Electronic Supporting Information

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

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
1M-d1	x,1+y,z	-2.29	8.3	non-specific
1M-d2	x,-1+y,z	-2.29	8.3	non-specific
1M-d3	1+x,y,z	-2.12	7.7	non-specific
1M-d4	1+x,-1+y,z	-0.40	1.4	non-specific
1M-d5	-1+x,y,z	-2.12	7.7	non-specific
1M-d6	-1+x,1+y,z	-0.40	1.4	non-specific
1M-d7	-x,1/2+y,1/2-z	-2.96	10.8	C-H...π 2.73 Å, 160˚
1M-d8	-x,1/2+y,-1/2-z	-2.96	10.8	C-H...π 2.73 Å, 160˚
1M-d9	-x,-1/2+y,1/2-z	-2.96	10.8	C-H...π 2.73 Å, 160˚
1M-d10	-x,-1/2+y,-1/2-z	-2.96	10.8	C-H...π 2.73 Å, 160˚
1M-d11	1-x,1/2+y,1/2-z	-1.52	5.5	non-specific
1M-d12	1-x,-1/2+y,1/2-z	-1.52	5.5	non-specific
1M-d13	-1-x,1/2+y,-1/2-z	-1.52	5.5	non-specific
1M-d14	-1-x,-1/2+y,-1/2-z	-1.52	5.5	non-specific
Total energy		-27.54		

Table S2. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal **1O.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
1O-d1	1/2-x,-y,1/2+z	-3.01	11.3	C-H...π 3.06 Å, 171°
1O-d2	1/2-x,-y,-1/2+z	-3.01	11.3	C-H...π 3.06 Å, 171°
1O-d3	-1/2-x,-y,1/2+z	-3.01	11.3	C-H...π 3.06 Å, 171°
1O-d4	-1/2-x,-y,-1/2+z	-3.01	11.3	C-H...π 3.06 Å, 171°
1O-d5	-x,1/2+y,1/2-z	-1.97	7.4	non-specific
1O-d6	-x,1/2+y,-1/2-z	-1.97	7.4	non-specific
1O-d7	-x,-1/2+y,1/2-z	-1.97	7.4	non-specific
1O-d8	-x,-1/2+y,-1/2-z	-1.97	7.4	non-specific
1O-d9	1/2+x,1/2-y,-z	-1.68	6.3	non-specific
1O-d10	1/2+x,-1/2-y,-z	-1.68	6.3	non-specific
1O-d11	-1/2+x,1/2-y,-z	-1.68	6.3	non-specific
1O-d12	-1/2+x,-1/2-y,-z	-1.68	6.3	non-specific
Total energy		-26.62		

Table S3. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal **2.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
2-d1	1+x,y,z	-5.69	19.7	stacking 3.42 Å
2-d2	-1+x,y,z	-5.69	19.7	stacking 3.42 Å
2-d3	-x,1/2+y,1/2-z	-1.26	4.4	C-H…O 2.72 Å
2-d4	-x,-1/2+y,1/2-z	-1.26	4.4	C-H…O 2.72 Å
2-d5	1-x,1/2+y,1/2-z	-1.55	5.4	C-H…O 2.74 Å
2-d6	1-x,-1/2+y,1/2-z	-1.55	5.4	C-H…O 2.74 Å
2-d7	-x,-y,-z	-1.75	6.1	non-specific
2-d8	-x,1-y,-z	-2.11	7.3	non-specific
2-d9	1-x,1-y,-z	-1.81	6.3	C-H…O 2.56 Å, 138°
2-d10	-1-x,1-y,-z	-0.88	3.0	non-specific
2-d11	x,1/2-y,1/2+z	-1.44	5.0	non-specific
2-d12	x,1/2-y,-1/2+z	-1.44	5.0	non-specific
2-d13	1+x,1/2-y,1/2+z	-1.23	4.3	C-H…O 2.57 Å, 122°
2-d14	1+x,1/2-y,1/2+z	-1.23	4.3	C-H…O 2.57 Å, 122°
Total energy		-28.91		

Table S4. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal **3.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
3-d1	1+x,y,z	-1.43	4.4	C-H…O 2.57, 124
3-d2	-1+x,y,z	-1.43	4.4	C-H…O 2.57, 124
3-d3	-x,1/2+y,1/2-z	-0.99	3.0	C-H…O 2.44, 129
3-d4	-x,-1/2+y,1/2-z	-0.99	3.0	C-H…O 2.44, 129
3-d5	1-x,1/2+y,1/2-z	-2.59	7.9	C-H…O 2.60, 142
3-d6	1-x,-1/2+y,1/2-z	-2.59	7.9	C-H…O 2.60, 142
3-d7	-x,1-y,-z	-0.89	2.7	non-specific
3-d8	-x,2-y,-z	-3.27	10.0	non-specific
3-d9	1-x,2-y,-z	-0.59	1.8	non-specific
3-d10	1-x,2-y,1-z	-0.67	2.0	non-specific
3-d11	x,3/2-y,1/2+z	-7.08	21.7	stacking C…C 3.70Å
3-d12	x,3/2-y,-1/2+z	-7.08	21.7	stacking C…C 3.70Å
3-d13	1+x,3/2-y,1/2+z	-1.53	4.7	C-H…O 2.65, 144
3-d14	-1+x,3/2-y,-1/2+z	-1.51	4.6	C-H…O 2.65, 144
Total energy		-32.64		

Table S5. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal **4.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
4-d1	x,y,1+z	-7.31	22.5	stacking C…C 3.44Å
4-d2	x,y,-1+z	-7.30	22.5	stacking C…C 3.44Å
4-d3	-x,1-y,1/2+z	-1.73	5.3	C-H…O 2.49 Å, 156°
4-d4	-x,1-y,-1/2+z	-1.73	5.3	C-H…O 2.49 Å, 156°
4-d5	-x,2-y,1/2+z	-1.39	4.3	C-H…O 2.46 Å, 152°
4-d6	-x,2-y,-1/2+z	-1.39	4.3	C-H…O 2.46 Å, 152°
4-d7	1/2+x,3/2-y,z	-1.70	5.2	C-H…O 2.46 Å, 152°
4-d8	1/2+x,3/2-y,1+z	-1.43	4.4	C-H…O 2.37 Å, 130°
4-d9	-1/2+x,3/2-y,z	-1.70	5.2	C-H…O 2.46 Å, 152°
4-d10	-1/2+x,3/2-y,-1+z	-1.44	4.4	C-H…O 2.37 Å, 130°
4-d11	1/2-x,1/2+y,1/2+z	-1.58	4.9	C-H…O 2.43 Å, 139°
4-d12	1/2-x,1/2+y,-1/2+z	-1.12	3.45	non-specific
4-d13	1/2-x,-1/2+y,1/2+z	-1.12	3.45	non-specific
4-d14	1/2-x,-1/2+y,-1/2+z	-1.50	4.6	C-H…O 2.43 Å, 139°
Total energy		-32.43		

Table S6. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal **5.**

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction
5-d1	x,y,1+z	-3.12	9.3	non-specific
5-d2	x,y,-1+z	-3.12	9.3	non-specific
5-d3	x,1+y,z	-4.01	12.0	non-specific
5-d4	x,1+y,1+z 0 0	-0.90	2.7	C-H…O 2.36, 155
5-d5	x,-1+y,z	-4.01	12.0	non-specific
5-d6	x,-1+y,-1+z 0 0	-0.90	2.7	C-H…O 2.36, 155
5-d7	1/2-x,1/2+y,1/2-z	-2.37	7.1	non-specific
5-d8	1/2-x,1/2+y,-1/2-z	-1.97	5.9	C-H…O 2.45 Å, 131°
5-d9	1/2-x,-1/2+y,1/2-z	-2.37	7.1	non-specific
5-d10	1/2-x,-1/2+y,-1/2-z	-1.98	5.9	C-H…O 2.37 Å, 130°
5-d11	-1/2-x,1/2+y,1/2-z	-1.98	5.9	C-H…O 2.43 Å, 139°
5-d12	-1/2-x,1/2+y,-1/2-z	-2.37	7.1	non-specific
5-d13	-1/2-x,-1/2+y,1/2-z	-1.97	5.9	C-H…O 2.45 Å, 131°
5-d14	-1/2-x,-1/2+y,-1/2-z	-2.37	7.1	non-specific
Total energy		-33.44		

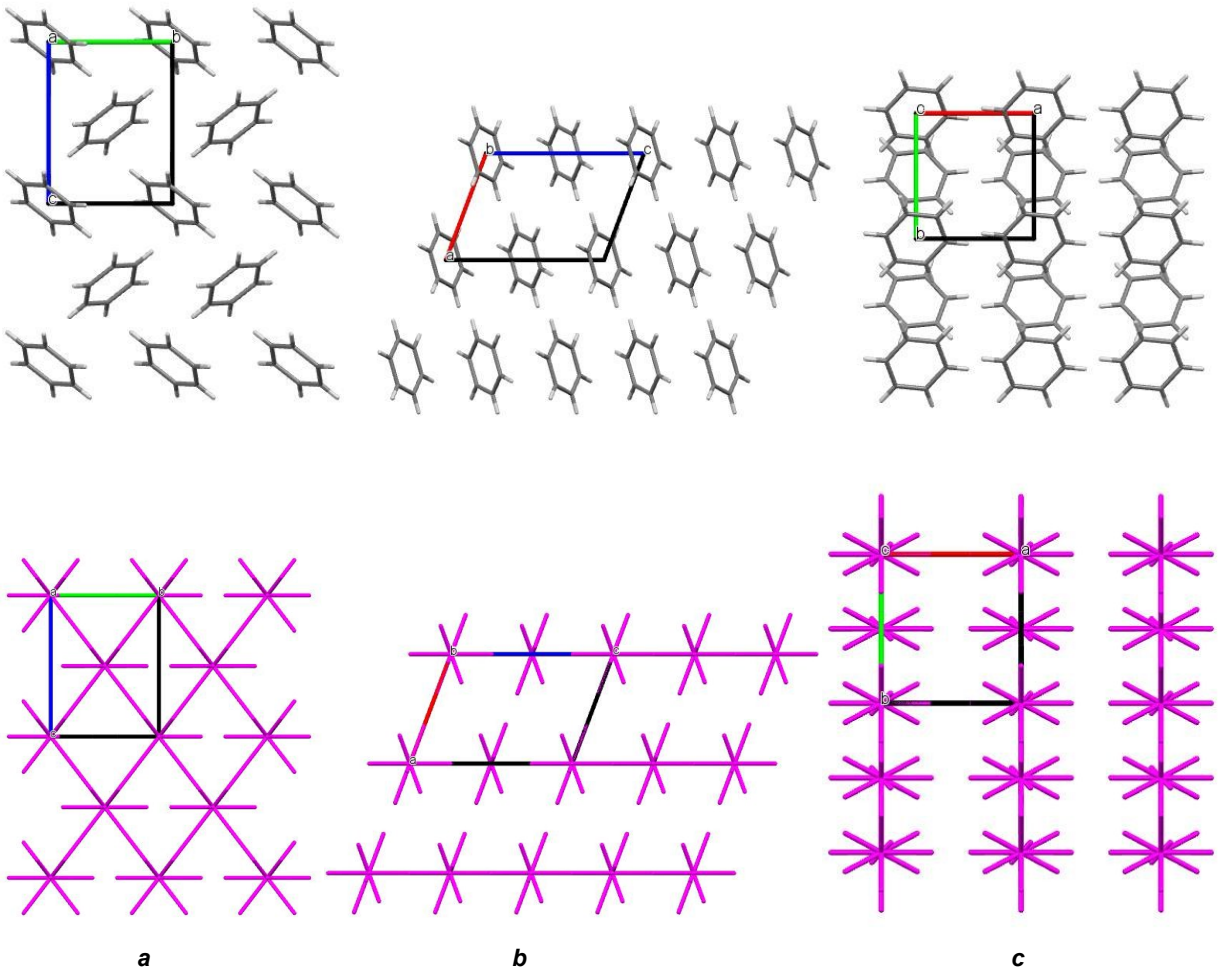


Figure S1. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **1M**. The projection along *a*, *b* and *c* crystallographic direction is presented.

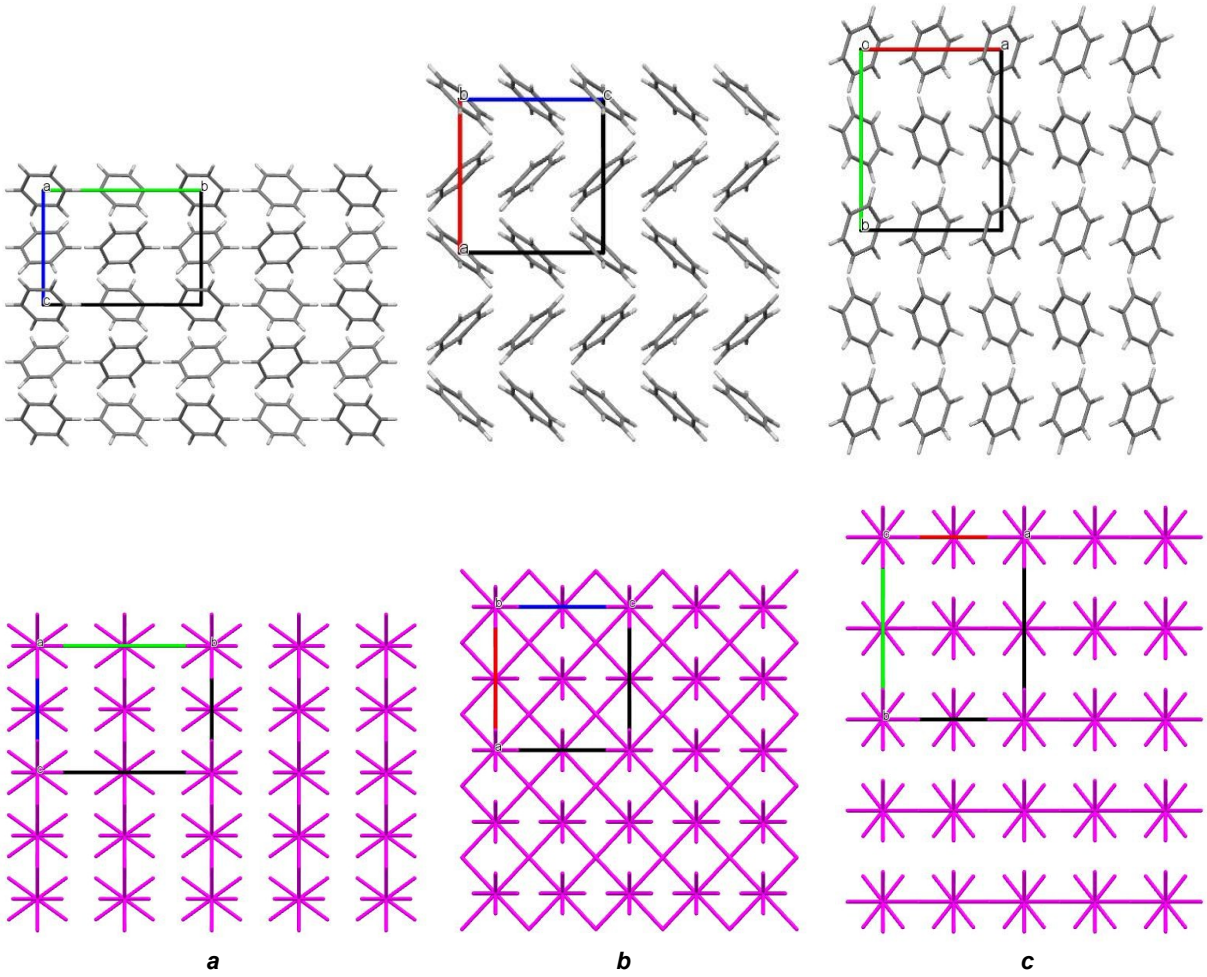


Figure S2. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **1O**. The projection along *a*, *b* and *c* crystallographic direction is presented.

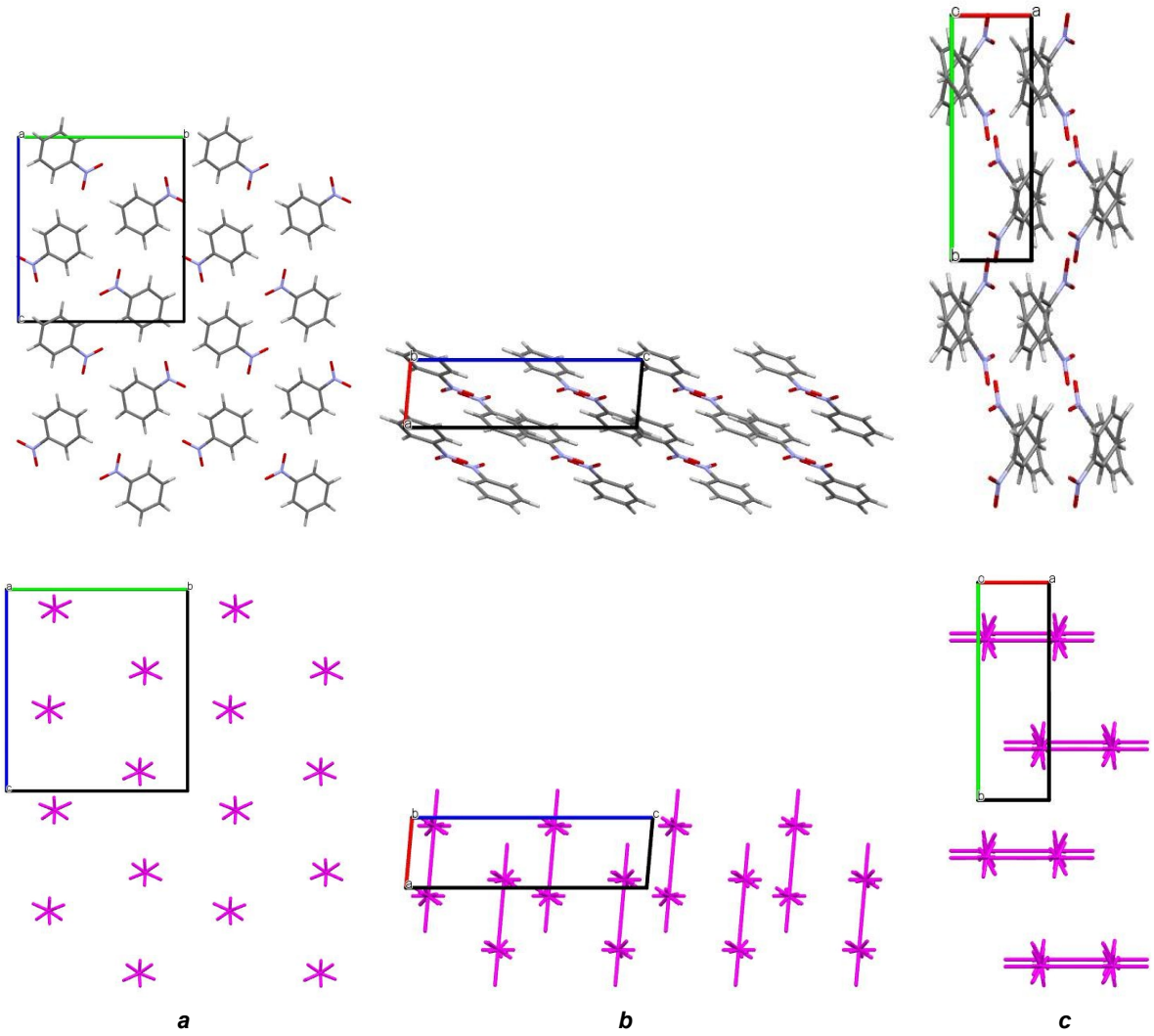


Figure S3. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **2**. The projection along *a*, *b* and *c* crystallographic direction is presented.

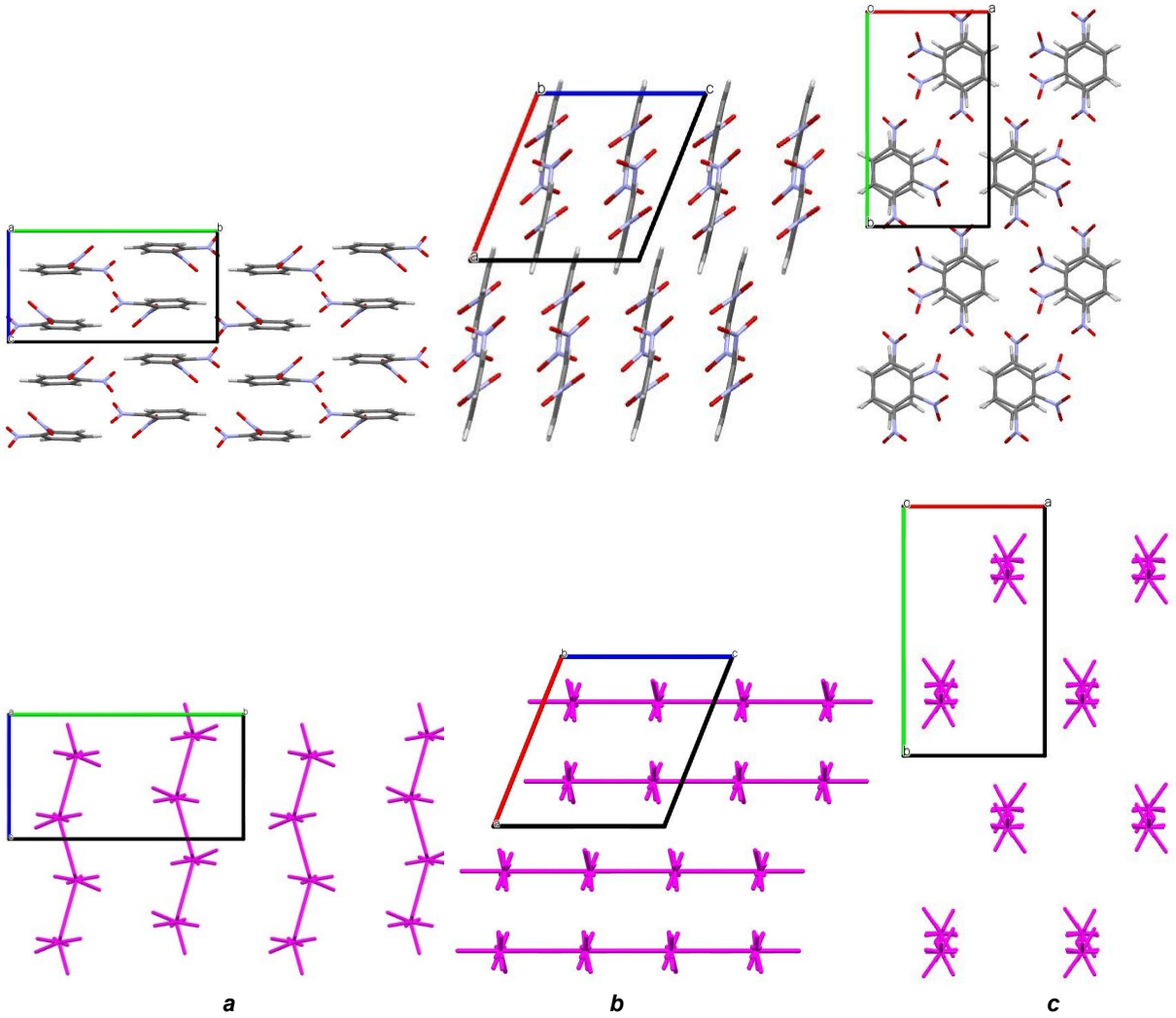


Figure S4. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **3**. The projection along *a*, *b* and *c* crystallographic direction is presented.

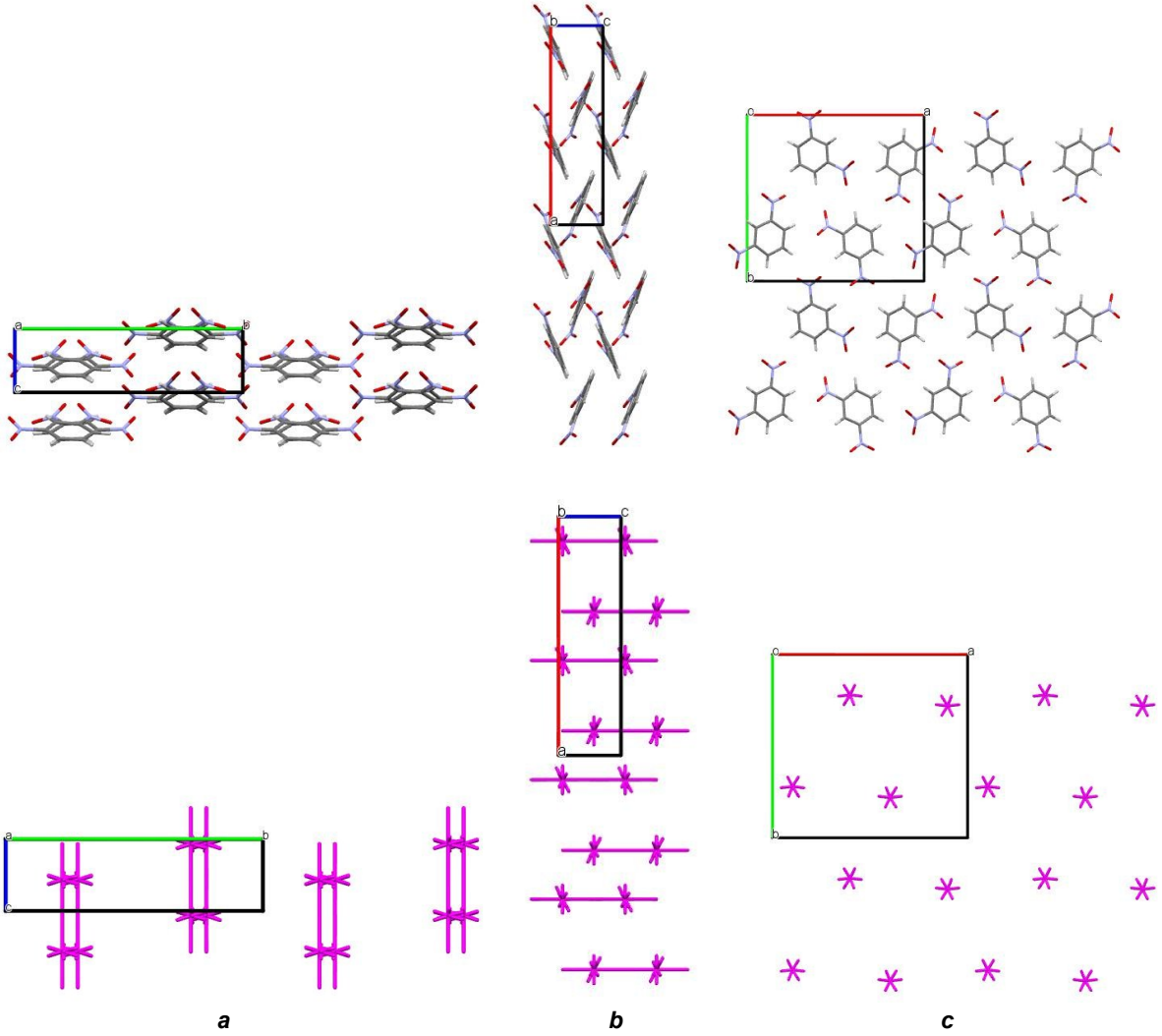
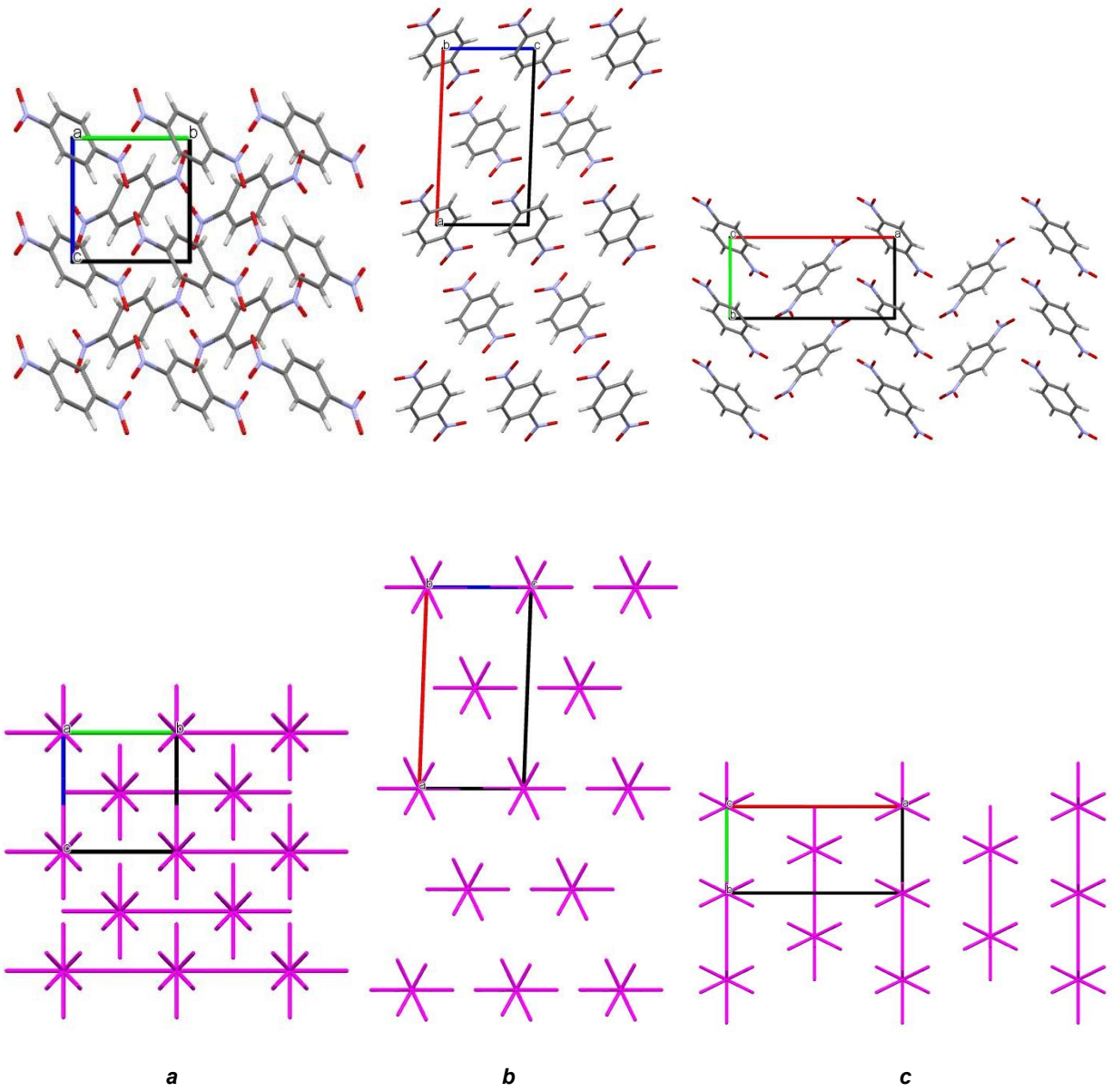


Figure S5. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals of **4**. The projection along *a*, *b* and *c* crystallographic direction is presented.



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

Figure S6. 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.