Electronic Supporting Information

For paper

Crystal Packing of Aminobenzenes: Study From the Energetic Viewpoint

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

Dimer	Molecules	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
Molecule A					
1m-d1	A-B	x,y,1+z	-3.40	9.2	N-H…N
1m-d2	A-A	x,1+y,z	-3.10	8.4	non-specific
1m -d3	A-B	x,1+y,1+z	-0.57	1.5	non-specific
1m -d4	A-A	x,-1+y,z	-3.10	8.4	non-specific
1m -d5	A-A	1-x,1/2+y,3/2-z	-1.96	5.3	non-specific
1m -d6	A-A	1-x,-1/2+y,3/2-z	-1.96	5.3	non-specific
1m -d7	A-A	1-x,1-y,2-z	-1.50	4.1	non-specific
1m -d8	A-A	x,1/2-y,1/2+z	-5.69	15.5	N-H…C(π)
1m -d9	A-B	x,1/2-y,1/2+z	-2.79	7.6	N-H…N
1m -d10	A-A	x,1/2-y,-1/2+z	-5.69	15.5	N-H…C(π)
1m -d11	A-B	x,3/2-y,1/2+z	-1.58	4.3	non-specific
1m -d12	A-A	x,3/2-y,1/2+z	-2.72	7.4	non-specific
1m -d13	A-A	x,3/2-y,-1/2+z	-2.72	7.4	non-specific
Total energy			-36.78		
Molecule B					
1m -d14	B-A	x,y,-1+z	-3.40	9.2	N-H…N
1m -d15	B-B	x,1+y,z	-3.19	8.6	non-specific
1m -d16	B-B	x,-1+y,z	-3.19	8.6	non-specific
1m -d17	B-A	x,-1+y,-1+z	-0.57	1.5	non-specific
1m -d18	B-B	2-x,1/2+y,1/2-z	-1.92	5.2	H…H
1m -d19	B-B	2-x,-1/2+y,1/2-z	-1.92	5.2	H…H
1m -d20	B-B	2-x,1-y,1-z	-1.54	4.2	non-specific
1m -d21	B-B	x,1/2-y,1/2+z	-5.76	15.6	N-H…C(π)
1m -d22	B-A	x,1/2-y,-1/2+z	-2.79	7.6	N-H…N
1m -d23	B-B	x,1/2-y,-1/2+z	-5.76	15.6	N-H…C(π)
1m -d24	B-B	x,3/2-y,1/2+z	-2.66	7.2	non-specific
1m -d25	B-B	x,3/2-y,-1/2+z	-2.66	7.2	non-specific
1m -d26	B-A	x,3/2-y,-1/2+z	-1.58	4.3	non-specific
Total energy			-36.95		

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

Dimer	Molecules	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
Molecule A					
1o-d1	A-A	x,1+y,z	-3.13	8.6	non-specific
1o -d2	A-A	x,-1+y,z	-3.13	8.6	non-specific
1o -d3	A-B	1+x,y,z	-1.57	4.3	non-specific
1o -d4	A-B	1/2-x,1/2+y,1/2+z	-1.57	4.3	non-specific
1o -d5	A-B	1/2-x,-1/2+y,1/2+z	-2.98	8.2	N-H…N
1o -d6	A-B	1-x,1-y,1/2+z	-3.10	8.5	N-H…N
1o -d7	A-B	1-x,2-y,1/2+z	-0.52	1.4	non-specific
1o -d8	A-A	1/2+x,1/2-y,z	-5.61	15.4	N-H…C(π)
1o -d9	A-B	1/2+x,1/2-y,z	-1.95	5.4	non-specific
1o -d10	A-A	1/2+x,3/2-y,z	-2.64	7.2	non-specific
1o -d11	A-B	1/2+x,3/2-y,z	-1.98	5.4	non-specific
1o -d12	A-A	-1/2+x,1/2-y,z	-5.61	15.4	N-H…C(π)
1o -d13	A-A	-1/2+x,3/2-y,z	-2.64	7.2	non-specific
Total energy			-36.43		
Molecule B					
1o -d14	B-B	x,1+y,z	-3.13	8.5	non-specific
1o -d15	B-B	x,-1+y,z	-3.13	8.5	non-specific
1o -d16	B-A	-1+x,y,z	-1.57	4.3	non-specific
1o -d17	B-A	1/2-x,1/2+y,-1/2+z	-2.98	8.1	N-H…N
1o -d18	B-A	1/2-x,-1/2+y,-1/2+z	-1.57	4.3	non-specific
1o -d19	B-A	1-x,1-y,-1/2+z	-3.10	8.4	N-H…N
1o -d20	B-A	1-x,2-y,-1/2+z	-0.52	1.4	non-specific
1o -d21	B-B	1/2+x,1/2-y,z	-2.65	7.2	non-specific
1o -d22	B-B	1/2+x,3/2-y,z	-5.83	15.8	N-H…C(π)
1o -d23	B-A	-1/2+x,1/2-y,z	-1.95	5.3	non-specific
1o -d24	B-B	-1/2+x,1/2-y,z	-2.65	7.2	non-specific
1o -d25	B-B	-1/2+x,3/2-y,z	-5.83	15.8	N-H…C(π)
1o -d26	B-A	-1/2+x,3/2-y,z	-1.98	5.4	non-specific
Total energy			-36.90		

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

Building unit is molecule

Dimer	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
2m-d1	1-x,1/2+y,3/2-z	-1.61	3.4	non-specific
2m-d2	1-x,-1/2+y,3/2-z	-1.61	3.4	non-specific
2m-d3	2-x,1/2+y,3/2-z	-5.29	11.1	N-H…N
2m-d4	2-x,-1/2+y,3/2-z	-5.29	11.1	N-H…N
2m-d5	1-x,-y,1-z	-2.87	6	non-specific
2m-d6	1-x,-y,2-z	-1.57	3.3	non-specific
2m-d7	2-x,-y,1-z	-6.40	13.5	N-H…N
2m-d8	2-x,-y,2-z	-4.76	10	non-specific
2m-d9	x,1/2-y,1/2+z	-4.30	9	C-H…N
2m-d10	x,1/2-y,-1/2+z	-4.30	9	C-H…N
2m-d11	x,-1/2-y,1/2+z	-4.76	10	N-H…C(π)
2m-d12	x,-1/2-y,-1/2+z	-4.76	10	N-H…C(π)
Total energy		-47.52		

Building unit is dimer

Dimer	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
2m_dim-d1	x,y,1+z	-6.03	7.2	N-H…N
2m_dim -d2	x,y,-1+z	-6.03	7.2	N-H…N
2m_dim -d3	1+x,y,z	-3.02	3.6	non-specific
2m_dim -d4	1+x,y,-1+z	-1.63	1.9	non-specific
2m_dim -d5	-1+x,y,z	-3.02	3.6	non-specific
2m_dim -d6	-1+x,y,1+z	-1.63	1.9	non-specific
2m_dim -d7	1-x,1/2+y,3/2-z	-1.71	2	non-specific
2m_dim -d8	1-x,-1/2+y,3/2-z	-1.71	2	non-specific
2m_dim -d9	2-x,1/2+y,1/2-z	-13.88	16.6	N-H…N, N-H…C(π)
2m_dim -d10	2-x,1/2+y,3/2-z	-13.88	16.6	N-H…N, N-H…C(π)
2m_dim-d11	2-x,-1/2+y,1/2-z	-13.88	16.6	N-H…N, N-H…C(π)
2m_dim-d12	2-x,-1/2+y,3/2-z	-13.88	16.6	N-H…N, N-H…C(π)
2m_dim-d13	3-x,1/2+y,1/2-z	-1.71	2	non-specific
2m_dim-d14	3-x,-1/2+y,1/2-z	-1.71	2	non-specific
Total energy		-83.71		

Table S4. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **2O.**

Building unit is molecule

Dimer	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
2o-d1	1/2+x,1/2-y,1-z	-5.33	11.3	N-H…N
2o-d2	1-x,1/2+y,1/2-z	-5.33	11.3	N-H…N
2o-d3	1-x,1/2+y,1/2-z	-1.77	3.8	non-specific
2o-d4	1-x,-1/2+y,1/2-z	-1.77	3.8	non-specific
2o-d5	1-x,-y,1-z	-4.78	10.2	non-specific
2o-d6	1-x,1-y,1-z	-6.10	13	N-H…N
2o-d7	1/2+x,y,1/2-z	-2.05	4.4	non-specific
2o-d8	-1/2+x,y,1/2-z	-2.05	4.4	non-specific
2o-d9	1/2-x,1/2+y,z	-4.81	10.2	N-H…C(π)
2o-d10	1/2-x,-1/2+y,z	-4.81	10.2	N-H…C(π)
2o-d11	3/2-x,1/2+y,z	-4.09	8.7	C-H…N
2o-d12	3/2-x,-1/2+y,z	-4.09	8.7	C-H…N
Total energy		-46.97		

Building unit is dimer

Dimer	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
2o_dim_d1	x,1+y,z	-5.91	7.1	N-H…N
2o_dim_d2	x,-1+y,z	-5.91	7.1	N-H…N
2o_dim_d3	1/2-x,1-y,1/2+z	-2.10	2.5	non-specific
fda_dim_d4	1/2-x,1-y,-1/2+z	-2.10	2.5	non-specific
fda_dim_d5	3/2-x,1-y,1/2+z	-2.10	2.5	non-specific
fda_dim_d6	3/2-x,1-y,-1/2+z	-2.10	2.5	non-specific
fda_dim_d7	1/2+x,1/2-y,1-z	-13.75	16.6	N-H…N, N-H…C(π)
fda_dim_d8	1/2+x,3/2-y,1-z	-13.75	16.6	N-H…N, N-H…C(π)
fda_dim_d9	-1/2+x,1/2-y,1-z	-13.75	16.6	N-H…N, N-H…C(π)
fda_dim_d10	-1/2+x,3/2-y,1-z	-13.75	16.6	N-H…N, N-H…C(π)
fda_dim_d11	1-x,1/2+y,1/2-z	-1.92	2.3	non-specific
2o_dim_d12	1-x,1/2+y,3/2-z	-1.92	2.3	non-specific
2o_dim_d13	1-x,-1/2+y,1/2-z	-1.92	2.3	non-specific
2o_dim_d14	1-x,-1/2+y,3/2-z	-1.92	2.3	non-specific
Total energy		-82.91		

Table S5. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **3.**

Dimer	Molecules	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
Molecule D					
3-d1	D-C	x,y,z	-7.47	14.7	N-H…C(π)
3-d2	D-A	x,y,z	-3.07	6	non-specific
3-d3	D-C	1+x,y,z	-7.91	15.5	N-H…C(π)
3-d4	D-B	1+x,y,z	-4.48	8.8	N-H…N
3-d5	D-A	1+x,y,z	-5.62	11	N-H…C(π)
3-d6	D-B	1+x,-1+y,z	-2.69	5.3	N-H…N
3-d7	D-C	1-x,1/2+y,1/2-z	-4.67	9.2	N-H…N
3-d8	D-B	1-x,-1/2+y,1/2-z	-6.24	12.2	N-H…N
3-d9	D-C	1-x,-1/2+y,1/2-z	-1.60	3.1	H…H
3-d10	D-D	2-x,1/2+y,1/2-z	-0.26	0.5	non-specific
3-d11	D-D	2-x,-1/2+y,1/2-z	-0.26	0.5	non-specific
3-d12	D-A	1-x,-y,-z	-4.69	9.2	N-H…N
3-d13	D-B	1-x,1-y,-z	-2.01	3.9	non-specific
Total energy			-50.98		
Molecule C					
3-d14	C-A	x,y,z	-5.30	10.5	N-H…N
3-d15	C-B	x,y,z	-3.39	6.7	N-H…N
3-d16	C-D	x,y,z	-7.47	14.8	N-H…C(π)
3-d17	C-B	x,-1+y,z	-1.83	3.6	non-specific
3-d18	C-D	-1+x,y,z	-7.91	15.7	N-H…C(π)
3-d19	C-B	-x,-1/2+y,1/2-z	-3.79	7.5	non-specific
3-d20	C-D	1-x,1/2+y,1/2-z	-1.60	3.2	H…H
3-d21	C-C	1-x,1/2+y,1/2-z	-3.16	6.3	N-H…N
3-d22	C-D	1-x,-1/2+y,1/2-z	-4.67	9.3	N-H…N
3-d23	C-C	1-x,-1/2+y,1/2-z	-3.16	6.3	N-H…N
3-d24	C-B	1-x,-1/2+y,1/2-z	-5.50	10.9	N-H…C(π)
3-d25	C-A	1-x,-y,-z	-0.26	0.5	non-specific
3-d26	C-A	x,1/2-y,1/2+z	-2.31	4.6	C-H…N
Total energy			-50.35		
Molecule B					
3-d27	B-C	x,y,z	-3.39	7.1	N-H…N
3-d28	B-A	x,y,z	-2.07	4.4	H…H
3-d29	B-C	x,1+y,z	-1.83	3.9	non-specific
3-d30	B-A	x,1+y,z	-2.90	6.1	N-H…N
3-d31	B-D	-1+x,y,z	-4.48	9.4	N-H…N
3-d32	B-D	-1+x,1+y,z	-2.69	5.7	N-H…N
3-d33	B-C	-x,1/2+y,1/2-z	-3.79	8	non-specific
3-d34	B-D	1-x,1/2+y,1/2-z	-6.24	13.2	N-H…N
3-d35	B-C	1-x,1/2+y,1/2-z	-5.50	11.6	N-H…C(π)

3-d36	B-A	-x,1-y,-z	-5.78	12.2	N-H…C(π)
3-d37	B-B	-x,1-y,-z	-1.59	3.4	non-specific
3-d38	B-A	1-x,1-y,-z	-5.14	10.8	C-H…C(π)
3-d39	B-D	1-x,1-y,-z	-2.01	4.2	non-specific
Total energy			-47.42		
Molecule A					
3-d40	A-C	x,y,z	-5.30	11.7	N-H…N
3-d41	A-D	x,y,z	-3.07	6.8	non-specific
3-d42	A-B	x,y,z	-2.07	4.6	H…H
3-d43	A-B	x,-1+y,z	-2.90	6.4	N-H…N
3-d44	A-D	-1+x,y,z	-5.62	12.4	N-H…C(π)
3-d45	A-B	-x,1-y,-z	-5.78	12.8	N-H…C(π)
3-d46	A-A	1-x,-y,-z	-7.61	16.8	N-H…C(π)
3-d47	A-D	1-x,-y,-z	-4.69	10.3	N-H…N
3-d48	A-C	1-x,-y,-z	-0.26	0.6	non-specific
3-d49	A-B	1-x,1-y,-z	-5.14	11.3	C-H…C(π)
3-d50	A-A	1-x,1-y,-z	-0.58	1.3	non-specific
3-d51	A-C	x,1/2-y,-1/2+z	-2.31	5.1	C-H…N
Total energy			-45.32		

Table S6. Pairwise interaction energies (kcal/mol) of the basic molecule with neighbouring ones in crystal of **4.**

Dimer	Molecules	Symmetry operation	E_{int}, kcal mol^{-1}	Contribution to the total interaction energy, %	Interaction
Molecule A					
4-d1	A-B	x,y,z	-5.08	9.4	N-H…N
4-d2	A-C	x,y,z	-4.41	8.19	N-H…N
4-d3	A-A	x,1+y,z	-4.17	7.7	non-specific
4-d4	A-C	x,1+y,z	-1.78	3.3	C-H…N
4-d5	A-A	x,-1+y,z	-4.17	7.7	non-specific
4-d6	A-B	x,-1+y,z	-0.80	1.5	non-specific
4-d7	A-A	1-x,1/2+y,3/2-z	-6.04	11.2	N-H…C(π)
4-d8	A-B	1-x,1/2+y,3/2-z	-2.73	5.1	N-H…N
4-d9	A-A	1-x,-1/2+y,3/2-z	-6.04	11.2	N-H…C(π)
4-d10	A-B	1-x,-1/2+y,3/2-z	-2.30	4.3	C-H…π
4-d11	A-A	2-x,1/2+y,3/2-z	-6.09	11.3	N-H…C(π)
4-d12	A-C	2-x,1/2+y,3/2-z	-4.16	7.7	N-H…N
4-d13	A-A	2-x,-1/2+y,3/2-z	-6.09	11.3	N-H…C(π)
Total energy			-53.84		
Molecule B					
4-d14	B-A	x,y,z	-5.08	10.2	N-H…N
4-d15	B-C	x,y,z	-3.54	7.1	non-specific
4-d16	B-B	x,1+y,z	-4.36	8.8	non-specific
4-d17	B-C	x,1+y,z	-6.04	12.2	N-H…C(π)
4-d18	B-A	x,1+y,z	-0.80	1.6	non-specific
4-d19	B-B	x,-1+y,z	-4.36	8.8	non-specific
4-d20	B-C	-1+x,y,z	-6.04	12.2	N-H…C(π)
4-d21	B-C	-1+x,1+y,z	-3.54	7.1	non-specific
4-d22	B-A	1-x,1/2+y,3/2-z	-2.30	4.6	non-specific
4-d23	B-A	1-x,-1/2+y,3/2-z	-2.73	5.5	N-H…N
4-d24	B-A	1-x,1-y,2-z	-0.80	1.6	non-specific
4-d25	B-A	1-x,2-y,2-z	-5.08	10.2	N-H…N
4-d26	B-A	x,3/2-y,1/2+z	-2.30	4.6	non-specific
4-d27	B-A	x,5/2-y,1/2+z	-2.73	5.5	N-H…N
Total energy			-49.70		
Molecule C					
4-d28	C-A	x,y,z	-4.41	9.2	N-H…N
4-d29	C-B	x,y,z	-3.54	7.4	non-specific
4-d30	C-C	x,1+y,z	-4.03	8.4	non-specific
4-d31	C-A	x,-1+y,z	-1.78	3.7	non-specific
4-d32	C-B	x,-1+y,z	-6.04	12.6	N-H…C(π)

4-d33	C-C	x,-1+y,z	-4.03	8.4	non-specific
4-d34	C-B	1+x,y,z	-6.04	12.6	N-H…C(π)
4-d35	C-B	1+x,-1+y,z	-3.54	7.4	non-specific
4-d36	C-A	2-x,-1/2+y,3/2-z	-4.16	8.7	N-H…N
4-d37	C-A	2-x,1-y,2-z	-4.41	8.7	N-H…N
4-d38	C-A	2-x,2-y,2-z	-1.78	3.7	C-H…N
4-d39	C-A	x,3/2-y,1/2+z	-4.16	8.7	N-H…N
Total energy			-47.92		

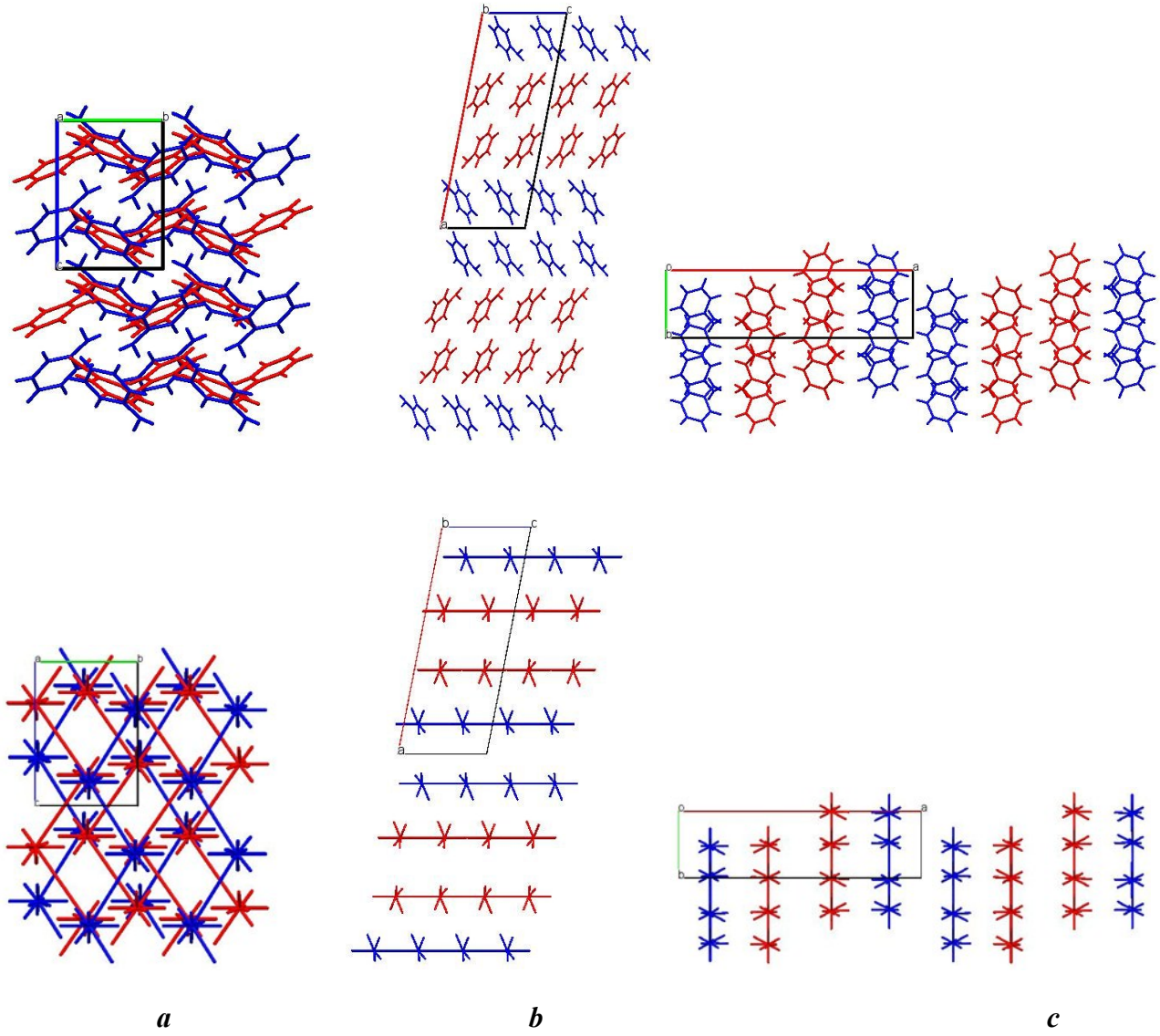
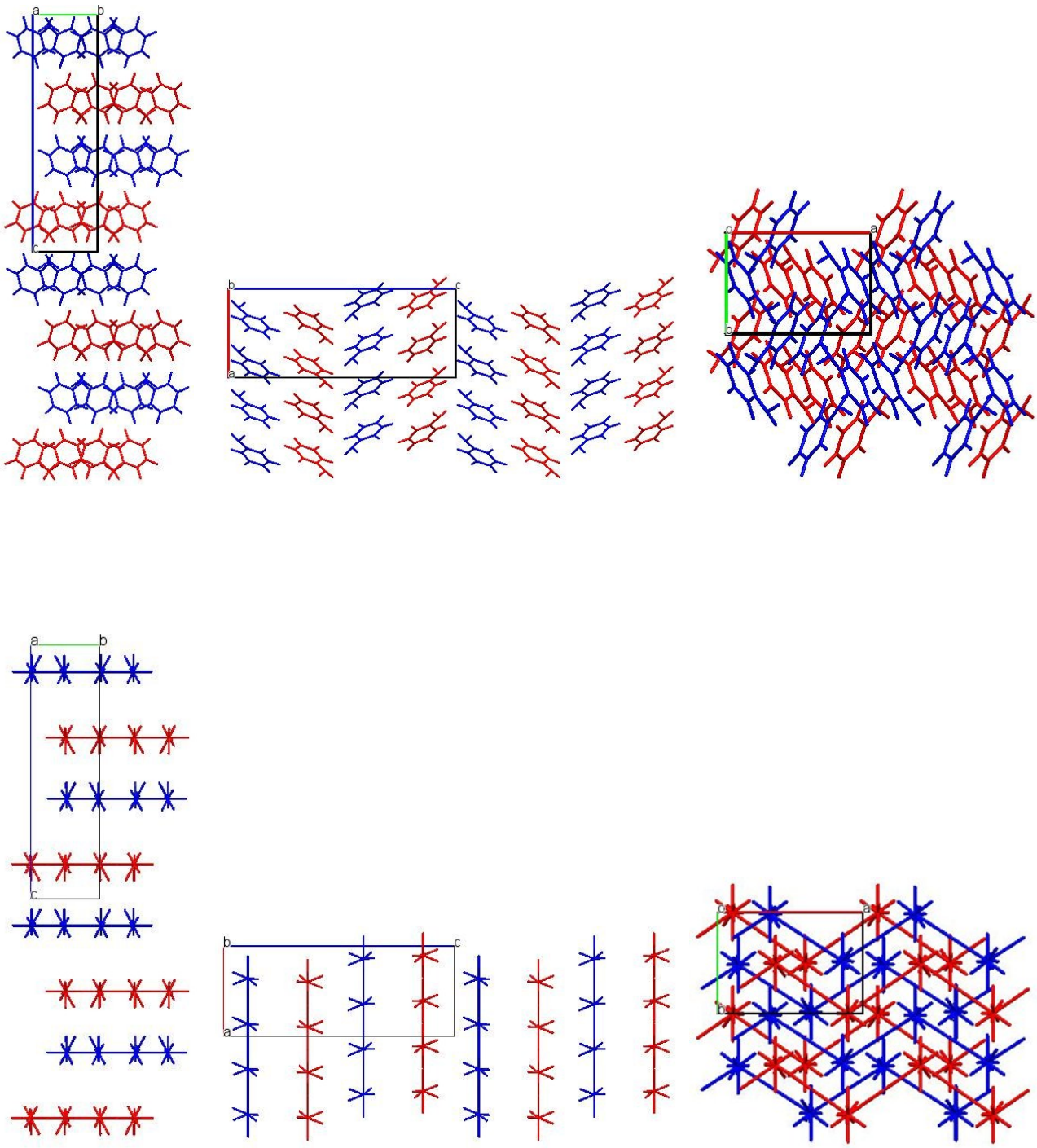


Figure S1. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals **1M**. The projection along *a*, *b* and crystallographic direction is presented. The chains/columns of the different molecules (A and B) are highlighted by different colors.



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

Figure S2. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals **1O**. The projection along *a*, *b* and *c* crystallographic direction is presented. The chains/columns of the different molecules (A and B) are highlighted by different colors.

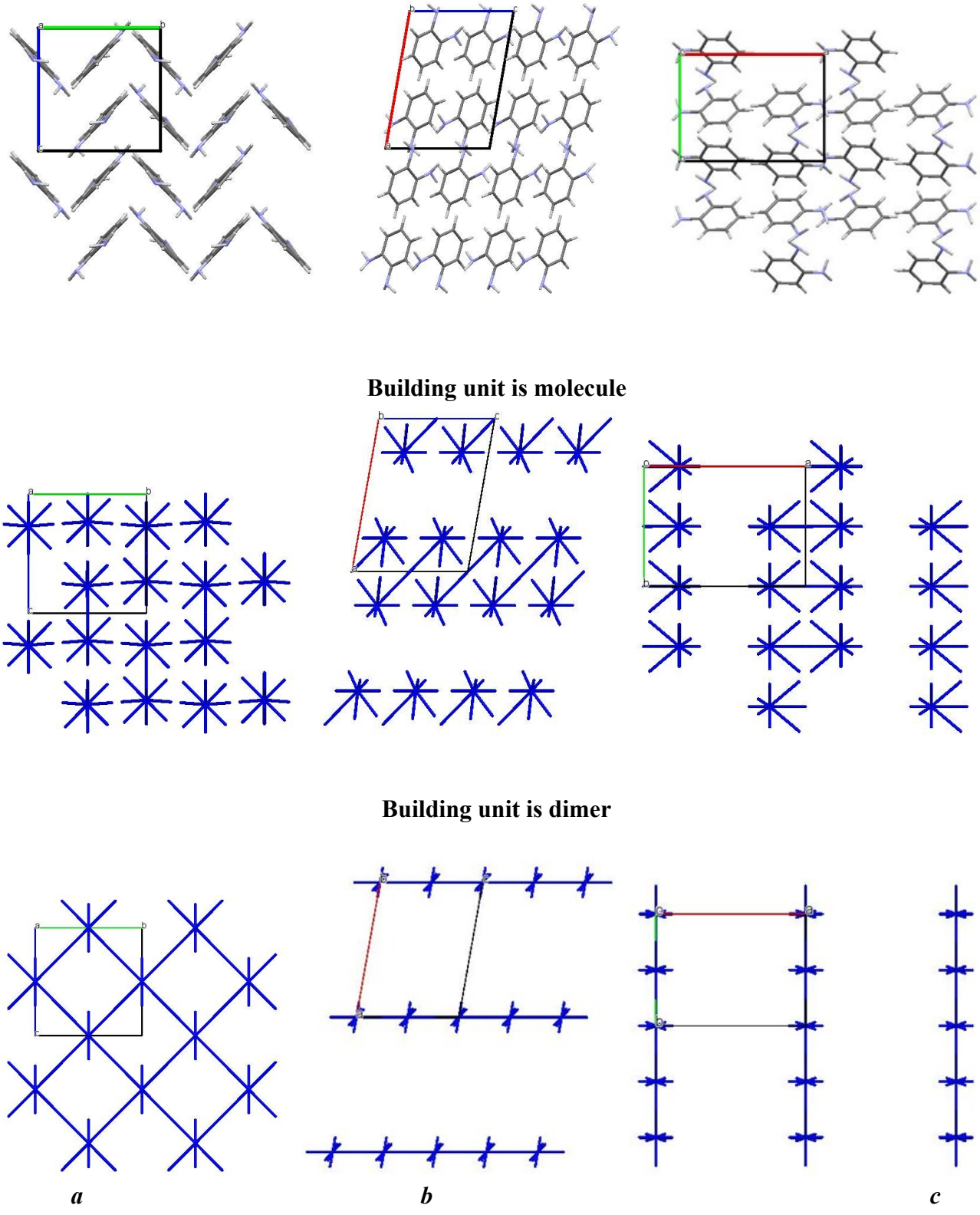
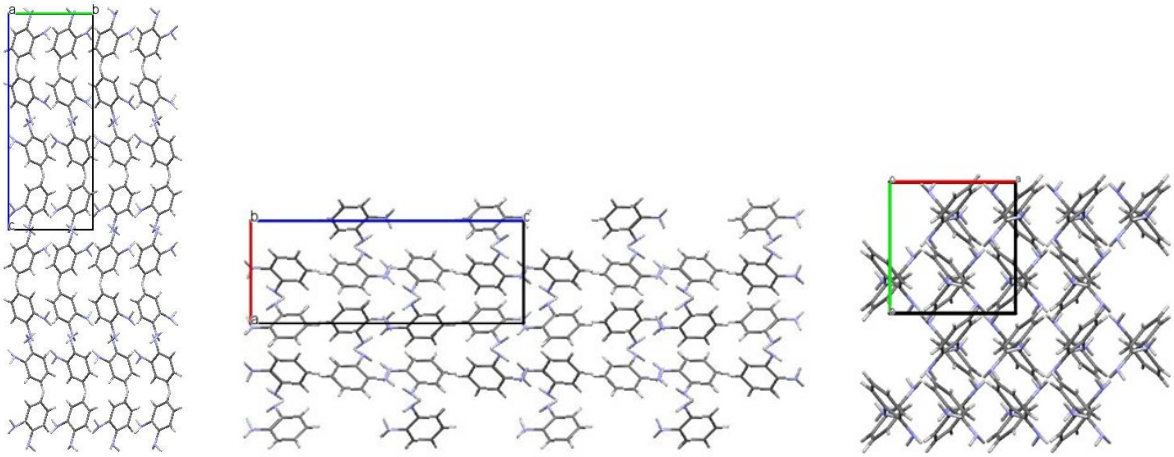
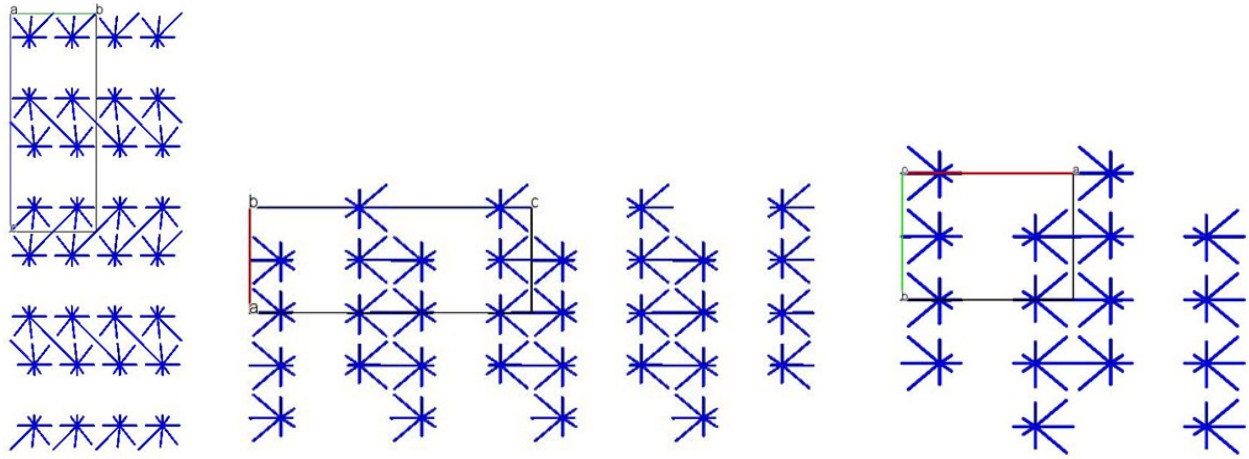


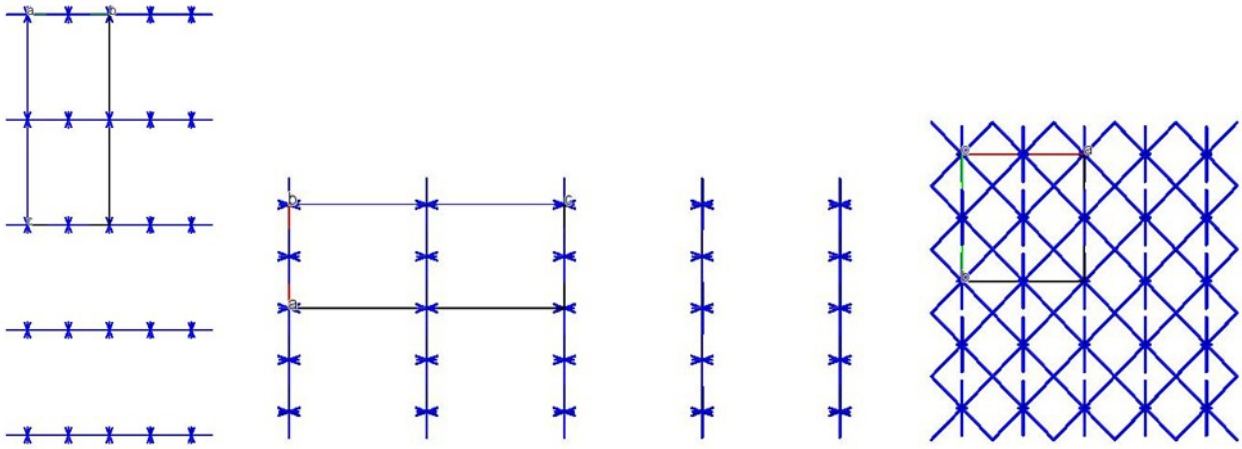
Figure S3. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals **2M**. The projection along *a*, *b* and *c* crystallographic direction is presented.



Building unit is molecule

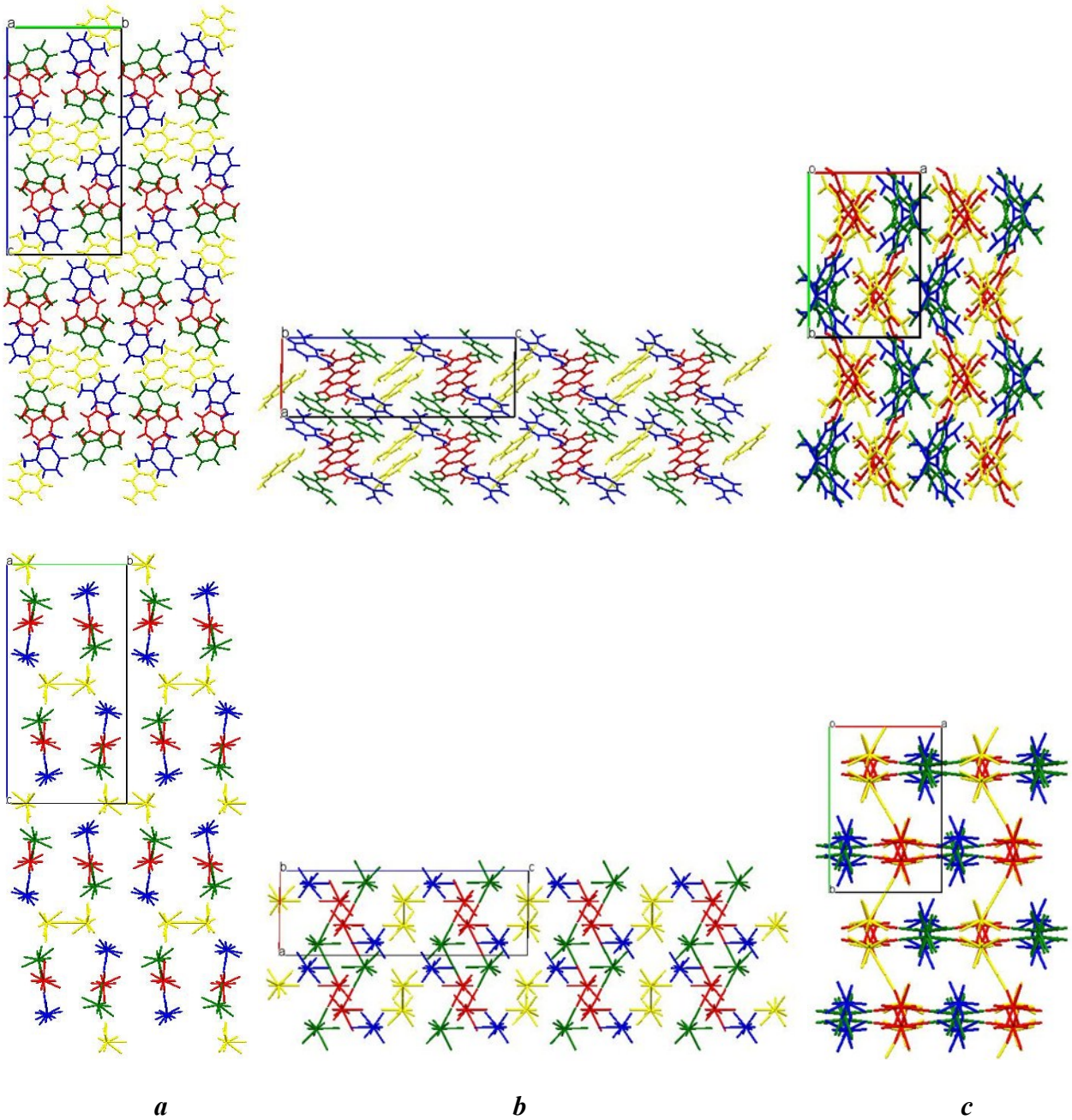


Building unit is dimer



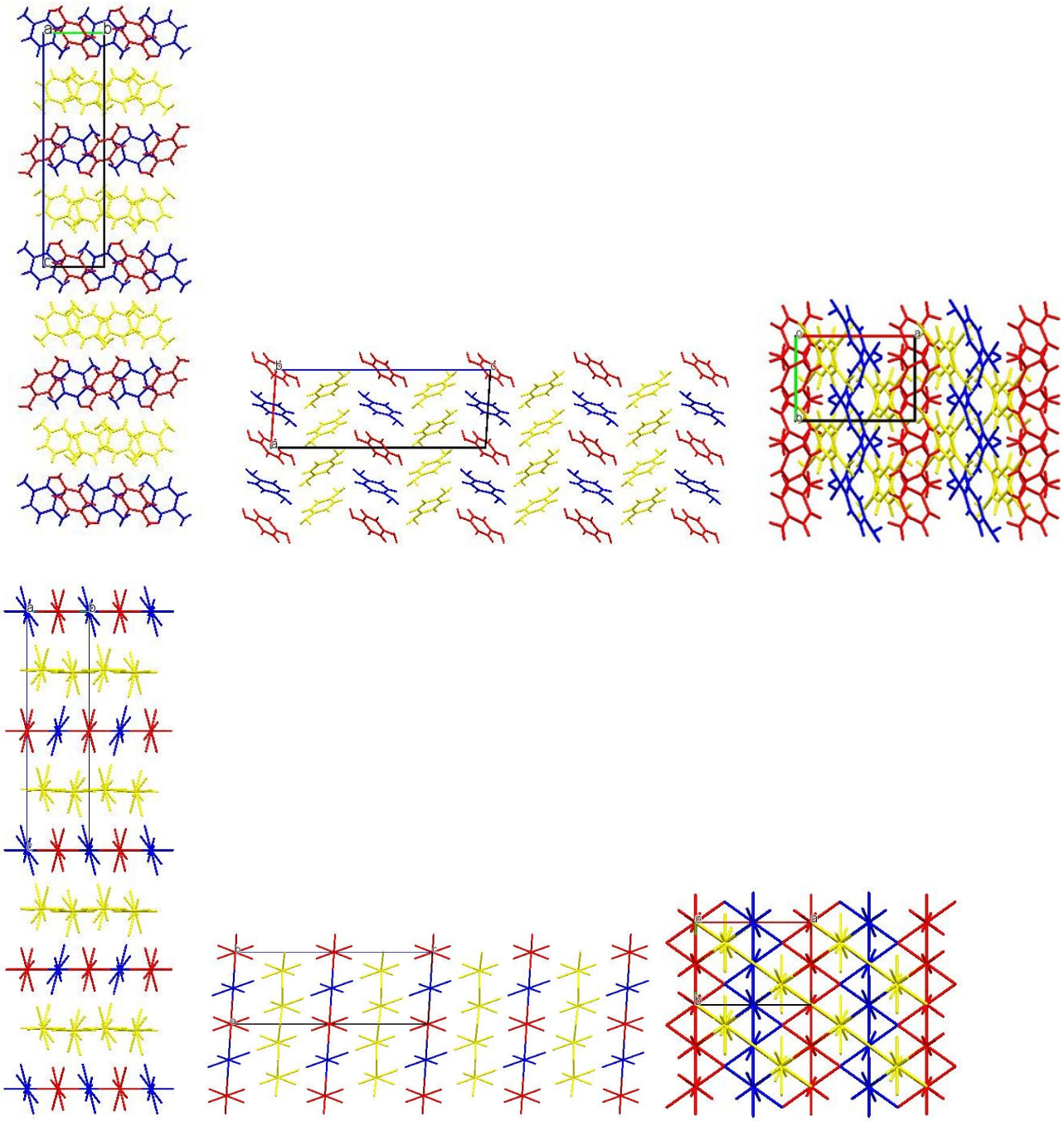
a ***b*** ***c***

Figure S4. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals **2O**. The projection along *a*, *b* and *c* crystallographic direction is presented.



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

Figure S5. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals **3**. The projection along *a*, *b* and *c* crystallographic direction is presented. The chains/columns of the different molecules (A, B, C and D) are highlighted by different colors.



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

Figure S6. Packing of molecules (top) and energetic vector diagram (bottom) in the crystals **4**. The projection along *a*, *b* and *c* crystallographic direction is presented. The chains/columns of the different molecules (A, B and C) are highlighted by different colors.