Electronic Supporting Information

Table S1. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **1.**

The building unit is a molecule

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
1-d1	x,1+y,z	-0.98	1.6	non-specific
1-d2	x,-1+y,z	-0.98	1.6	non-specific
1-d3	1/2-x,1/2+y,1/2-z	-1.26	2.1	non-specific
1-d4	1/2-x,-1/2+y,1/2-z	-1.26	2.1	non-specific
1-d5	3/2-x,1/2+y,1/2-z	-6.89	11.4	C-H…C(π)
1-d6	3/2-x,-1/2+y,1/2-z	-6.89	11.4	C-H…C(π)
1-d7	1-x,1-y,-z	-5.34	8.8	C-H…O
1-d8	1-x,2-y,-z	-10.78	17.8	stacking
1-d9	2-x,2-y,-z	-2.89	4.8	non-specific
1-d10	1/2+x,3/2-y,-1/2+z	-7.34	12.1	N-H…O
1-d11	1/2+x,5/2-y,-1/2+z	-4.26	7.0	N-H…O
1-d12	-1/2+x,3/2-y,1/2+z	-7.34	12.1	N-H…O
1-d13	-1/2+x,5/2-y,1/2+z	-4.26	7.0	N-H…O
Total energy		-60.46		

The building unit is a dimer

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
1_dim-d1	x,1+y,z	-7.07	9.3	C-H…O
1_dim -d2	x,-1+y,z	-7.07	9.3	C-H…O
1_dim -d3	1+x,y,z	-1.09	1.4	C-H…O
1_dim -d4	-1+x,y,z	-1.09	1.4	C-H…O
1_dim -d5	1/2-x,1/2+y,1/2-z	-9.39	12.3	N-H…O
1_dim -d6	1/2-x,1/2+y,-1/2-z	-5.54	7.3	C-H…C(π)
1_dim -d7	1/2-x,-1/2+y,1/2-z	-9.40	12.3	N-H…O
1_dim -d8	1/2-x,-1/2+y,-1/2-z	-5.53	7.3	C-H…C(π)
1_dim -d9	3/2-x,1/2+y,1/2-z	-5.53	7.3	C-H…C(π)
1_dim -d10	3/2-x,1/2+y,-1/2-z	-9.40	12.3	N-H…O
1_dim -d11	3/2-x,-1/2+y,1/2-z	-5.54	7.3	C-H…C(π)
1_dim -d12	3/2-x,-1/2+y,-1/2-z	-9.39	12.3	N-H…O
Total energy		-76.04		

Table S2. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **2.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
2-d1	1+x,y,z	-6.31	8.5	stacking
2-d2	-1+x,y,z	-6.31	8.5	stacking
2-d3	3/2-x,2-y,1/2+z	-9.58	12.9	N-H…O
2-d4	3/2-x,2-y,-1/2+z	-9.58	12.9	N-H…O
2-d5	5/2-x,2-y,1/2+z	-2.31	3.1	non-specific
2-d6	5/2-x,2-y,-1/2+z	-2.31	3.1	non-specific
2-d7	1-x,1/2+y,1/2-z	0.27	0.4	non-specific
2-d8	1-x,-1/2+y,1/2-z	0.27	0.4	non-specific
2-d9	2-x,1/2+y,1/2-z	-4.74	6.4	N-H…N
2-d10	2-x,-1/2+y,1/2-z	-4.74	6.4	N-H…N
2-d11	1/2+x,3/2-y,-z	-7.06	9.5	C-H…C(π), C-H…O
2-d12	1/2+x,5/2-y,-z	-7.47	10.0	N-H…O
2-d13	-1/2+x,3/2-y,-z	-7.06	9.5	C-H…C(π), C-H…O
2-d14	-1/2+x,5/2-y,-z	-7.47	10.0	N-H…O
Total energy		-74.38		

Table S3. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **3.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
3-d1	x,1+y,z	-7.67	13.0	stacking
3-d2	x,-1+y,z	-7.67	13.0	stacking
3-d3	-x,1/2+y,1/2-z	-4.12	7.0	N-H…N
3-d4	-x,-1/2+y,1/2-z	-4.12	7.0	N-H…N
3-d5	1-x,1/2+y,1/2-z	-3.24	5.5	non-specific
3-d6	1-x,-1/2+y,1/2-z	-3.24	5.5	non-specific
3-d7	-x,1-y,-z	-6.69	11.3	N-H…O
3-d8	-x,2-y,-z	-3.32	5.6	non-specific
3-d9	1-x,2-y,1-z	-2.64	4.5	non-specific
3-d10	1-x,3-y,1-z	-1.35	2.3	non-specific
3-d11	x,3/2-y,1/2+z	-4.92	8.3	N-H…O
3-d12	x,3/2-y,-1/2+z	-4.92	8.3	N-H…O
3-d13	x,5/2-y,1/2+z	-2.56	4.3	non-specific
3-d14	x,5/2-y,-1/2+z	-2.56	4.3	non-specific
Total energy		-59.00		

Table S4. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **4.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
4-d1	1+x,y,z	-4.18	7.0	stacking
4-d2	-1+x,y,z	-4.18	7.0	stacking
4-d3	1/2+x,3/2-y,1/2+z	-3.50	5.9	N-H…O
4-d4	1/2+x,3/2-y,-1/2+z	-5.44	9.2	N-H…O
4-d5	-1/2+x,3/2-y,1/2+z	-5.44	9.2	N-H…O
4-d6	-1/2+x,3/2-y,-1/2+z	-3.50	5.9	N-H…O
4-d7	-x,2-y,-z	-4.96	8.4	non-specific
4-d8	-x,2-y,1-z	0.75	1.3	non-specific
4-d9	-1-x,2-y,-z	-5.27	8.9	non-specific
4-d10	1/2-x,1/2+y,1/2-z	-5.69	9.6	N-H…N
4-d11	1/2-x,-1/2+y,1/2-z	-5.69	9.6	N-H…N
4-d12	-1/2-x,1/2+y,1/2-z	-6.12	10.3	N-H…N
4-d13	-1/2-x,-1/2+y,1/2-z	-6.12	10.3	N-H…N
Total energy		-59.34		

Table S5. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **5.**

The building unit is a molecule

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
5-d1	x,1+y,z	1.07	1.2	non-specific
5-d2	x,-1+y,z	1.07	1.2	non-specific
5-d3	1/2-x,1/2+y,1/2-z	-1.18	1.3	non-specific
5-d4	1/2-x,1/2+y,-1/2-z	1.37	1.5	non-specific
5-d5	1/2-x,-1/2+y,1/2-z	-1.18	1.3	non-specific
5-d6	1/2-x,-1/2+y,-1/2-z	1.37	1.5	non-specific
5-d7	-x,1-y,-z	-12.98	14.7	non-specific
5-d8	-x,2-y,-z	-14.68	16.6	N-H…O
5-d9	1-x,-y,-z	-14.08	15.9	N-H…O
5-d10	1-x,1-y,-z	-17.86	20.2	stacking
5-d11	1/2+x,1/2-y,1/2+z	-6.38	7.2	N-H…O
5-d12	1/2+x,3/2-y,1/2+z	-9.36	10.6	N-H…O
5-d13	-1/2+x,1/2-y,-1/2+z	-6.38	7.2	N-H…O
5-d14	-1/2+x,3/2-y,-1/2+z	-9.36	10.6	N-H…O
Total energy		-88.56		

The building unit is a dimer

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
5_dim-d1	x,1+y,z	-13.64	13.7	N-H…O
5_dim-d2	x,-1+y,z	-13.64	13.7	N-H…O
5_dim-d3	1+x,y,z	-6.47	6.5	stacking
5_dim-d4	1+x,-1+y,z	-6.21	6.2	N-H…O
5_dim -d5	-1+x,y,z	-6.47	6.5	stacking
5_dim-d6	-1+x,1+y,z	-6.21	6.2	N-H…O
5_dim-d7	1/2-x,1/2+y,1/2-z	-2.01	2.0	non-specific
5_dim-d8	1/2-x,1/2+y,-1/2-z	-9.80	9.8	N-H…O
5_dim-d9	1/2-x,-1/2+y,1/2-z	-2.01	2.0	non-specific
5_dim-d10	1/2-x,-1/2+y,-1/2-z	-9.63	9.7	N-H…O
5_dim -d11	3/2-x,1/2+y,1/2-z	-9.63	9.7	N-H…O
5_dim-d12	3/2-x,1/2+y,-1/2-z	-2.01	2.0	non-specific
5_dim-d13	3/2-x,-1/2+y,1/2-z	-9.80	9.8	N-H…O
5_dim-d14	3/2-x,-1/2+y,-1/2-z	-2.01	2.0	non-specific
Total energy		-99.55		

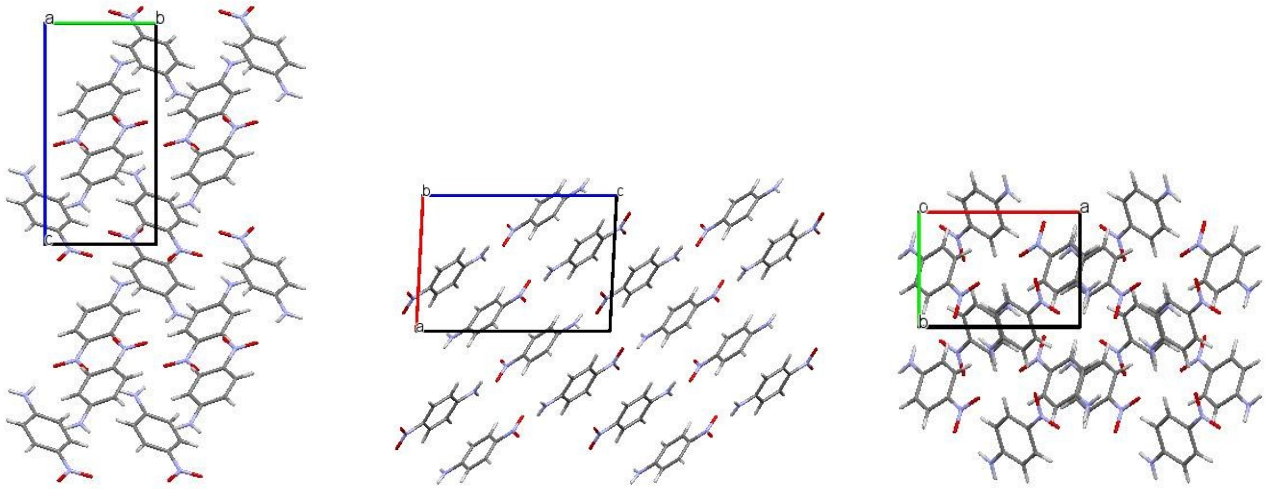
Table S6. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **6.**

The building unit is a molecule

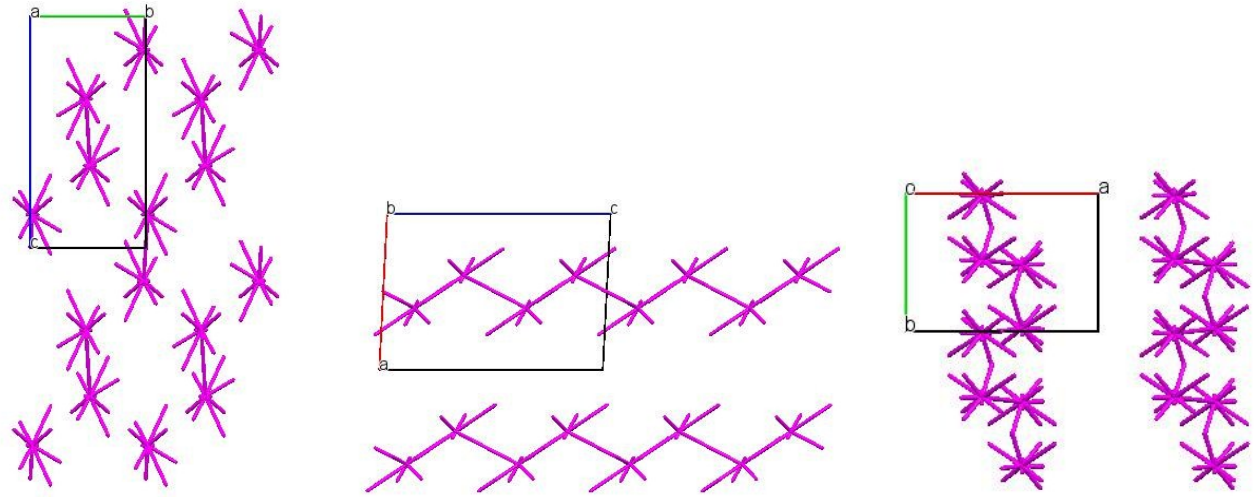
Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
6-d1	x,y,1+z	-3.20	4.6	N-H…O
6-d2	x,y,-1+z	-3.20	4.6	N-H…O
6-d3	x,1+y,z	-8.18	11.8	N-H…O
6-d4	x,1+y,-1+z	-0.43	0.6	N-H…O
6-d5	x,-1+y,z	-8.18	11.8	N-H…O
6-d6	x,-1+y,1+z	-0.43	0.6	N-H…O
6-d7	-x,1-y,1-z	-3.31	4.8	non-specific
6-d8	-x,1-y,2-z	-6.53	9.4	non-specific
6-d9	-x,2-y,1-z	-12.14	17.5	stacking
6-d10	1-x,-y,2-z	-2.05	3.0	non-specific
6-d11	1-x,1-y,1-z	-10.43	15.1	stacking
6-d12	1-x,1-y,2-z	-7.35	10.6	stacking
6-d13	1-x,2-y,1-z	-3.84	5.5	non-specific
Total energy		-69.28		

The building unit is a dimer

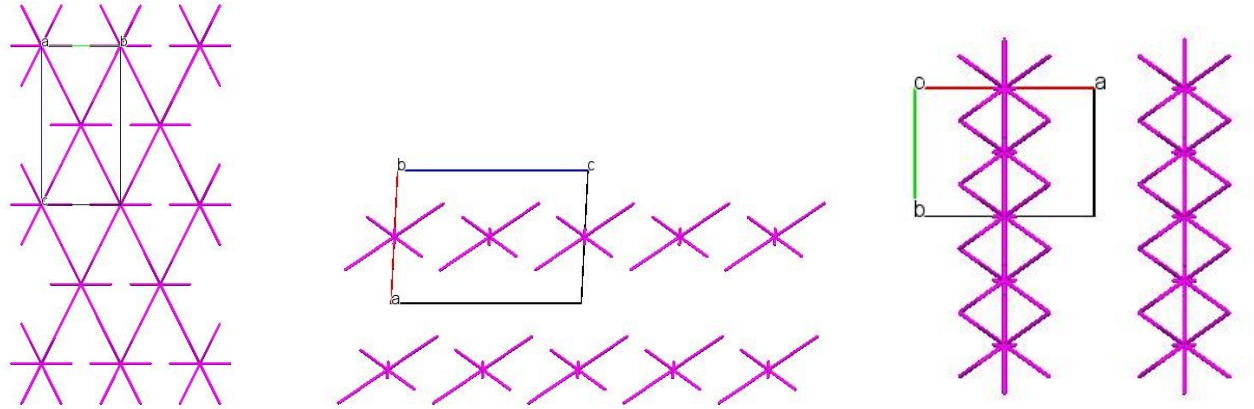
Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
6-d-d1	x,y,1+z	-6.63	7.3	N-H…O
6-d-d2	x,y,-1+z	-6.63	7.3	N-H…O
6-d-d3	x,1+y,z	-14.02	15.5	N-H…O
6-d-d4	x,1+y,-1+z	-6.55	7.2	N-H…O
6-d-d5	x,-1+y,z	-14.02	15.5	N-H…O
6-d-d6	x,-1+y,1+z	-6.55	7.2	N-H…O
6-d-d7	1+x,y,z	-4.35	4.8	non-specific
6-d-d8	1+x,-1+y,z	-7.78	8.6	stacking
6-d-d9	1+x,-1+y,1+z	-4.69	5.2	non-specific
6-d-d10	1+x,-2+y,1+z	-1.32	1.5	non-specific
6-d-d11	-1+x,y,z	-4.32	4.8	non-specific
6-d-d12	-1+x,1+y,z	-7.78	8.6	stacking
6-d-d13	-1+x,1+y,-1+z	-4.69	5.2	non-specific
6-d-d14	-1+x,2+y,-1+z	-1.32	1.5	non-specific
Total energy		-90.65		



The building unit is a molecule

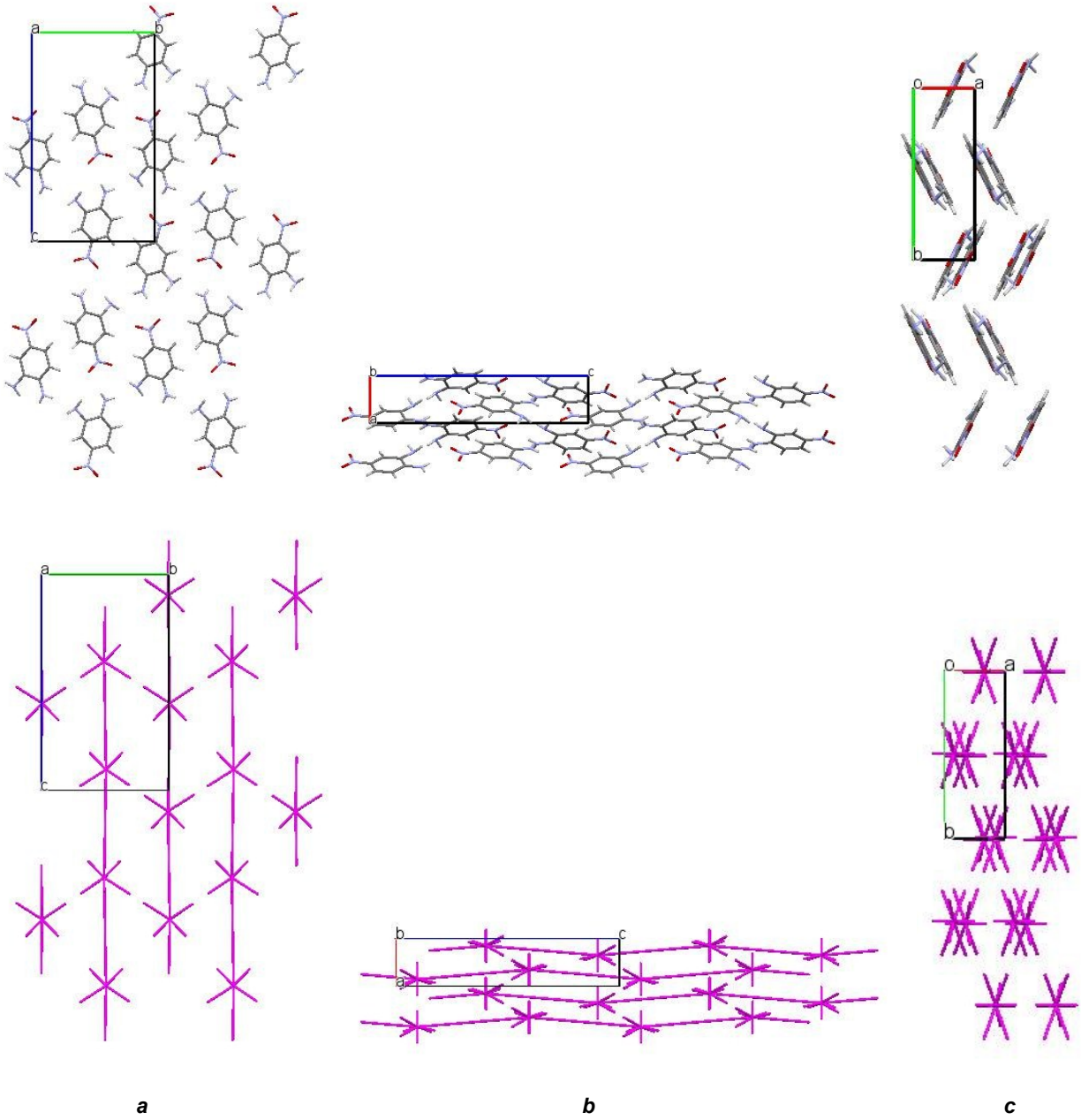


The building unit is a dimer



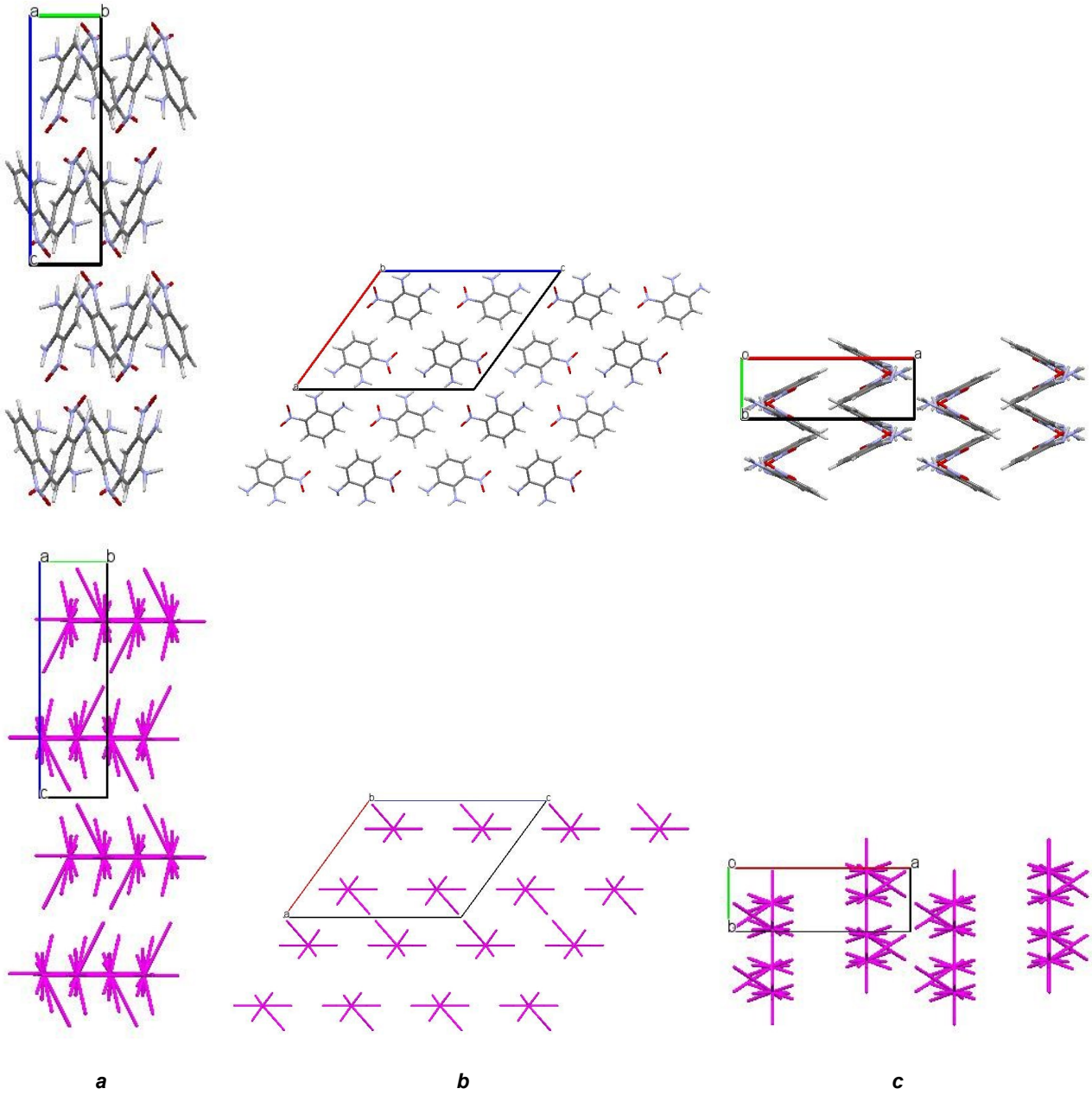
a ***b*** ***c***

Figure S1. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **1**. The projection along *a*, *b* and *c* crystallographic direction is presented.



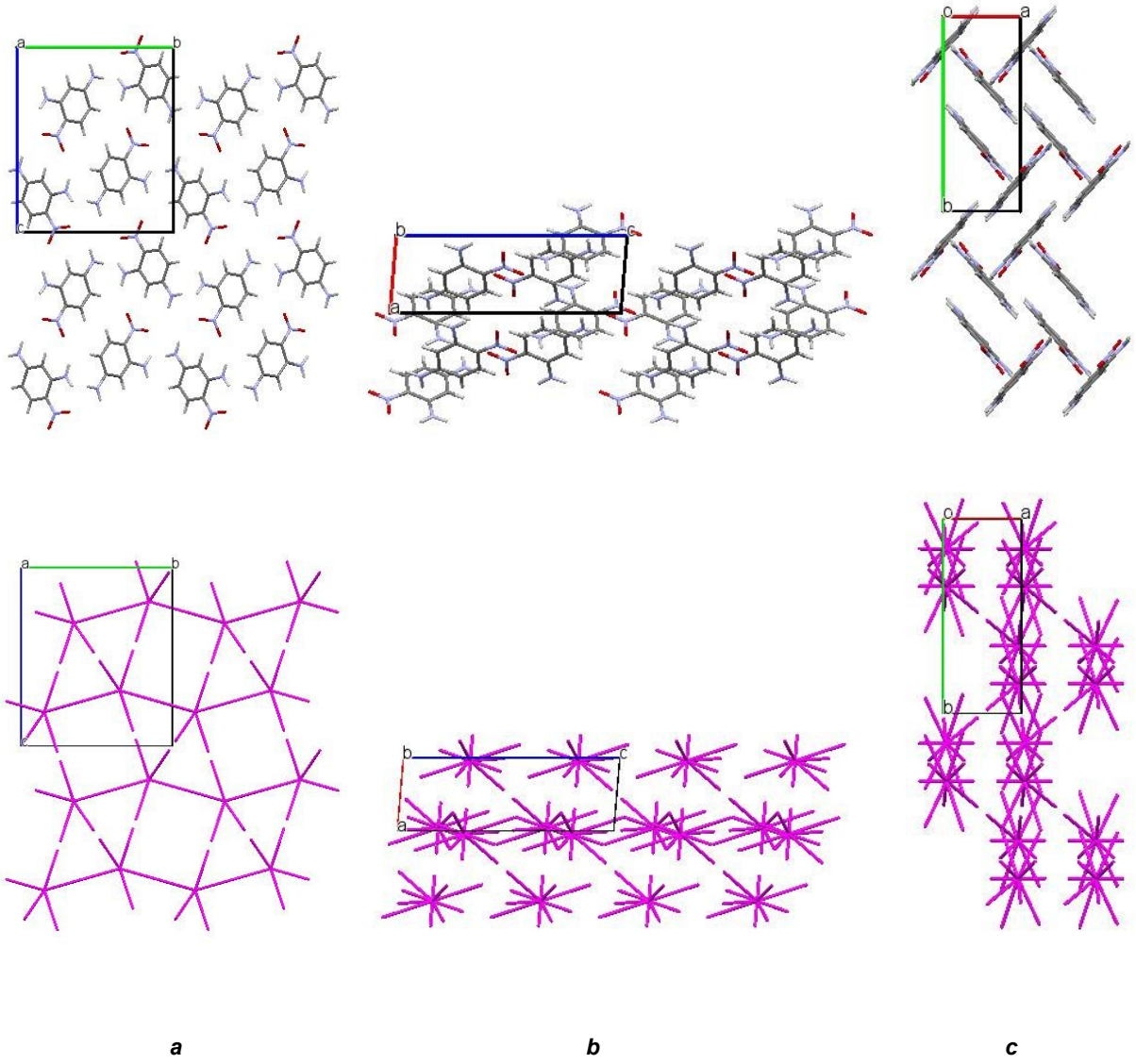
a ***b*** ***c***

Figure S2. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **2**. The projection along *a*, *b* and *c* crystallographic direction is presented.



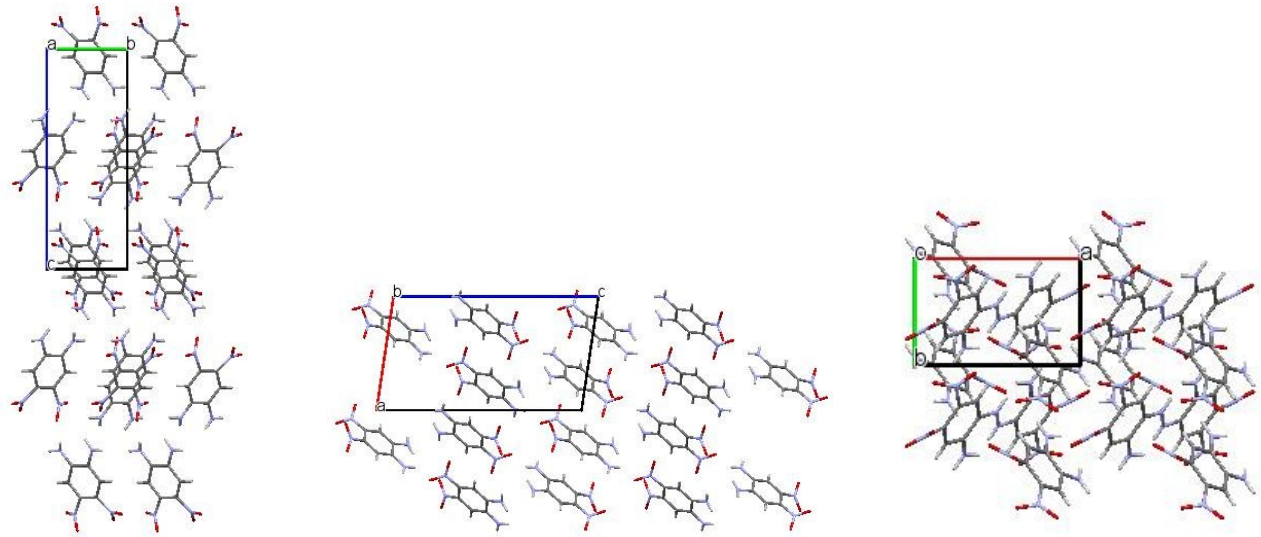
a ***b*** ***c***

Figure S3. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **3**. The projection along *a*, *b* and *c* crystallographic direction is presented.

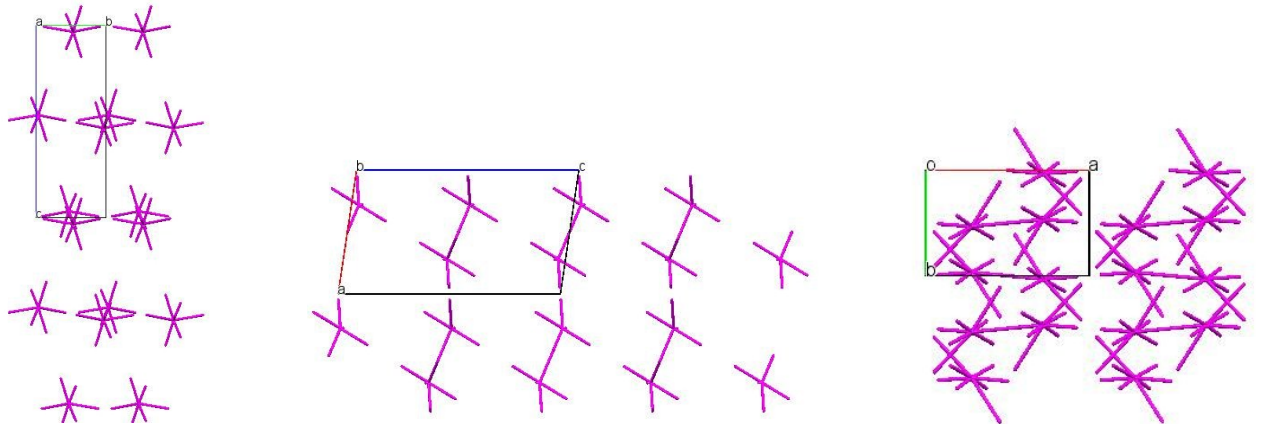


a ***b*** ***c***

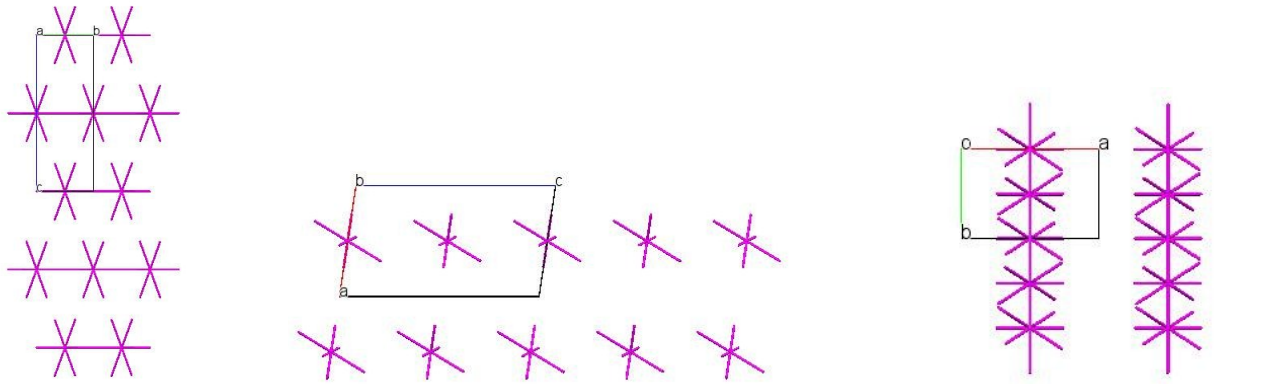
Figure S4. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **4**. The projection along *a*, *b* and *c* crystallographic direction is presented.



The building unit is a molecule

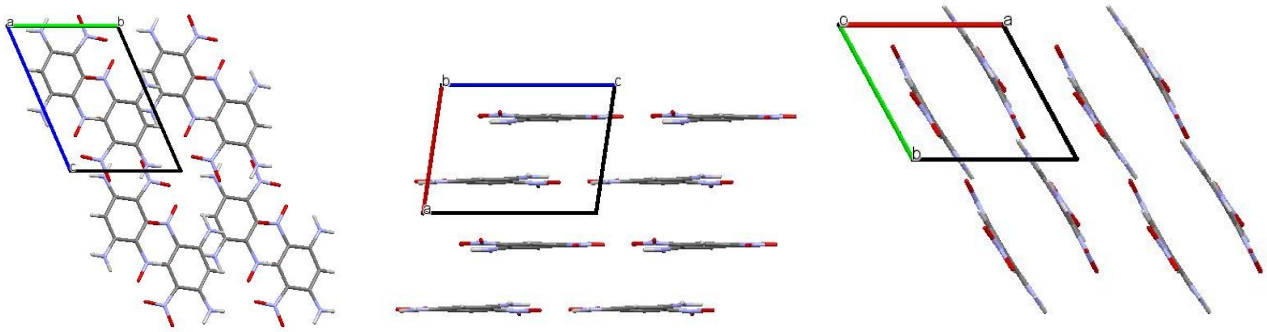


The building unit is a dimer

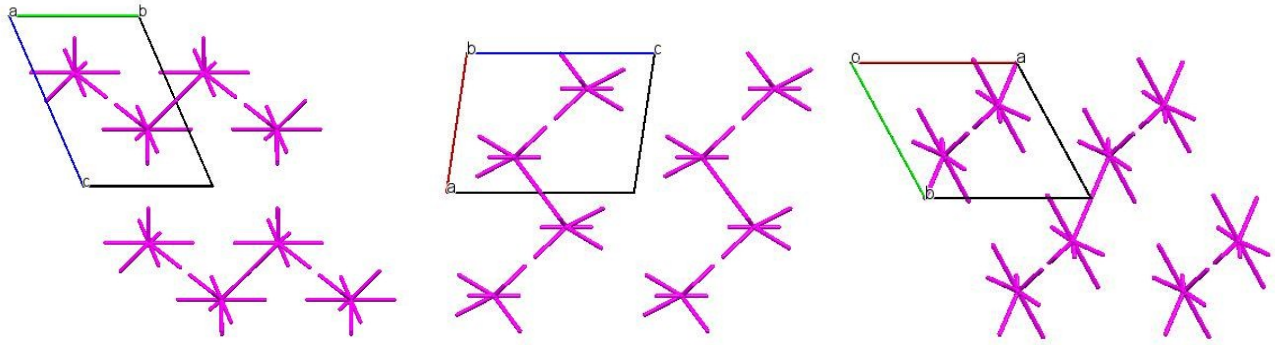


a ***b*** ***c***

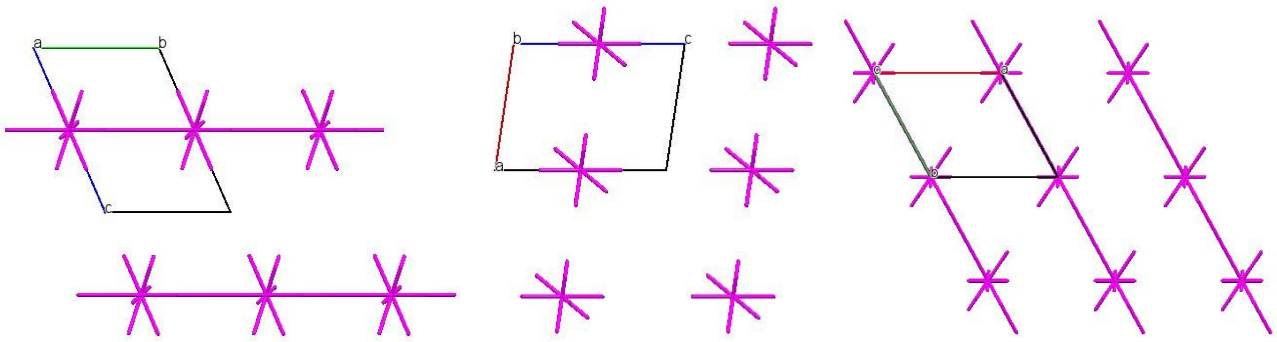
Figure S5. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **5**. The projection along *a*, *b* and *c* crystallographic direction is presented.



The building unit is a molecule



The building unit is a dimer



a ***b*** ***c***

Figure S6. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **6**. The projection along *a*, *b* and *c* crystallographic direction is presented.