-z**	**-2.68**
5-10	**1-x,1-y,-z**	**-10.23**
5-11	**1-x,1-y,1-z**	**-10.40**
5-12	2-x,-y,1-z	-1.44
5-13	2-x,1-y,1-z	-2.00

Table S6. Energy of interactions of basic molecule **6** with molecules belonging to its first coordination sphere. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry code	$E_{int.}$, kcal/mol
6-1	**x,y,-1+z**	**-3.30**
6-2	**x,y,1+z**	**-3.30**
6-3	-0.5+x,0.5-y,1-z	-6.16
6-4	-0.5+x,0.5-y,2-z	-3.66
6-5	0.5+x,0.5-y,1-z	-6.16
6-6	0.5+x,0.5-y,2-z	-3.66
6-7	1-x,-0.5+y,1.5-z	-3.26
6-8	1-x,0.5+y,1.5-z	-3.26
6-9	**0.5-x,1-y,-0.5+z**	**-13.18**
6-10	**0.5-x,1-y,0.5+z**	**-13.18**
6-11	1.5-x,1-y,-0.5+z	-5.00
6-12	1.5-x,1-y,0.5+z	-5.00