STRUCTURAL CHEMISTRY

Volume 75 (2019)

Supporting information for article:

Polymorphism of 3-(5-phenyl-1,3,4-oxadiazol-2-yl)- and 3-[5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl]-2*H*-chromen-2-ones

Svitlana V. Shishkina, Irina S. Konovalova, Pavlo V. Trostianko, Anna O. Geleverya, Sergiy M. Kovalenko and Natalya D. Bunyatyan

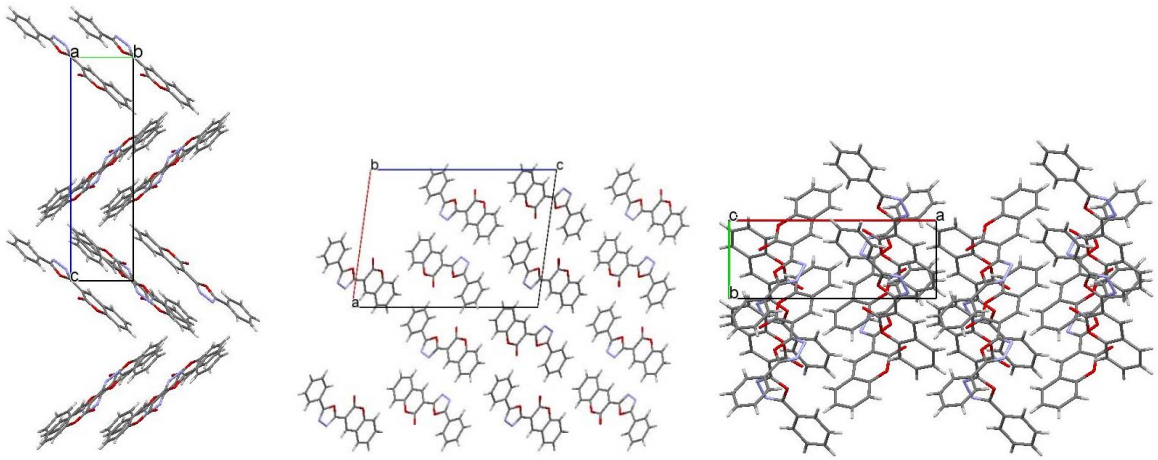

Fig. S1. Molecules packing in structure **1A**.

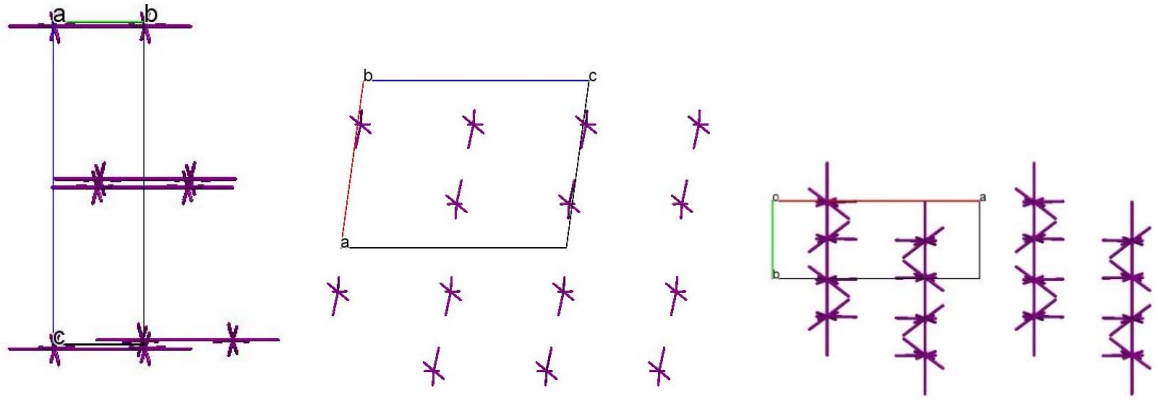

Fig. S2. Packing of energy-vector diagrams in structure **1A**.

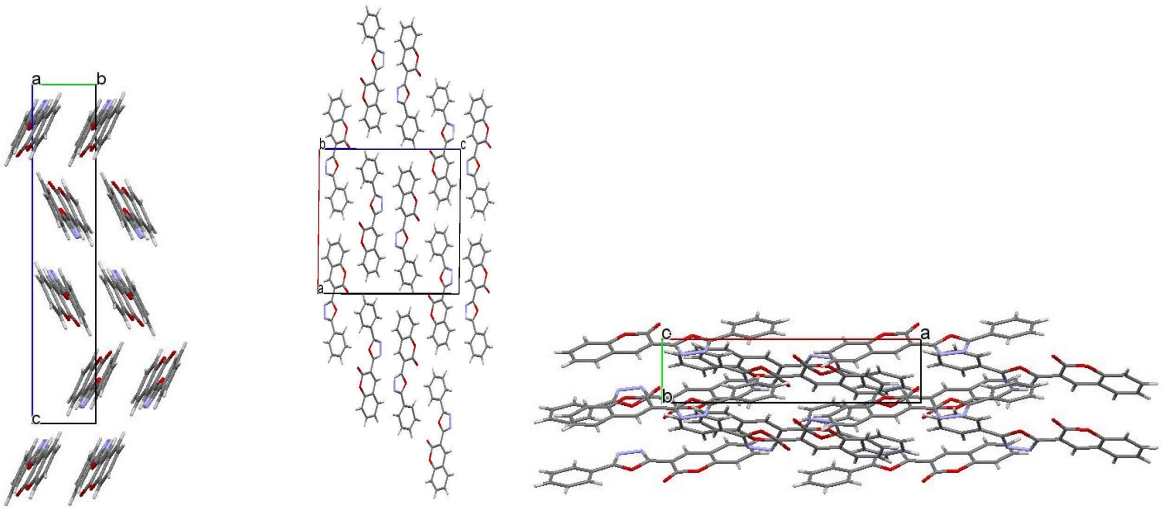

Fig. S3. Molecules packing in structure **1B**.

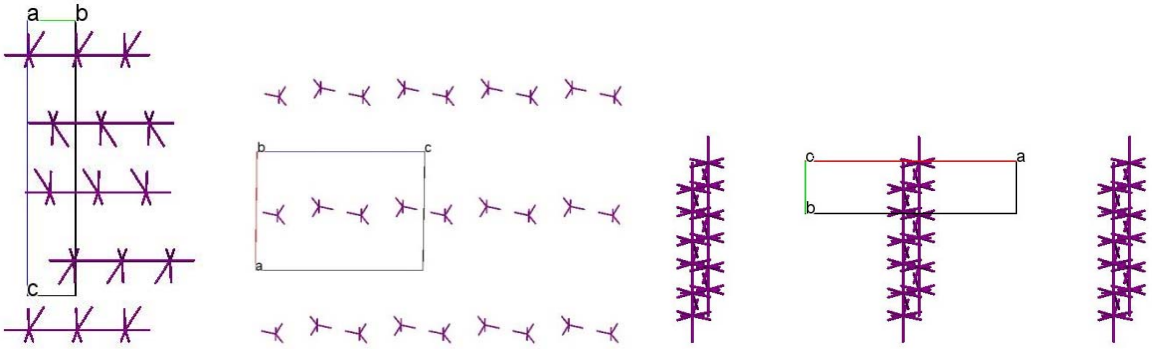

Fig. S4. Packing of energy-vector diagrams in structure **1B**.

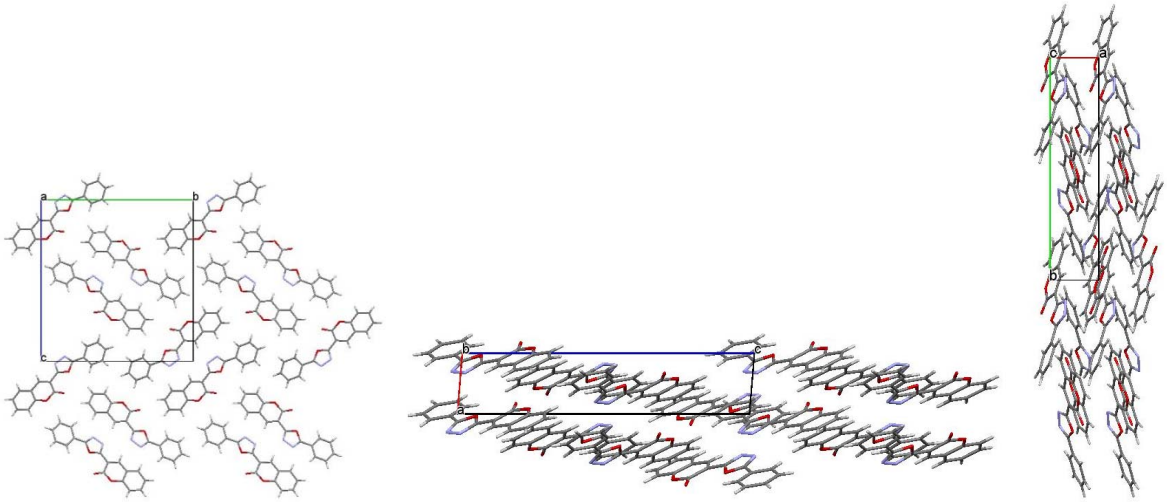

Fig. S5. Molecules packing in structure **1C**.

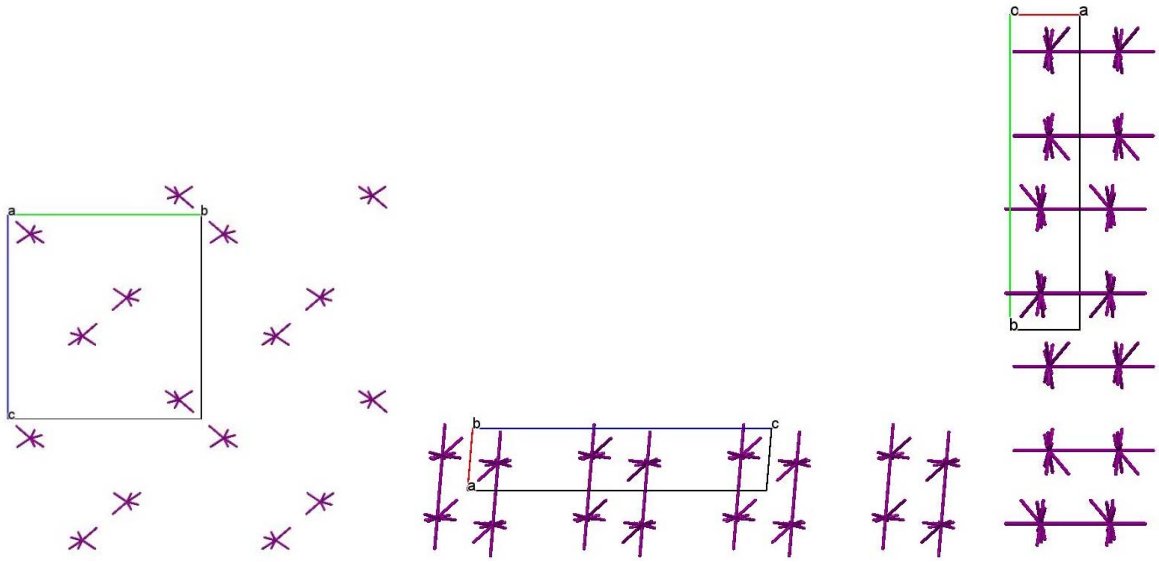

Fig. S6. Packing of energy-vector diagrams in structure **1C**.

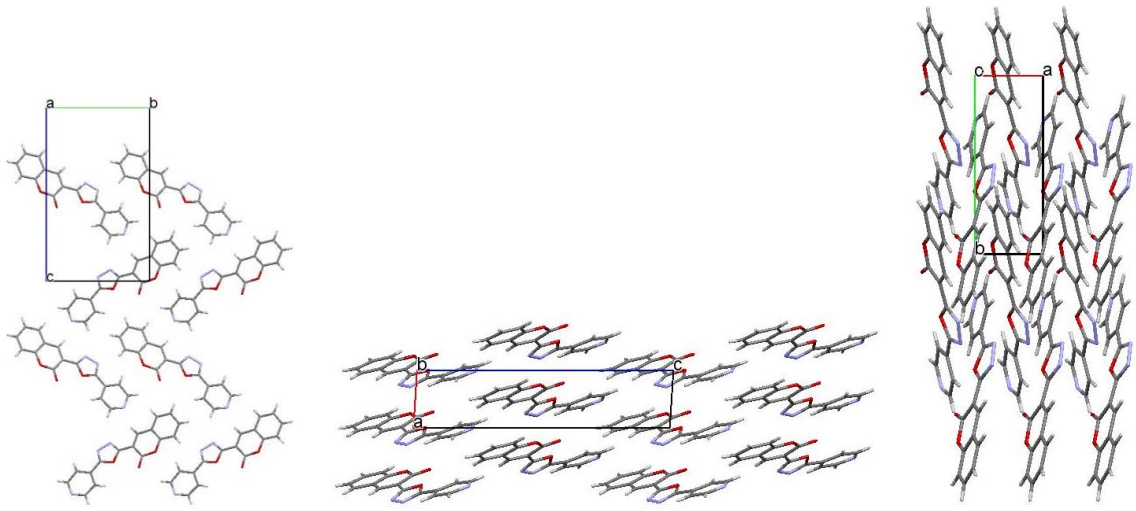

Fig. S7. Molecules packing in structure **2A**.

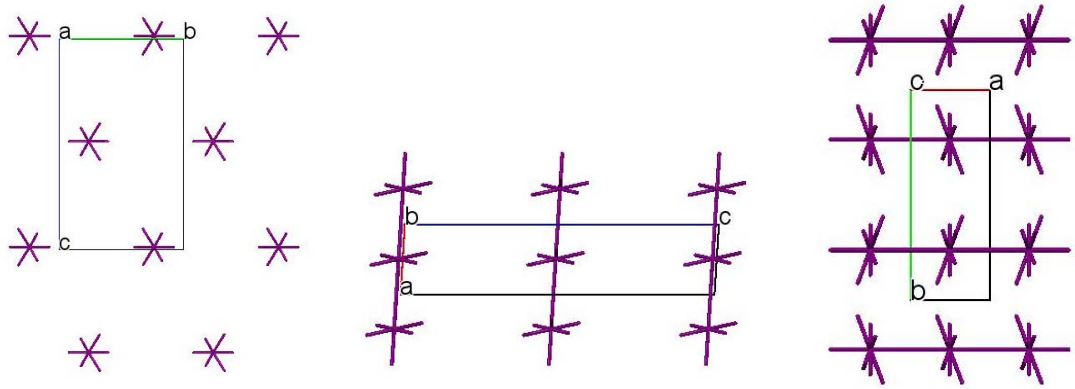

Fig. S8. Packing of energy-vector diagrams in structure **2A**.

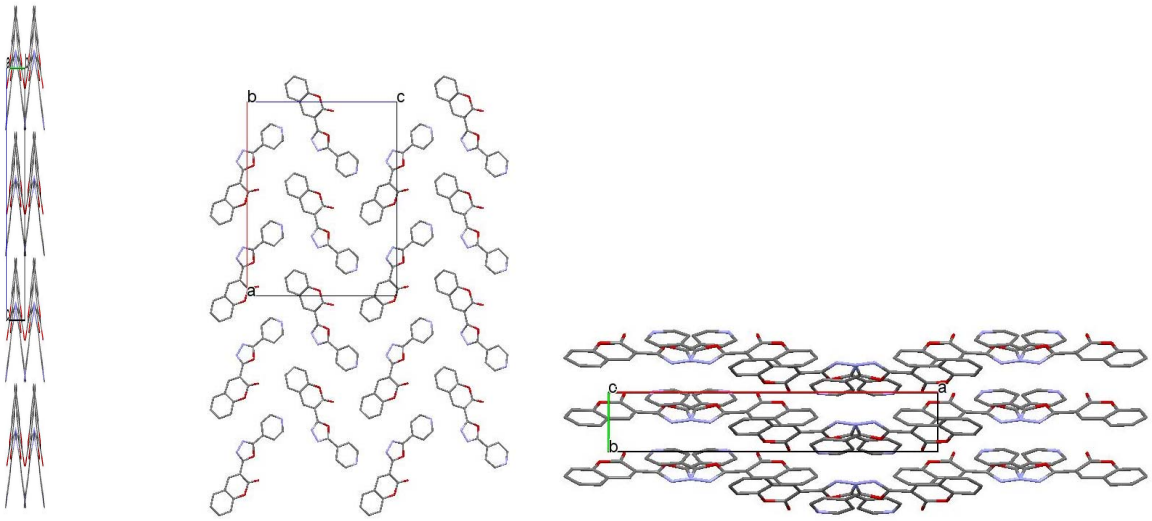

Fig. S9. Molecules packing in structure **2B**.

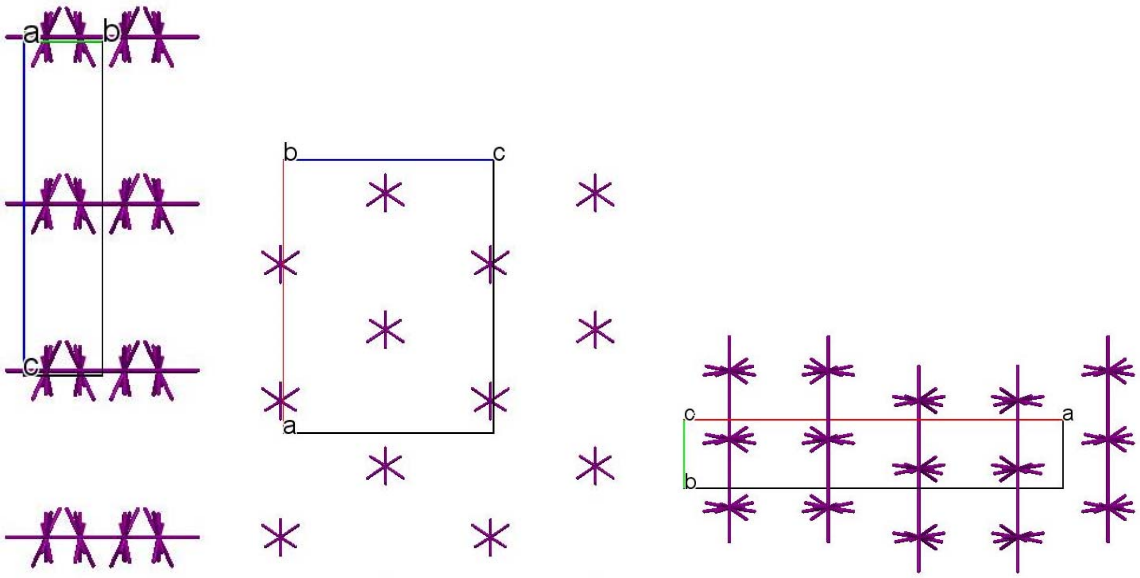

Fig. S10. Packing of energy-vector diagrams in structure **2B**.

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
1A_1	x,1+y,z	-16.10	21.0
1A_2	x,-1+y,z	-16.10	21.0
1A_3	1-x,1-y,1-z	-9.49	12.4
1A_4	1-x,2-y,1-z	-7.00	9.1
1A_5	2-x,-y,1-z	-5.28	6.9
1A_6	1/2+x,3/2-y,1/2+z	-3.17	4.1
1A_7	-1/2+x,3/2-y,-1/2+z	-3.17	4.1
1A_8	2-x,1-y,1-z	-3.11	4.0
1A_9	3/2-x,1/2+y,1/2-z	-2.66	3.5
1A_10	3/2-x,-1/2+y,1/2-z	-2.66	3.5
1A_11	1/2+x,1/2-y,1/2+z	-2.63	3.4
1A_12	-1/2+x,1/2-y,-1/2+z	-2.63	3.4
1A_13	3/2-x,1/2+y,3/2-z	-1.36	1.8
1A_14	3/2-x,-1/2+y,3/2-z	-1.36	1.8
		-76.71	

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
1B_1	x,1+y,z	-15.95	20.5
1B_2	x,-1+y,z	-15.95	20.5
1B_3	1-x,2-y,1-z	-10.50	13.5
1B_4	1-x,1-y,1-z	-9.78	12.5
1B_5	1/2-x,1/2+y,1/2-z	-5.30	6.8
1B_6	1/2-x,-1/2+y,1/2-z	-5.30	6.8
1B_7	3/2-x,1/2+y,1/2-z	-4.67	6.0
1B_8	3/2-x,-1/2+y,1/2-z	-4.67	6.0
1B_9	1+x,y,z	-1.70	2.2
1B_10	-1+x,y,z	-1.70	2.2
1B_11	1+x,1+y,z	-1.22	1.6
1B_12	-1+x,-1+y,z	-1.22	1.6
		-77.98	

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

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
1C_1	1+x,y,z	-15.76	20.2
1C_2	-1+x,y,z	-15.76	20.2
1C_3	2-x,1-y,1-z	-10.02	12.8
1C_4	1-x,1-y,1-z	-10.01	12.8
1C_5	3/2-x,1/2+y,3/2-z	-4.25	5.4
1C_6	3/2-x,-1/2+y,3/2-z	-4.25	5.4
1C_7	1/2-x,1/2+y,3/2-z	-3.04	3.9
1C_8	1/2-x,-1/2+y,3/2-z	-3.04	3.9
1C_9	1/2+x,1/2-y,-1/2+z	-2.49	3.2
1C_10	-1/2+x,1/2-y,1/2+z	-2.49	3.2
1C_11	1-x,-y,1-z	-2.36	3.0
1C_12	1/2+x,1/2-y,1/2+z	-1.73	2.2
1C_13	-1/2+x,1/2-y,-1/2+z	-1.73	2.2
1C_14	-x,-y,1-z	-1.25	1.6
		-78.20	

Table S4 Symmetry codes, interaction energy of the basic molecule with neighbouring ones (E_{int}, kcal/mol) and the contribution of this energy to the total interaction energy (%) in crystals **2A**.

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
2A_1	1+x,y,z	-16.04	19.7
2A_2	-1+x,y,z	-16.04	19.7
2A_3	1/2+x,1-y,-1/2+z	-5.51	6.8
2A_4	-1/2+x,1-y,1/2+z	-5.51	6.8
2A_5	1+x,1+y,z	-5.06	6.2
2A_6	-1+x,-1+y,z	-5.06	6.2
2A_7	1/2+x,-y,-1/2+z	-4.12	5.1
2A_8	-1/2+x,-y,1/2+z	-4.12	5.1
2A_9	x,1+y,z	-3.78	4.7
2A_10	x,-1+y,z	-3.78	4.7
2A_11	1/2+x,1-y,1/2+z	-3.54	4.3
2A_12	-1/2+x,1-y,-1/2+z	-3.54	4.3
2A_13	1/2+x,-y,1/2+z	-2.62	3.2
2A_14	-1/2+x,-y,-1/2+z	-2.62	3.2
		-81.33	

Table S5 Symmetry codes, interaction energy of the basic molecule with neighbouring ones (E_{int}, kcal/mol) and the contribution of this energy to the total interaction energy (%) in crystals **2B**.

Dimer	Symmetry operation	E_{int}, kcal/mol	The contribution to the total interaction energy, %
2B_1	x,1+y,z	-15.91	19.3
2B_2	x,-1+y,z	-15.91	19.3
2B_3	3/2-x,1+y,1/2+z	-5.44	6.6
2B_4	3/2-x,-1+y,-1/2+z	-5.44	6.6
2B_5	1-x,1-y,1/2+z	-4.63	5.6
2B_6	1-x,1-y,-1/2+z	-4.63	5.6
2B_7	3/2-x,y,1/2+z	-4.47	5.4
2B_8	3/2-x,y,-1/2+z	-4.47	5.4
2B_9	1/2+x,1-y,z	-4.20	5.1
2B_10	-1/2+x,1-y,z	-4.20	5.1
2B_11	1/2+x,2-y,z	-3.84	4.6
2B_12	-1/2+x,2-y,z	-3.84	4.6
2B_13	1-x,2-y,1/2+z	-2.79	3.4
2B_14	1-x,2-y,-1/2+z	-2.79	3.4
		-82.56	