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Supporting information for article:

Polymorphism of methyl 4-amino-3-phenylisothiazole-5-carboxylate: an experimental and theoretical study

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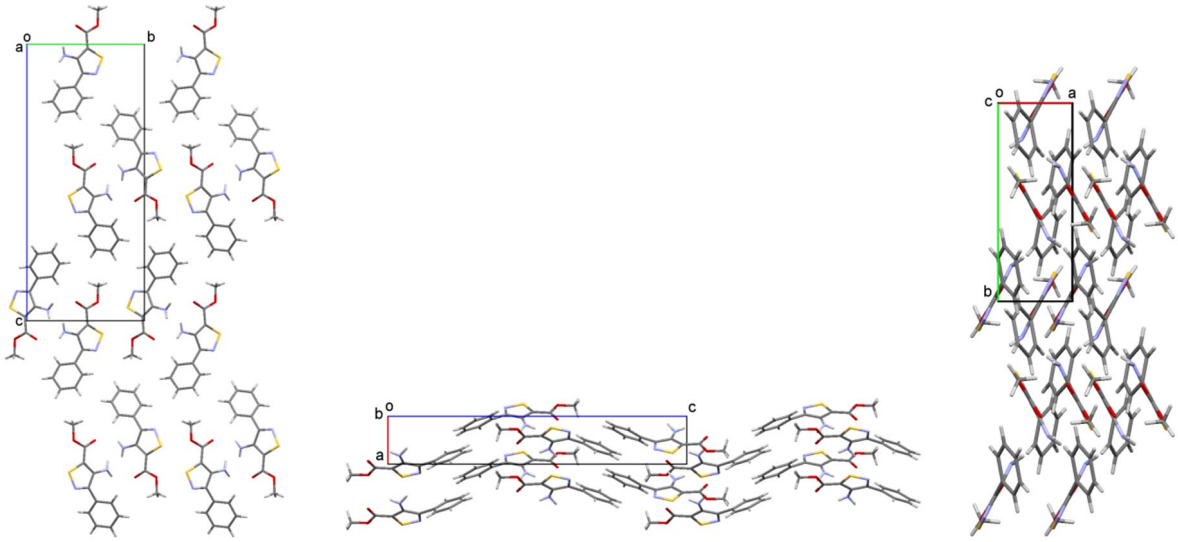

Fig. S1. Molecules packing in structure **1a**.

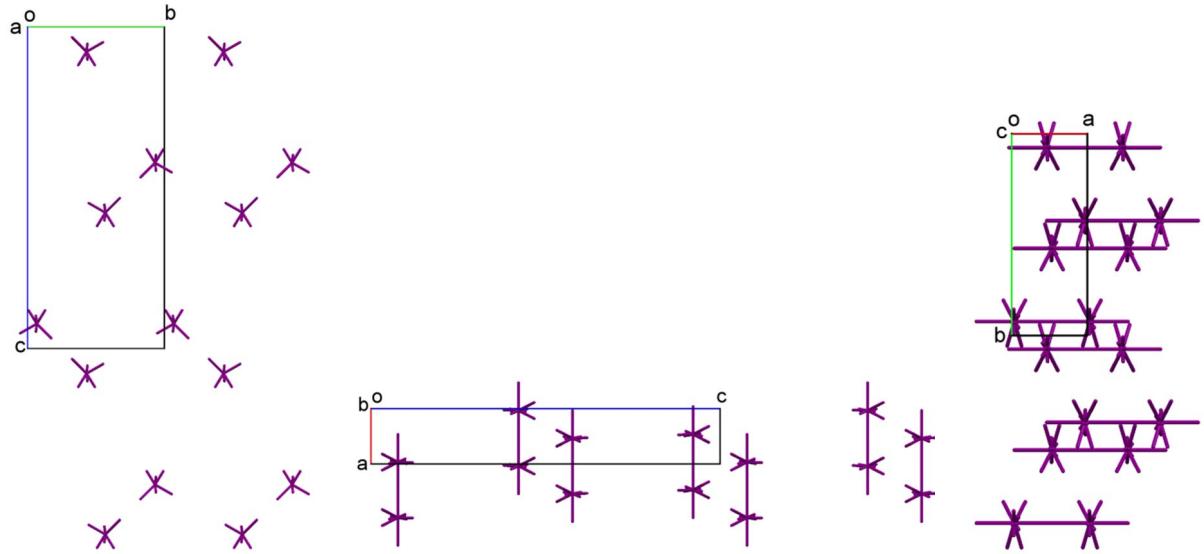

Fig. S2. Packing of energy-vector diagrams in structure **1a**.

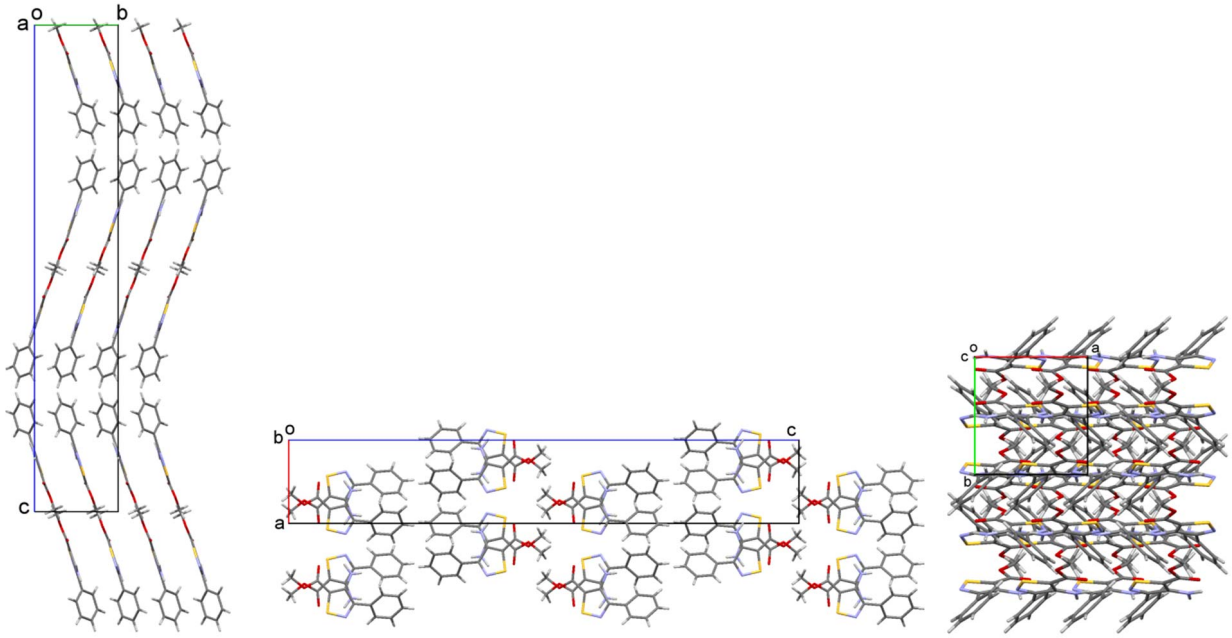

Fig. S3. Molecules packing in structure **1b**.

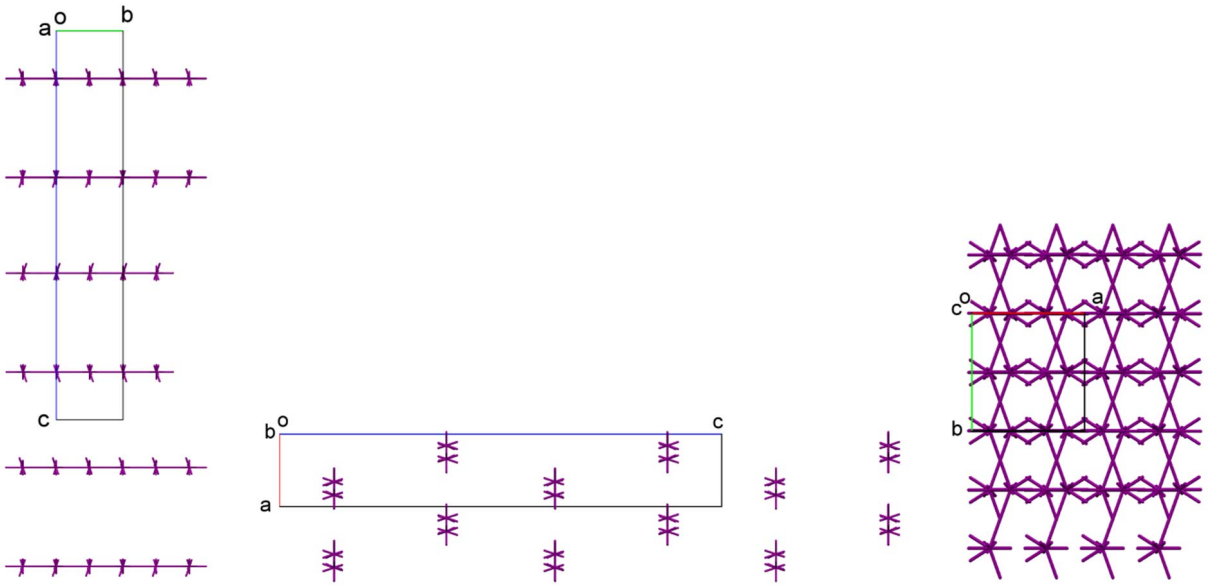

Fig. S2. Packing of energy-vector diagrams in structure **1b**.

Table S1 Symmetry codes, interaction energy of the basic molecule with neighbouring ones (E_{int}, kJ/mol) and the contribution of this energy to the total interaction energy (%) in crystals **1a**.

Dimer	Symmetry operation	E_{int}, kJ/mol	The contribution to the total interaction energy, %	Type of interaction
d1	-1+x,y,z	-53.09	20.0	stacking
d2	1+x,y,z	-53.09	20.0	stacking
d3	1/2+x,3/2-y,1-z	-30.73	11.6	N-H…O/N-H…N
d4	-1/2+x,3/2-y,1-z	-30.73	11.6	N-H…O/N-H…N
d5	1/2+x,1/2-y,1-z	-20.14	7.6	dispersion
d6	-1/2+x,1/2-y,1-z	-20.14	7.6	dispersion
d7	1-x,1/2+y,3/2-z	-12.81	4.8	dispersion
d8	1-x,-1/2+y,3/2-z	-12.81	4.8	dispersion
d9	2-x,-1/2+y,3/2-z	-6.41	2.4	dispersion
d10	2-x,1/2+y,3/2-z	-6.41	2.4	dispersion
d11	1/2-x,1-y,1/2+z	-5.15	1.9	dispersion
d12	1/2-x,1-y,-1/2+z	-5.15	1.9	dispersion
d13	3/2-x,1-y,-1/2+z	-4.10	1.5	dispersion
d14	3/2-x,1-y,1/2+z	-4.10	1.5	dispersion
	Total E_{int}, kcal/mol	-264.81		

Table S2 Symmetry codes, interaction energy of the basic molecule with neighbouring ones (E_{int}, kJ/mol) and the contribution of this energy to the total interaction energy (%) in crystals **1b**.

Dimer	Symmetry operation	E_{int}, kJ/mol	The contribution to the total interaction energy, %	Type of interaction
d1	3/2-x,-1/2+y,z	-53.97	21.2	stacking
d2	3/2-x,1/2+y,z	-53.97	21.2	stacking
d3	1/2-x,1/2+y,z	-22.69	8.9	dispersion
d4	1/2-x,-1/2+y,z	-22.69	8.9	dispersion
d5	1+x,y,z	-20.05	7.9	N-H…N
d6	-1+x,y,z	-20.05	7.9	N-H…N
d7	-1/2+x,3/2-y,1-z	-10.59	4.2	dispersion
d8	1/2+x,3/2-y,1-z	-10.59	4.2	dispersion
d9	2-x,1-y,1-z 0 0	-7.75	3.1	dispersion
d10	-1/2+x,y,3/2-z 0 0	-7.70	3.0	dispersion
d11	1/2+x,y,3/2-z 0 0	-7.70	3.0	dispersion
d12	1-x,1/2+y,3/2-z 0 0	-6.95	2.7	dispersion
d13	1-x,-1/2+y,3/2-z 0 0	-6.95	2.7	dispersion
d14	2-x,2-y,1-z 0 0	-2.64	1.0	dispersion
	Total E_{int}, kcal/mol	-254.26		