Electronic Supporting Information

For paper

The formation of two thiotriazoline polymorphs: study from the energetic view point

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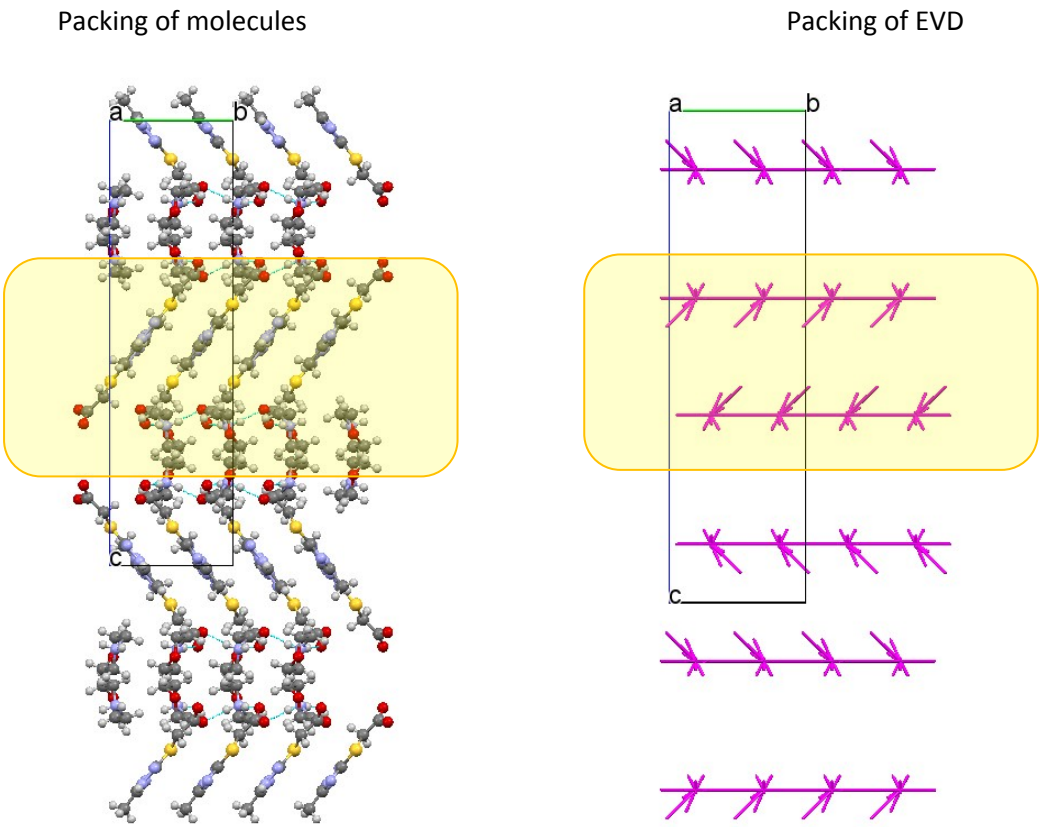

Figure S1. Crystal structure of orthorhombic modification presented as packing of molecules and energy-vector-diagram of intermolecular interactions. Projection along *a* axis. Columns are highlighted.

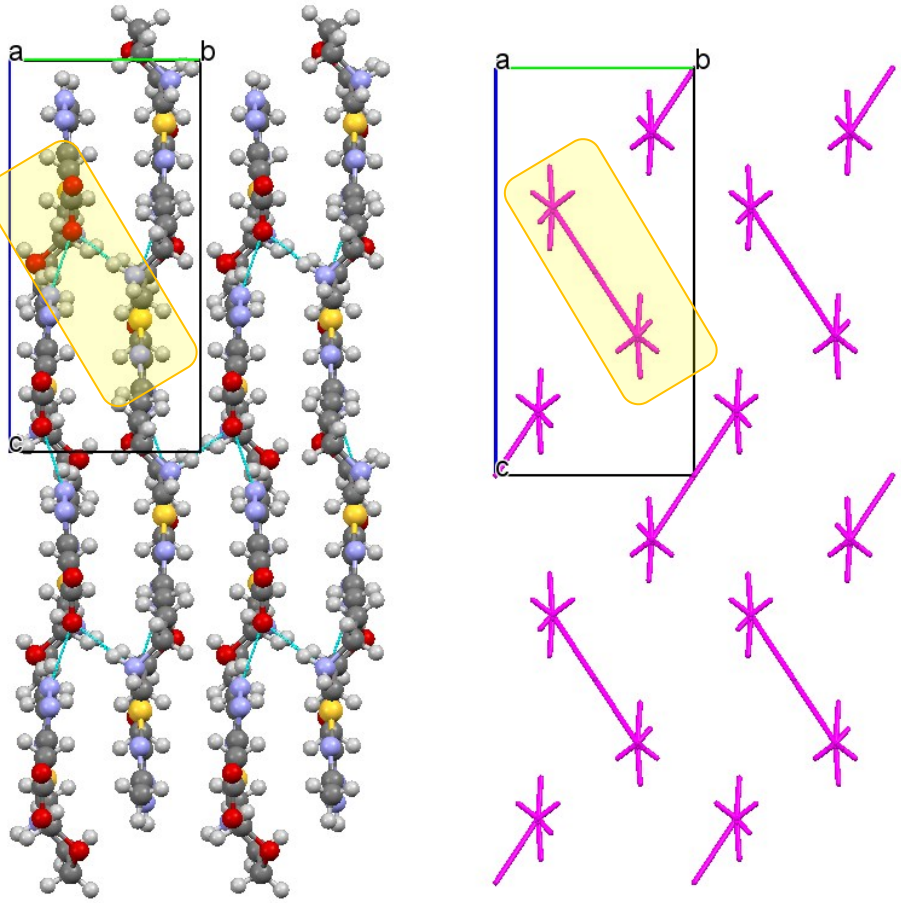

Figure S2. Crystal structure of monoclinic modification presented as packing of molecules and energy-vector-diagram of intermolecular interactions. Projection along *a* axis. Dimers are highlighted.

Table S1. Numbering of dimers, symmetry operation of second ion of dimer and energy of intermolecular interactions in dimers formed by the basic cation (**OMc**) or anion (**OMa**) in the orthorhombic crystals of thiotriazoline.

Dimer	Mole-cules	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Bonding type	H…A, Å	D-H…A, deg
OMa_1	A-C	x,y,z	-20,7	13,5	N-H…O	1.73	165
OMa_2	A-C	x,-1+y,z	-3,9	2,5			
OMa_3	A-C	-x,-1/2+y,1/2-z	-4,5	2,9			
OMa_4	A-C	1/2+x,1/2-y,1-z	-1,2	0,8			
OMa_5	A-A	1/2+x,-1/2-y,1-z	-9,3	6,1			
OMa_6	A-A	-1/2+x,-1/2-y,1-z	-9,3	6,0			
OMa_7	A-A	-x,-y,1-z	-4,6	3,0			
OMa_8	A-C	-x,-y,1-z	-1,7	1,1			
OMa_9	A-A	-x,-1-y,1-z	-2,2	1,5			
OMa_100	A-C	1/2+x,y,1/2-z	-2,5	1,6			
OMa_11	A-A	1/2-x,1/2+y,z	-5,1	3,3			
OMa_12	A-A	1/2-x,-1/2+y,z	-5,1	3,3			
OMa_13	A-C	1/2-x,-1/2+y,z	-18,8	12,2	N-H…O	1.73	175
OMa_14	A-C	-1/2-x,-1/2+y,z	-3,3	2,2			
OMc_1	C-A	x,y,z	-20,7	13,5	N-H…O	1.73	165
OMc_2	C-A	x,1+y,z	-3,9	2,5			
OMc_3	C-A	-x,1/2+y,1/2-z	-4,5	2,9			
OMc_4	C-C	-x,1/2+y,1/2-z	0,0	-0,0			
OMc_5	C-C	-x,-1/2+y,1/2-z	0,0	-0,0			
OMc_6	C-A	-1/2+x,1/2-y,1-z	-1,2	0,8			
OMc_7	C-A	-x,-y,1-z	-1,7	1,1			
OMc_8	C-C	1/2+x,y,1/2-z	-0,5	0,4			
OMc_9	C-C	-1/2+x,y,1/2-z	-0,5	0,4			
OMc_10	C-A	-1/2+x,y,1/2-z	-2,5	1,6			
OMc_11	C-A	1/2-x,1/2+y,z	-19,2	12,5	N-H…O	1.73	175
OMc_12	C-A	-1/2-x,1/2+y,z	-3,3	2,2			
OMc_13	C-C	-1/2-x,1/2+y,z	-1,8	1,2			
OMc_14	C-C	-1/2-x,-1/2+y,z	-1,8	1,2			

Table S2. Numbering of dimers, symmetry operation of second cation-anion pair of dimer and energy of intermolecular interactions in dimers formed by the cation-anion pair (**OMs**) in the orthorhombic crystals of thiotriazoline. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Bonding type	H…A, Å	D-H…A, deg
OMs_1	x,1+y,z	-3,2	-3,1			
OMs_2	x,-1+y,z	-3,2	-3,1			
OMs_3	-x,1/2+y,1/2-z	-4,2	-4,3			
OMs_4	-x,-1/2+y,1/2-z	-4,2	-4,3			
OMs_5	1/2+x,1/2-y,1-z	-0,9	-0,9			
OMs_6	1/2+x,-1/2-y,1-z	-9,8	-9,6	N-H…N (1)	1.87	167
OMs_7	-1/2+x,1/2-y,1-z	-0,9	-0,9			
OMs_8	-1/2+x,-1/2-y,1-z	-9,7	-9,6	N-H…N (1)	1.87	167
OMs_9	-x,-y,1-z	-7,4	-7,3	dispersion		
OMs_10	-x,-1-y,1-z	-2,6	-2,6			
OMs_11	1/2+x,y,1/2-z	-2,6	-2,6			
OMs_12	-1/2+x,y,1/2-z	-2,6	-2,6			
OMs_13	**1/2-x,1/2+y,z**	**-20,2**	**-19,9**	**N-H…O** **C-H…O**	**1.73** **2.38**	**175** **174**
OMs_14	**1/2-x,-1/2+y,z**	**-20,2**	**-19,9**	**N-H…O** **C-H…O**	**1.73** **2.38**	**175** **174**
OMs_15	-1/2-x,1/2+y,z	-4,8	-4,7			
OMs_16	-1/2-x,-1/2+y,z	-4,8	-4,7			

Table S3. Numbering of dimers, symmetry operation of second ion of dimer and energy of intermolecular interactions in dimers formed by the basic cation (**MMc**) or anion (**MMa**) in the monoclinic crystals of thiotriazoline.

Dimer	Mole-cules	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Bonding type	H…A, Å	D-H…A, deg
MMa_1	A-	x,y,z	-5,5	3,7			
MMa_2	A-C	x,1+y,z	-6,1	4,1			
MMa_3	A-A	-x,1/2+y,1/2-z	-1,4	0,9			
MMa_4	A-C	-x,1/2+y,1/2-z	-19,4	12,9	N-H…O	1.68	172
MMa_5	A-A	-x,-1/2+y,1/2-z	-1,4	0,9			
MMa_6	A-A	1-x,1/2+y,1/2-z	-3,5	2,3			
MMa_7	A-C	1-x,1/2+y,1/2-z	-4,6	3,1			
MMa_8	A-A	1-x,-1/2+y,1/2-z	-3,5	2,3			
MMa_9	A-C	-x,-y,-z	-5,1	3,4			
MMa_10	A-C	1-x,-y,-z	-1,5	1,0			
MMa_11	A-A	1-x,1-y,-z	-0,4	0,2			
MMa_12	A-A	x,1/2-y,1/2+z	-7,5	5,0			
MMa_13	A-C	x,1/2-y,1/2+z	-17,3	11,5	N-H…O	1.86	169
MMa_14	A-A	x,1/2-y,-1/2+z	-7,5	5,0			
MMa_15	A-C	x,-1/2-y,1/2+z	-4,2	2,8			
MMc_1	C-A	x,y,z	-5,6	3,7			
MMc_2	C-A	x,-1+y,z	-6,1	4,1			
MMc_3	C-A	-x,-1/2+y,1/2-z	-19,5	12,9	N-H…O	1.68	172
MMc_4	C-A	1-x,-1/2+y,1/2-z	-4,6	3,1			
MMc_5	C-C	-x,-y,-z	2,0	-1,4			
MMc_6	C-A	-x,-y,-z	-5,1	3,4			
MMc_7	C-C	-x,-1-y,-z	0,2	-0,2			
MMc_8	C-A	1-x,-y,-z	-1,5	1,0			
MMc_9	C-A	x,1/2-y,-1/2+z	-17,3	11,5	N-H…O	1.86	169
MMc_10	C-A	x,-1/2-y,-1/2+z	-4,2	2,8			

Table S4. Numbering of dimers, symmetry operation of second cation-anion pair of dimer and energy of intermolecular interactions in dimers formed by the cation-anion pair (**MMs**) in the monoclinic crystals of thiotriazoline. Dimers belonging to basic structural motif are highlighted in bold.

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Bonding type	H…A, Å	D-H…A, deg
MMs_1	1+x,y,z	-3,7	-3,6			
MMs_2	-1+x,y,z	-3,7	-3,6			
MMs_3	-x,1/2+y,1/2-z	-11,7	-11,7	C-H…N (2)	2.64	127
MMs_4	-x,-1/2+y,1/2-z	-11,7	-11,6	C-H…N (2)	2.64	127
MMs_5	1-x,1/2+y,1/2-z	-3,9	-3,8			
MMs_6	1-x,-1/2+y,1/2-z	-3,9	-3,8			
MMs_7	-x,-y,1-z	-6,5	-6,5	dispersion		
MMs_8	**-x,1-y,1-z**	**-29,3**	**-29,2**	**N-H…O (2)**	**1.86**	**168**
MMs_9	1-x,1-y,-z	-0,6	-0,6			
MMs_10	x,1/2-y,1/2+z	-11,7	-11,6	N-H…O (1)	1.89	146
MMs_11	x,1/2-y,-1/2+z	-11,7	-11,7	N-H…O (1)	1.89	146
MMs_12	1+x,1/2-y,-1/2+z	-1,1	-1,1			
MMs_13	-1+x,1/2-y,1/2+z	-1,1	-1,1			