



STRUCTURAL  
CHEMISTRY

**Volume 76 (2020)**

**Supporting information for article:**

**Conformational polymorphs of 3-cyclopropyl-5-(3-methyl-[1,2,4]triazolo[4,3-*a*]pyridin-7-yl)-1,2,4-oxadiazole**

**Svitlana V. Shishkina, Irina S. Konovalova, Svitlana S. Kovalenko, Lyudmila L. Nikolaeva, Natalya D. Bunyatyan and Sergiy M. Kovalenko**

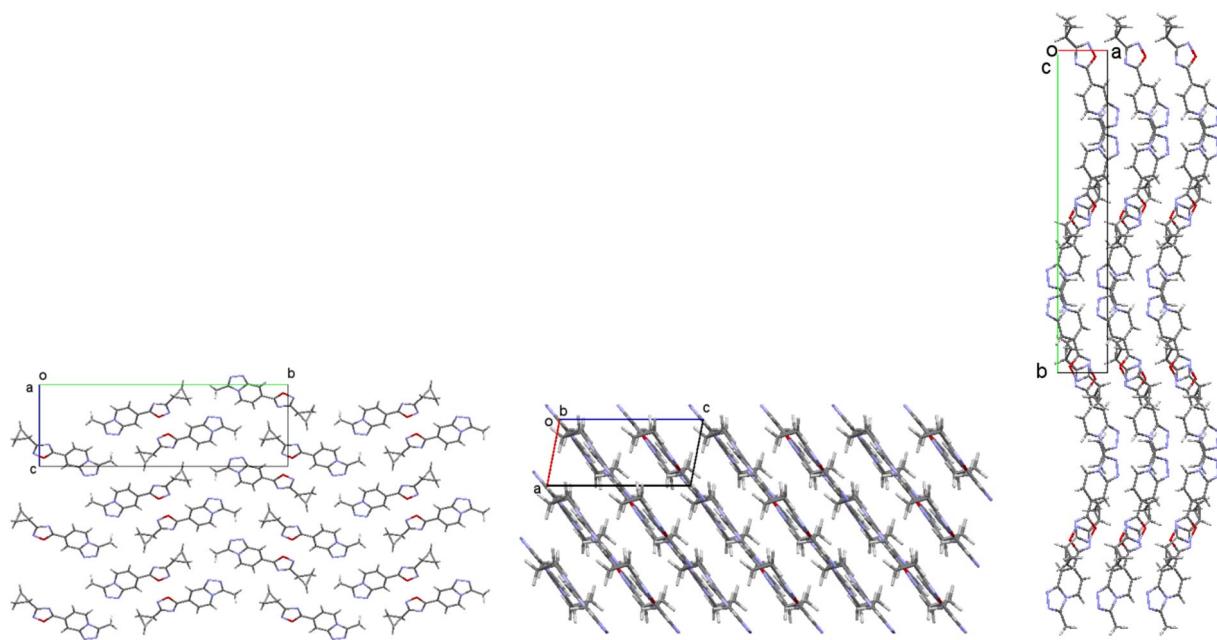


Fig. S1. Molecules packing in structure **1m**.

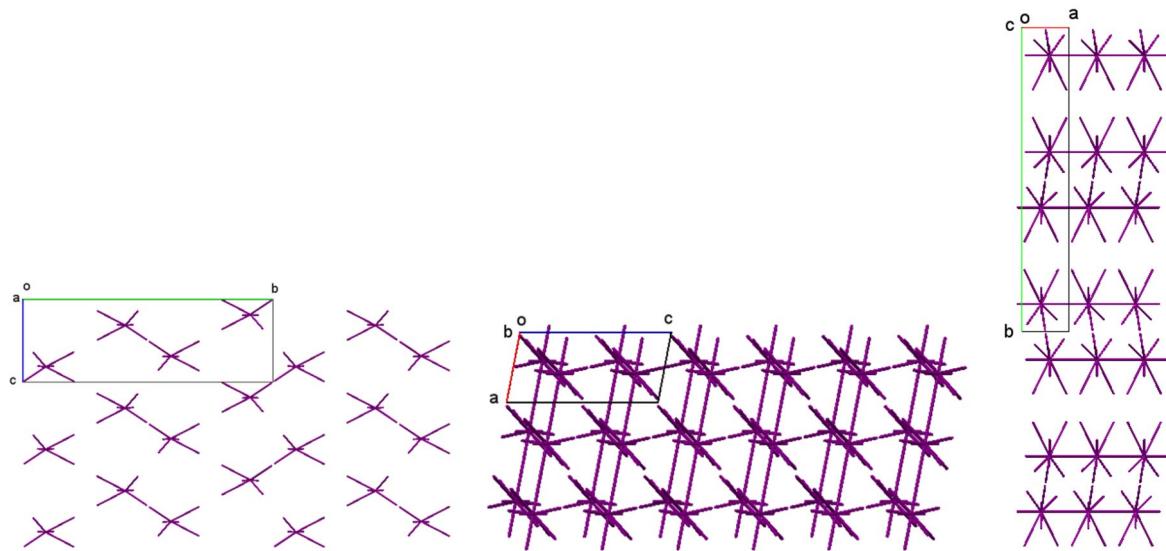
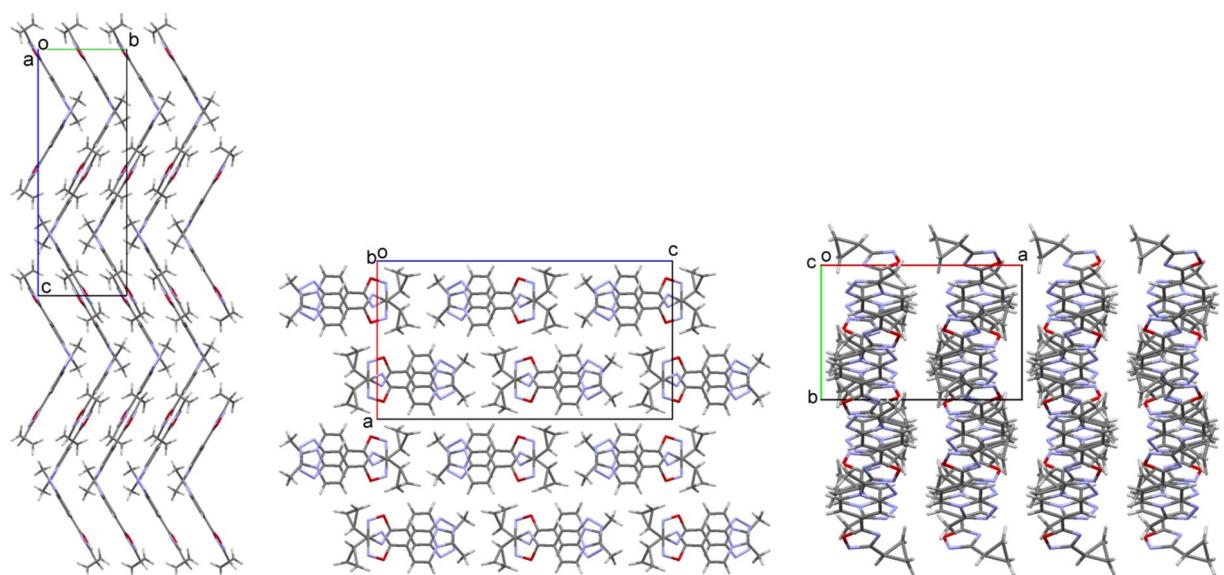
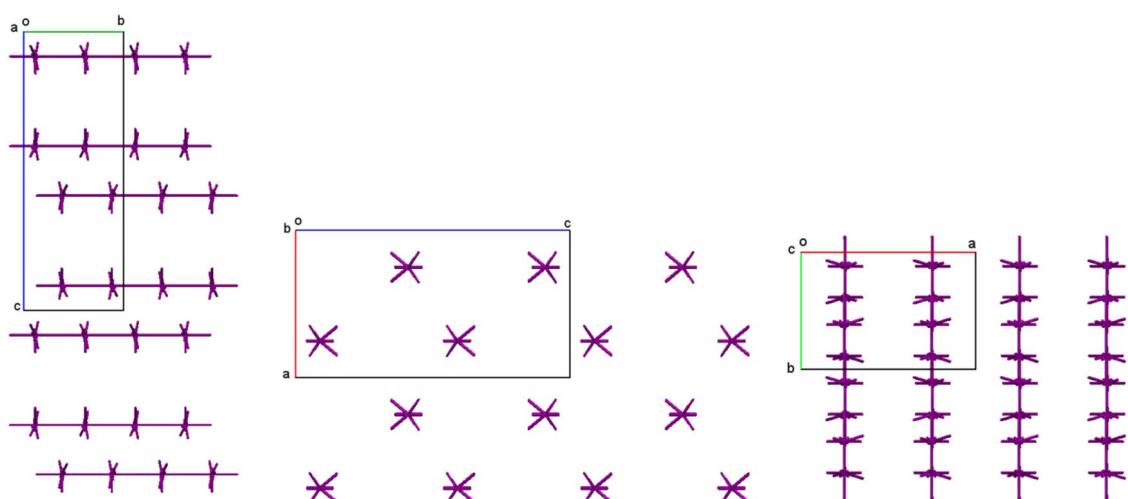


Fig. S2. Packing of energy-vector diagrams in structure **1m**.

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 ( $E_{\text{int}}$ , kcal/mol) and the contribution of this energy to the total interaction energy (%) in crystals **1m**.

Dimer	Symmetry operation	$E_{\text{int}}$ , kcal/mol	The contribution to the total interaction energy, %	Type of interaction
<b>1m_d1</b>	-1+x,y,z	-9.35	14.2	Stacking “head-to-head”
<b>1m_d2</b>	1+x,y,z	-9.35	14.2	Stacking “head-to-head”
<b>1m_d3</b>	1-x,1-y,1-z	-8.68	13.2	dispersion
<b>1m_d4</b>	-x,1-y,1-z	-6.75	10.3	C-H...N
<b>1m_d5</b>	1+x,3/2-y,1/2+z	-6.59	10.0	C-H...N
<b>1m_d6</b>	-1+x,3/2-y,-1/2+z	-6.59	10.0	C-H...N
<b>1m_d7</b>	2-x,1-y,2-z	-5.08	7.7	C-H...N, (propyl)
<b>1m_d8</b>	1-x,1-y,2-z	-4.86	7.4	dispersion
<b>1m_d9</b>	x,3/2-y,-1/2+z	-3.15	4.8	dispersion
<b>1m_d10</b>	x,3/2-y,1/2+z	-3.15	4.8	dispersion
<b>1m_d11</b>	1-x,-1/2+y,3/2-z	-1.15	1.7	dispersion
<b>1m_d12</b>	1-x,1/2+y,3/2-z	-1.15	1.7	dispersion
Total $E_{\text{int}}$ , kcal/mol		-65.87		

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

Dimer	Symmetry operation	$E_{\text{int}}$ , kcal/mol	The contribution to the total interaction energy, %	Type of interaction
<b>1r_d1</b>	3/2-x,-1/2+y,z	-16.61	22.8	Stacking “head-to-tail”
<b>1r_d2</b>	3/2-x,1/2+y,z	-16.61	22.8	Stacking “head-to-tail”
<b>1r_d3</b>	1-x,1-y,1-z	-6.93	9.5	dispersion
<b>1r_d4</b>	-1/2+x,y,3/2-z	-6.32	8.7	$C_{\text{sp}}^3\text{-H...N}$
<b>1r_d5</b>	1/2+x,y,3/2-z	-6.32	8.7	$C_{\text{sp}}^3\text{-H...N}$
<b>1r_d6</b>	2-x,1-y,1-z	-3.92	5.4	$C_{\text{ar}}\text{-H...N}$
<b>1r_d7</b>	x,1/2-y,-1/2+z	-3.13	4.3	dispersion
<b>1r_d8</b>	x,1/2-y,1/2+z	-3.13	4.3	dispersion
<b>1r_d9</b>	1/2+x,3/2-y,1-z	-1.39	1.9	dispersion
<b>1r_d10</b>	-1/2+x,3/2-y,1-z	-1.39	1.9	dispersion
<b>1r_d11</b>	3/2-x,1-y,-1/2+z	-1.31	1.8	dispersion
<b>1r_d12</b>	3/2-x,1-y,1/2+z	-1.31	1.8	dispersion
<b>1r_d13</b>	-1/2+x,1/2-y,1-z	-1.26	1.7	dispersion
<b>1r_d14</b>	1/2+x,1/2-y,1-z	-1.26	1.7	dispersion
<b>1r_d15</b>	2-x,-1/2+y,3/2-z	-0.92	1.3	dispersion
<b>1r_d16</b>	2-x,1/2+y,3/2-z	-0.92	1.3	dispersion
<b>-72.76</b>				