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Supporting information for article:

Polymorphic transition due to grinding: the case of 3-(1-(t-butoxy-carbonyl)azetidin-3-yl)-1,2-oxazole-4-carboxylic acid

Irina S. Konovalova, Anna M. Shaposhnyk, Vyacheslav N. Baumer, Bohdan A. Chalyk and Svitlana V. Shishkina

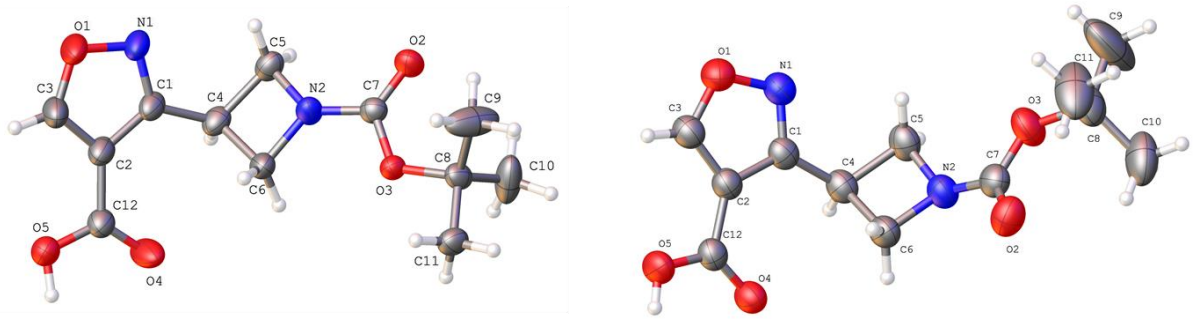

Figure S1 **Figure S1** Molecular structure of compound **1** in polymorphic structure **1a** (on the left) and **1b** (on the right).

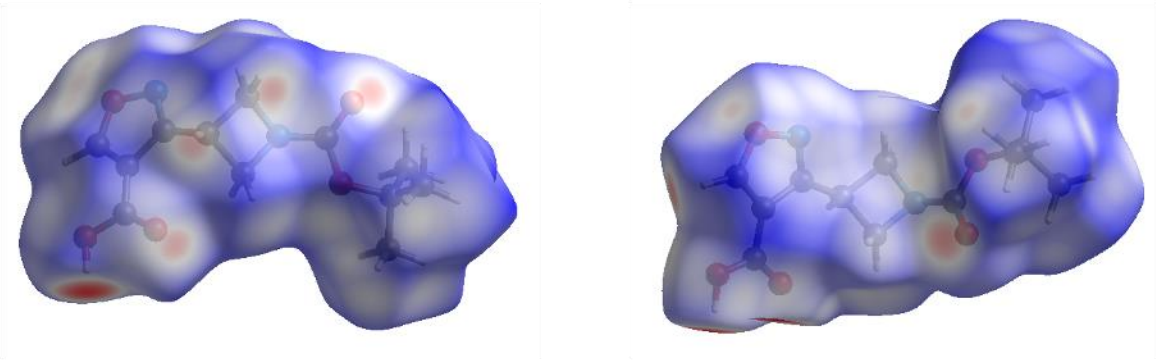

Figure S2 **Figure S2** Hirshfeld surfaces with mapped d_{norm} property projected and transparency to show the conformation of the molecules found in structure **1a** (on the left) and **1b** (on the right).

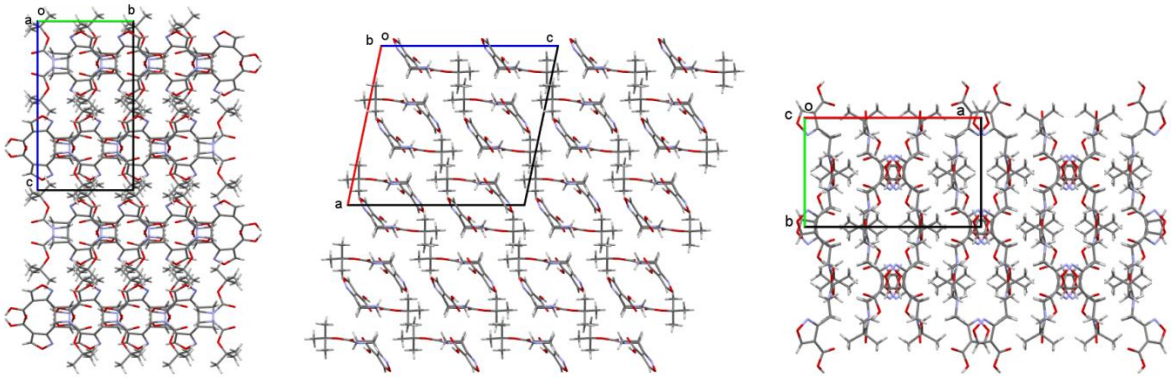

Figure S3 **Figure S3** Molecules packing in structure **1a**.

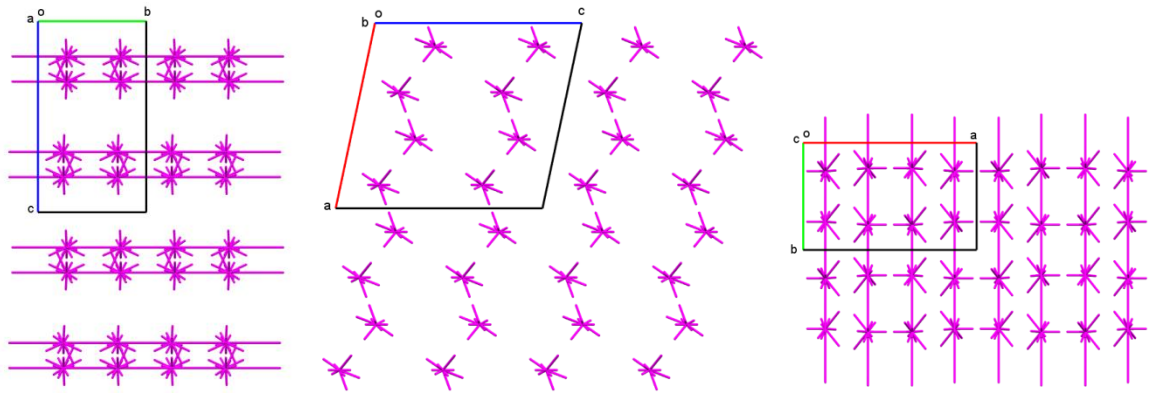

Figure S4 **Figure S4** Packing of energy-vector diagrams in structure **1a**.

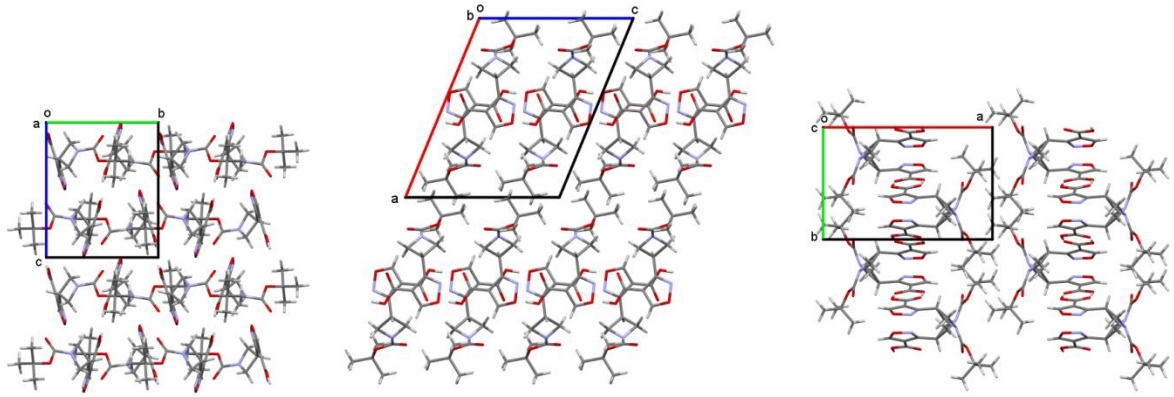

Figure S5 **Figure S5** Molecules packing in structure **1b**.

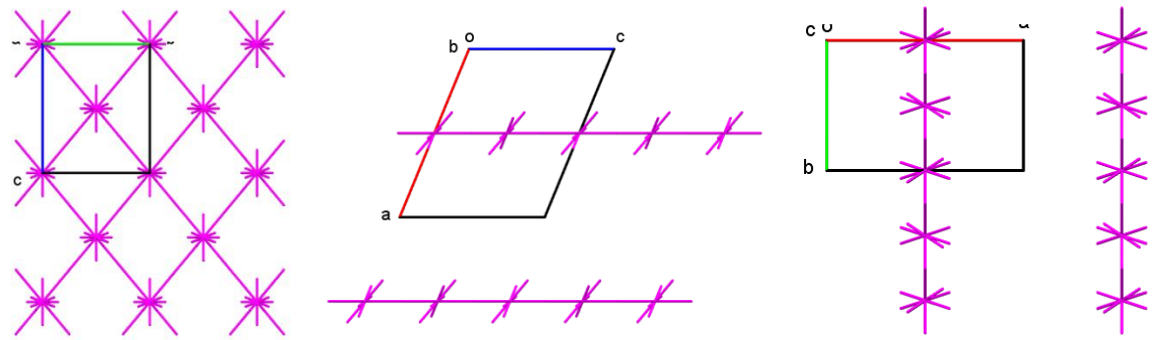

Figure S6 **Figure S6** Packing of energy-vector diagrams in structure **1b**.

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

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
1a_m1	x,1+y,z	-10.99	15.2	O-H…O
1a_m2	x,-1+y,z	-10.99	15.2	O-H…O
1a_m3	-x,y,1/2-z	-8.97	12.4	C-H…N(lp)
1a_m4	1/2-x,1/2+y,1/2-z	-6.98	9.7	C-H…O
1a_m5	1/2-x,-1/2+y,1/2-z	-6.98	9.7	C-H…O
1a_m6	1/2-x,1/2-y,1-z	-5.26	7.3	non-specific
1a_m7	-x,-y,-z	-3.57	5.0	non-specific
1a_m8	x,1-y,1/2+z	-2.25	3.1	non-specific
1a_m9	x,1-y,-1/2+z	-2.25	3.1	non-specific
1a_m10	1/2-x,3/2-y,1-z	-2.06	2.9	non-specific
1a_m11	-x,1+y,1/2-z	-2.01	2.8	non-specific
1a_m12	-x,-1+y,1/2-z	-2.01	2.8	non-specific
1a_m13	-x,1-y,1-z	-1.88	2.6	non-specific
1a_m14	x,-y,1/2+z	-1.69	2.3	non-specific
1a_m15	x,-y,-1/2+z	-1.69	2.3	non-specific
1a_m16	1/2+x,1/2-y,1/2+z	-1.29	1.8	non-specific
1a_m17	-1/2+x,1/2-y,-1/2+z	-1.29	1.8	non-specific
	Total E_{int}, kcal/mol	-72.17		

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

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
1b_m1	1-x,-y,-z	-21.14	27.5	O–H…O
1b_m2	1-x,1/2+y,1/2-z	-8.78	11.4	C–H…O
1b_m3	1-x,-1/2+y,1/2-z	-8.78	11.4	C–H…O
1b_m4	x,1/2-y,1/2+z	-6.59	8.6	non-specific
1b_m5	x,1/2-y,-1/2+z	-6.59	8.6	non-specific
1b_m6	1-x,-y,1-z	-5.16	6.7	non-specific
1b_m7	-x,1/2+y,1/2-z	-3.77	4.9	non-specific
1b_m8	-x,-1/2+y,1/2-z	-3.77	4.9	non-specific
1b_m9	-x,1-y,-z	-2.63	3.4	non-specific
1b_m10	x,3/2-y,1/2+z	-2.02	2.6	non-specific
1b_m11	x,3/2-y,-1/2+z	-2.02	2.6	non-specific
1b_m12	1-x,1-y,1-z	-1.64	2.1	non-specific
1b_m13	x,1+y,z	-1.59	2.1	non-specific
1b_m14	x,-1+y,z	-1.59	2.1	non-specific
1b_m15	-x,1-y,1-z	-0.88	1.1	non-specific
	Total E_{int}, kcal/mol	-76.96		

Table S3 **Table S3** Symmetry codes, interaction energy of the basic molecule with neighbouring ones (E_{int}, kcal/mol), the contribution of this energy to the total interaction energy (%) and bonding type in crystals **1b** (building unit is a centrosymmetric dimer).

Dimer	Symmetry operation	E_{int}, kcal/mol	Contribution to the total interaction energy, %	Interaction type
1b_d1	1-x,1/2+y,1/2-z	-15.40	13.3	C-H…O
1b_d2	1-x,1/2+y,-1/2-z	-15.40	13.3	C-H…O
1b_d3	1-x,-1/2+y,1/2-z	-15.40	13.3	C-H…O
1b_d4	1-x,-1/2+y,-1/2-z	-15.40	13.3	C-H…O
1b_d5	x,y,1+z	-5.49	4.7	non-specific
1b_d6	x,y,-1+z	-5.49	4.7	non-specific
1b_d7	x,1+y,z	-4.44	3.8	non-specific
1b_d8	x,-1+y,z	-4.44	3.8	non-specific
1b_d9	2-x,1/2+y,-1/2-z	-3.80	3.3	non-specific
1b_d10	2-x,-1/2+y,-1/2-z	-3.80	3.3	non-specific
1b_d11	-x,1/2+y,1/2-z	-3.80	3.3	non-specific
1b_d12	-x,-1/2+y,1/2-z	-3.80	3.3	non-specific
1b_d13	1+x,-1+y,z	-2.75	2.4	non-specific
1b_d14	-1+x,1+y,z	-2.75	2.4	non-specific
1b_d15	1-x,3/2+y,1/2-z	-2.19	1.9	non-specific
1b_d16	1-x,3/2+y,-1/2-z	-2.19	1.9	non-specific
1b_d17	1-x,-3/2+y,1/2-z	-2.19	1.9	non-specific
1b_d18	1-x,-3/2+y,-1/2-z	-2.19	1.9	non-specific
1b_d19	x,1+y,1+z	-1.74	1.5	non-specific
1b_d20	x,-1+y,-1+z	-1.74	1.5	non-specific
1b_d21	1+x,-1+y,-1+z	-0.89	0.8	non-specific
1b_d22	-1+x,1+y,1+z	-0.89	0.8	non-specific
	Total E_{int}, kcal/mol	-116.16		