STRUCTURAL CHEMISTRY

Volume 76 (2020)

Supporting information for article:

Concomitant polymorphic forms of 3-cyclopropyl-5-(2-hydrazinylpyridin-3-yl)-1,2,4-oxadiazole

Svitlana V. Shishkina, Irina S. Konovalova, Veronika R. Karpina, Svitlana S. Kovalenko, Sergiy M. Kovalenko and Natalya D. Bunyatyan

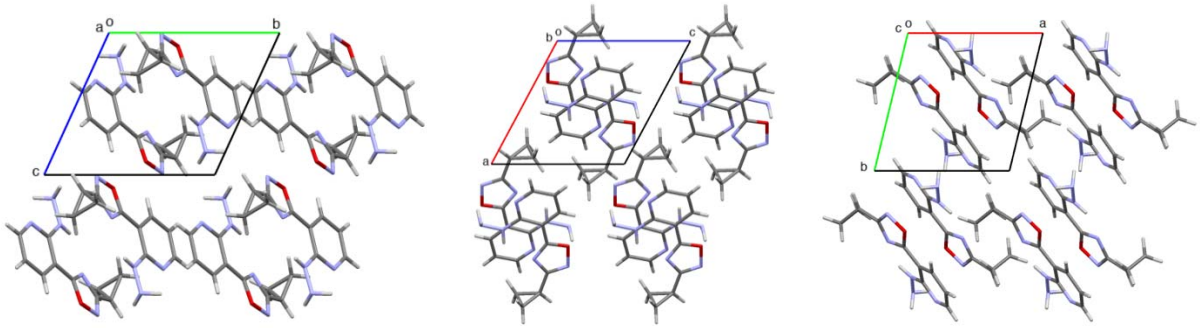

Fig. S1. Molecules packing in structure **1t**.

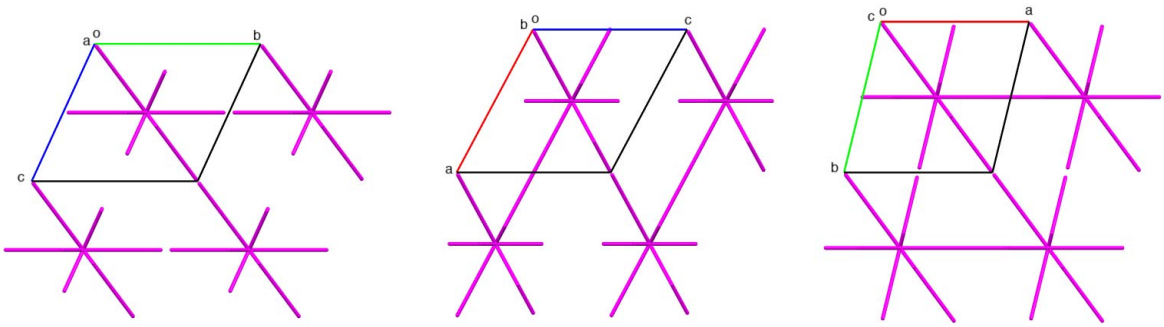

Fig. S2. Packing of energy-vector diagrams in structure **1t**.

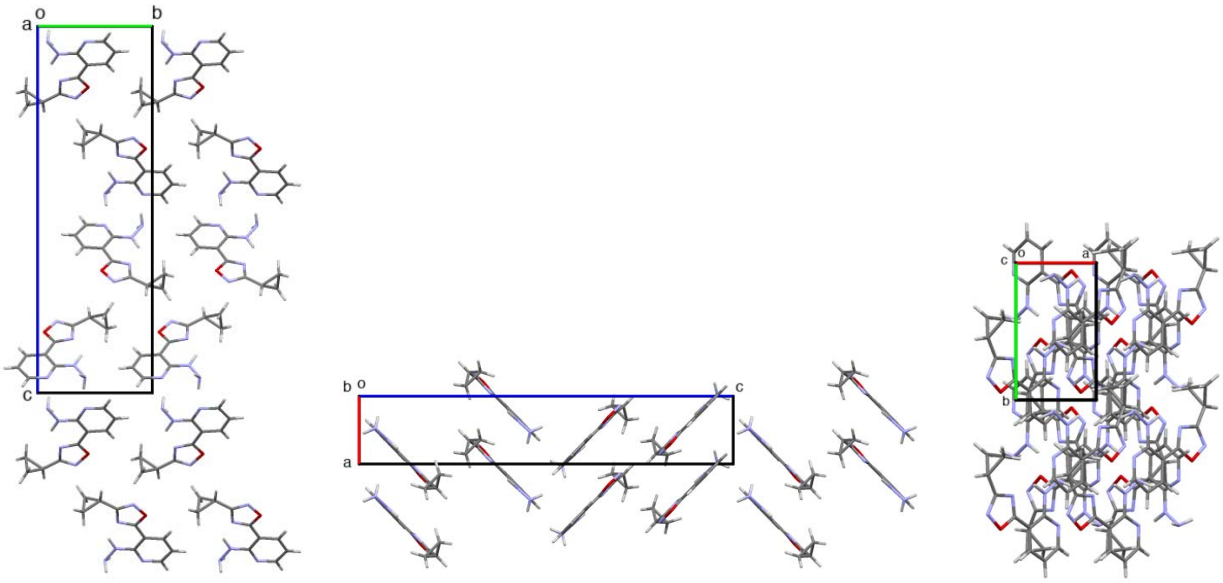

Fig. S3. Molecules packing in structure **1r**.

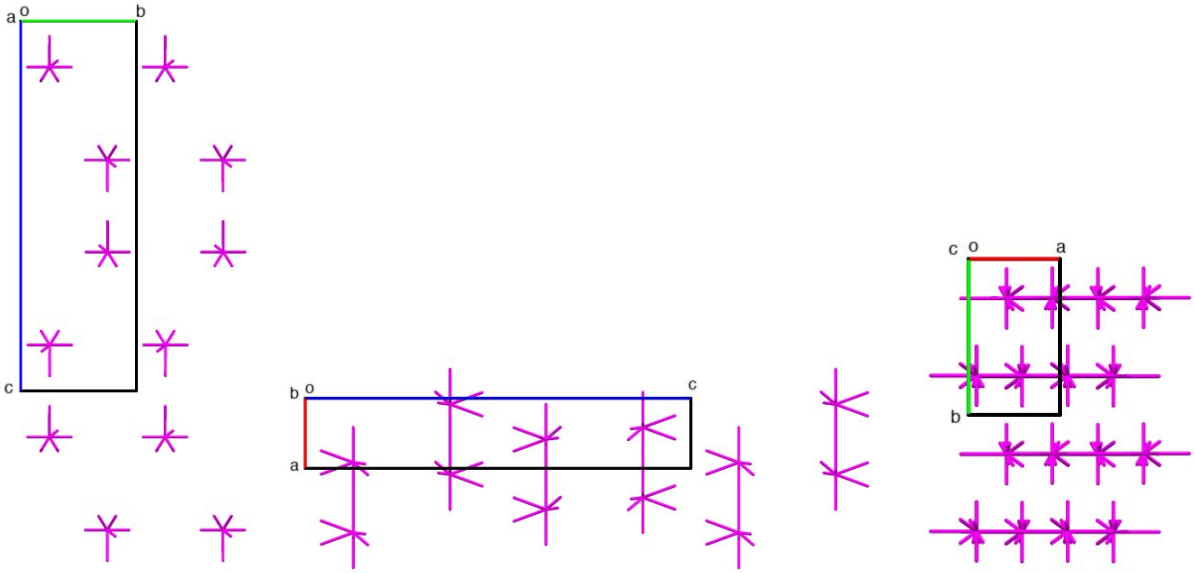

Fig. S2. Packing of energy-vector diagrams in structure **1t**.

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %	Type of interaction
1t_m1	1-x,1-y,1-z	-14.07	23.6	stacking, N-H…pi
1t_m2	1-x,-y,1-z	-9.41	15.8	stacking, N-H…pi
1t_m3	2-x,1-y,1-z	-6.38	10.7	dispersion
1t_m4	2-x,1-y,2-z	-5.74	9.6	dispersion
1t_m5	1-x,1-y,2-z	-4.78	8.0	C-H…O
1t_m6	1+x,1+y,1+z	-4.15	7.0	C-H…N(pyr)
1t_m7	-1+x,-1+y,-1+z	-4.15	7.0	C-H…N(pyr)
1t_m8	1+x,y,z	-2.25	3.8	dispersion
1t_m9	-1+x,y,z	-2.25	3.8	dispersion
1t_m10	1-x,-y,-z	-1.51	2.5	dispersion
1t_m11	-x,-y,1-z	-1.39	2.3	dispersion
1t_m12	x,y,-1+z	-1.01	1.7	dispersion
1t_m13	x,y,1+z	-1.01	1.7	dispersion
1t_m14	1+x,1+y,z	-0.74	1.2	dispersion
1t_m15	-1+x,-1+y,z	-0.74	1.2	dispersion
	Total E_{int}, kcal/mol	-59.59		

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %	Type of interaction
1t_d1	1+x,y,z	-10.84	11.1	dispersion
1t_d2	-1+x,y,z	-10.84	11.1	dispersion
1t_d3	1+x,1+y,1+z	-10.47	10.7	C-H…N(pyr)
1t_d4	-1+x,-1+y,-1+z	-10.47	10.7	C-H…N(pyr)
1t_d5	x,-1+y,z	-10.12	10.3	stacking pyr-pyr
1t_d6	x,1+y,z	-10.12	10.3	stacking pyr-pyr
1t_d7	x,y,-1+z	-6.48	6.6	C-H….O (2)
1t_d8	x,y,1+z	-6.48	6.6	C-H….O (2)
1t_d9	-1+x,y,-1+z	-6.19	6.3	dispersion
1t_d10	1+x,y,1+z	-6.19	6.3	dispersion
1t_d11	1+x,1+y,z	-2.72	2.8	dispersion
1t_d12	-1+x,-1+y,z	-2.72	2.8	dispersion
1t_d13	x,-1+y,-1+z	-2.12	2.2	dispersion
1t_d14	x,1+y,1+z	-2.12	2.2	dispersion
	Total E_{int}, kcal/mol	-97.90		

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %	Type of interaction
1r_m1	1+x,y,z	-10.46	17.4	stacking diaz-pyr
1r_m2	-1+x,y,z	-10.46	17.4	stacking diaz-pyr
1r_m3	1/2+x,3/2-y,1-z	-6.99	11.7	N-H…N (pyr)
1r_m4	-1/2+x,3/2-y,1-z	-6.99	11.7	N-H…N (pyr)
1r_m5	x,-1+y,z	-3.96	6.6	C-H…N (lp)
1r_m6	x,1+y,z	-3.96	6.6	C-H…N (lp)
1r_m7	-x,1/2+y,3/2-z	-3.14	5.2	dispersion
1r_m8	-x,-1/2+y,3/2-z	-3.14	5.2	dispersion
1r_m9	1-x,-1/2+y,3/2-z	-2.53	4.2	dispersion
1r_m10	1-x,1/2+y,3/2-z	-2.53	4.2	dispersion
1r_m11	1+x,-1+y,z	-1.46	2.4	dispersion
1r_m12	-1+x,1+y,z	-1.46	2.4	dispersion
1r_m13	1/2+x,1/2-y,1-z	-1.45	2.4	dispersion
1r_m14	-1/2+x,1/2-y,1-z	-1.45	2.4	dispersion
	Total E_{int}, kcal/mol	-59.97		