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Supporting information for article:

Concomitant polymorphs of 2-imino-2*H*-chromene-3-carboxylic acid amide: experimental and quantum chemical study

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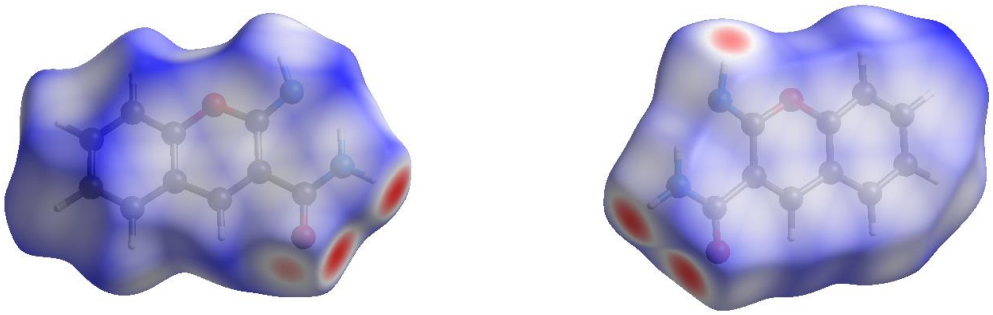
Supporting information



1m **1t**

Figure S1 Hirshfeld surfaces with mapped d_{norm} property projected and transparency to show the conformation of the molecules.

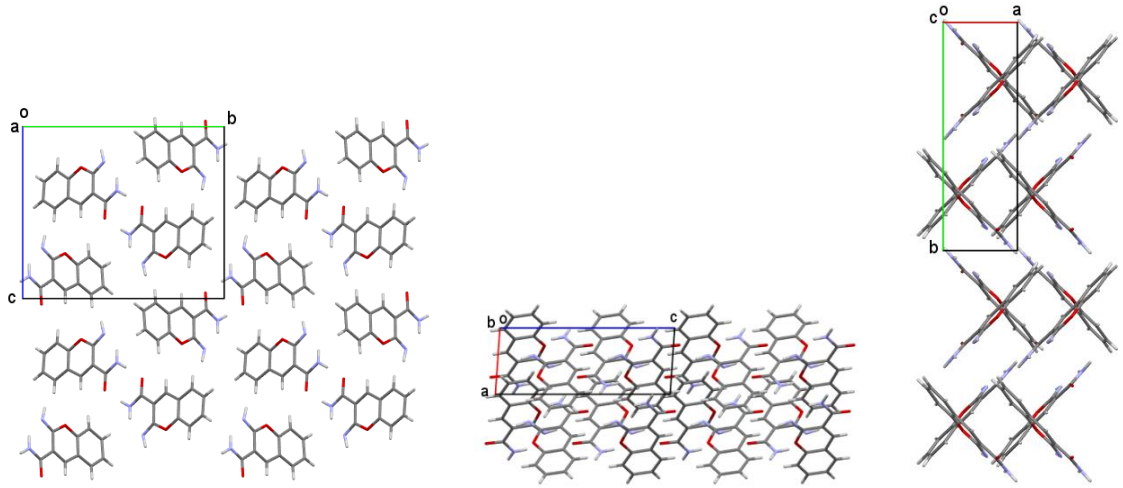


Figure S2 Molecules packing in structure **1m**.

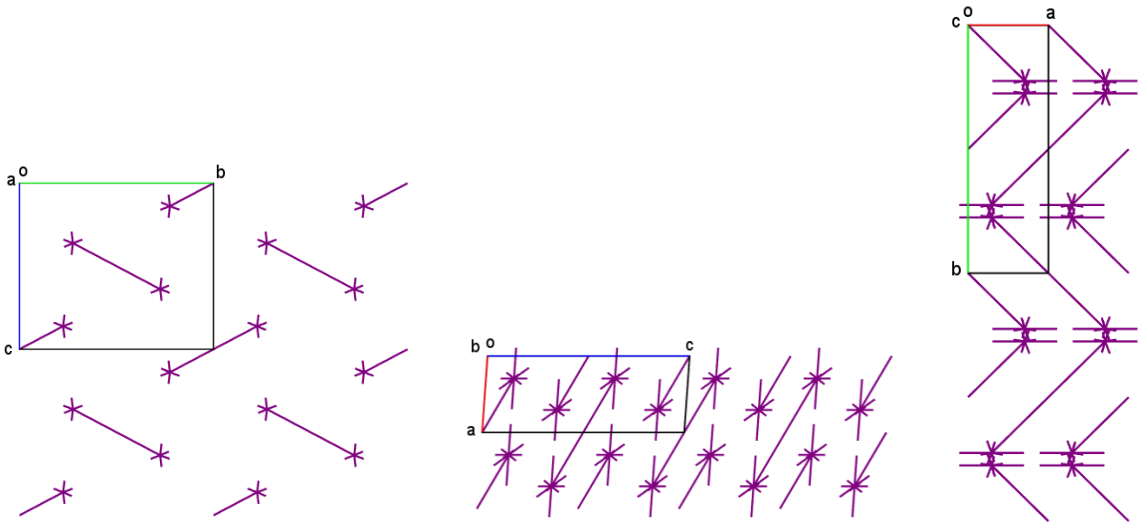


Figure S3 Packing of energy-vector diagrams in structure **1m**.

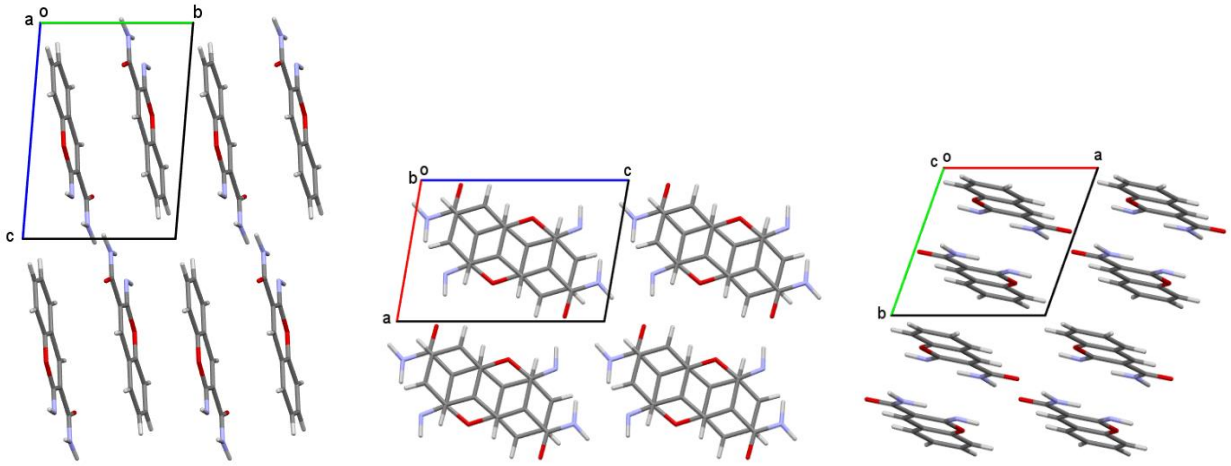


Figure S4 Molecules packing in structure **1t**.

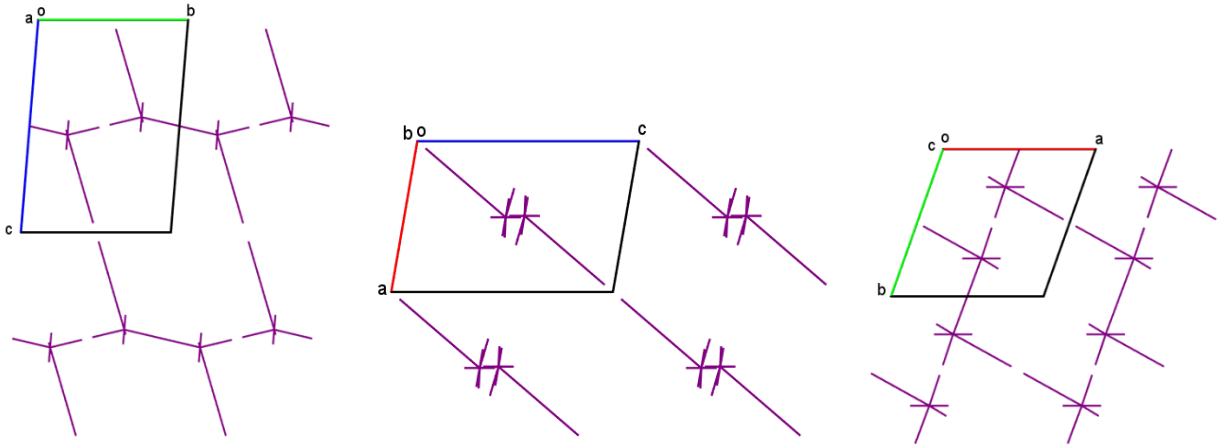


Figure S5 Packing of energy-vector diagrams in structure **1t**.

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

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1m_1	-x,1-y,1-z	-52.70	19.6	N2–H…O2
1m_2	-1+x,y,z	-42.47	15.8	stacking
1m_3	1+x,y,z	-42.47	15.8	stacking
1m_4	1+x,1/2-y,-1/2+z	-14.73	5.5	C2–H…O2
1m_5	-1+x,1/2-y,1/2+z	-14.73	5.5	C2–H…O2
1m_6	x,1/2-y,1/2+z	-14.01	5.2	non-specific
1m_7	x,1/2-y,-1/2+z	-14.01	5.2	non-specific
1m_8	1-x,1-y,1-z	-10.65	4.0	non-specific
1m_9	2-x,1/2+y,1/2-z	-10.35	3.9	C3–H…N1
1m_10	2-x,-1/2+y,1/2-z	-10.35	3.9	C3–H…N1
1m_11	2-x,-y,1-z	-8.69	3.2	non-specific
1m_12	-1+x,1/2-y,-1/2+z	-8.16	3.0	non-specific
1m_13	1+x,1/2-y,1/2+z	-8.16	3.0	non-specific
1m_14	1-x,-1/2+y,1/2-z	-7.84	2.9	non-specific
1m_15	1-x,1/2+y,1/2-z	-7.84	2.9	non-specific
1m_16	3-x,-y,1-z	-1.66	0.6	non-specific
		E_{int}(total) -268.8 kJ/mol		

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

Dimer	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %	Interaction type
1t_1	1-x,-y,1-z	-57.57	22.7	stacking of type 2
1t_2	2-x,1-y,2-z	-52.21	20.6	N2–H…O2
1t_3	1-x,1-y,1-z	-49.61	19.5	stacking of type 1
1t_4	2-x,1-y,1-z	-22.14	8.7	non-specific
1t_5	-x,-y,1-z	-15.72	6.2	non-specific
1t_6	-1+x,y,z	-14.48	5.7	N1–H…O2
1t_7	1+x,y,z	-14.48	5.7	N1–H…O2
1t_8	1-x,1-y,2-z	-8.27	3.3	non-specific
1t_9	x,y,-1+z	-7.97	3.1	non-specific
1t_10	x,y,1+z	-7.97	3.1	non-specific
1t_11	1-x,-y,-z	-2.54	1.0	non-specific
1t_12	-x,-y,-z	-0.81	0.3	non-specific
		E_{int}(total) -253.8 kJ/mol		