

Supporting Information for

Knowledge-Based Approaches to H-Bonding Patterns in Heterocycle-1-Carbohydrazoneamides

Anna V. Vologzhanina,^{†,} Andrey V. Sokolov,[‡] Petr P. Purygin,[§] Pavel N. Zolotarev,[§] Vladislav A. Blatov[§]*

[†] A. N. Nesmeyanov Institute of Organoelement Compounds, Vavilova str., 28, Moscow 1199911, Russia [‡] Samara State Medical University, Chapaevskaya str., 89, Samara 443099, Russia [§] Samara Center for Theoretical Materials Science (SCTMS), Samara State Aerospace University (National Research University) named after academician S.P.Korolyev, Moskovskoe Shosse 34, Samara 443086, Russia

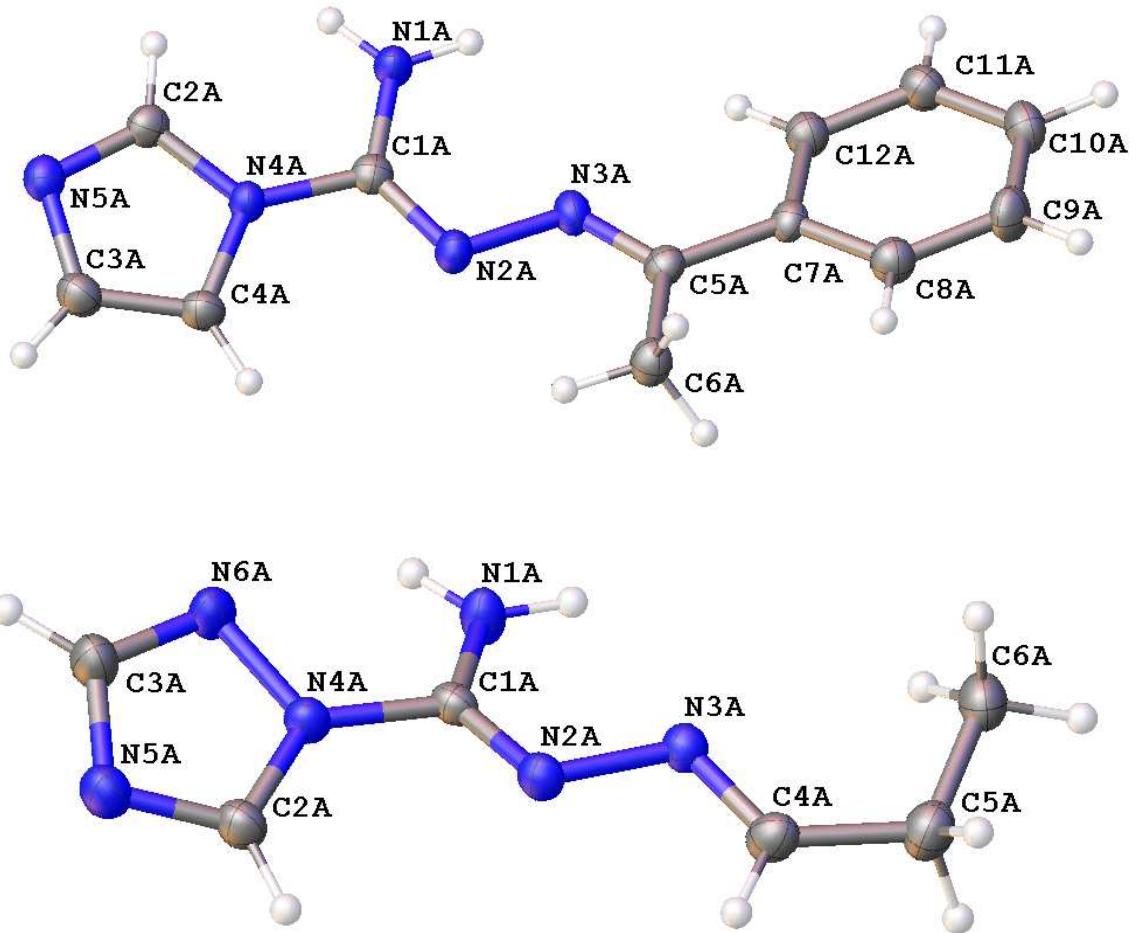


Figure S1. General view of the second molecule of **2** and **3** in representation of atoms with thermal ellipsoids (given with $p = 50\%$).

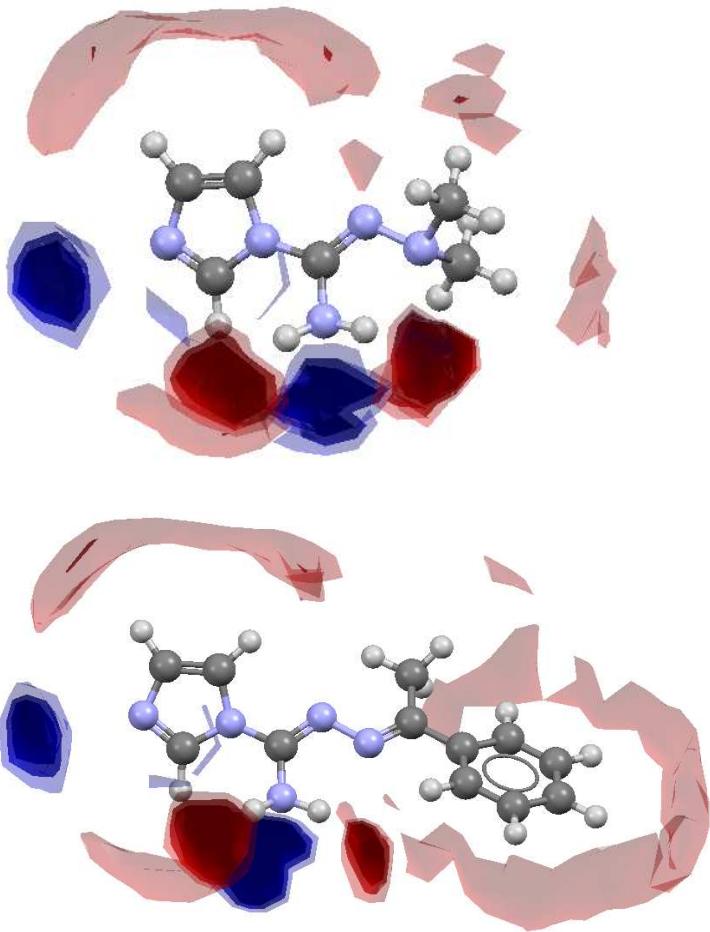


Figure S2. Interaction maps shown for isolated molecules of **1** (top) and **2** (bottom) without correction of geometry for amino group.

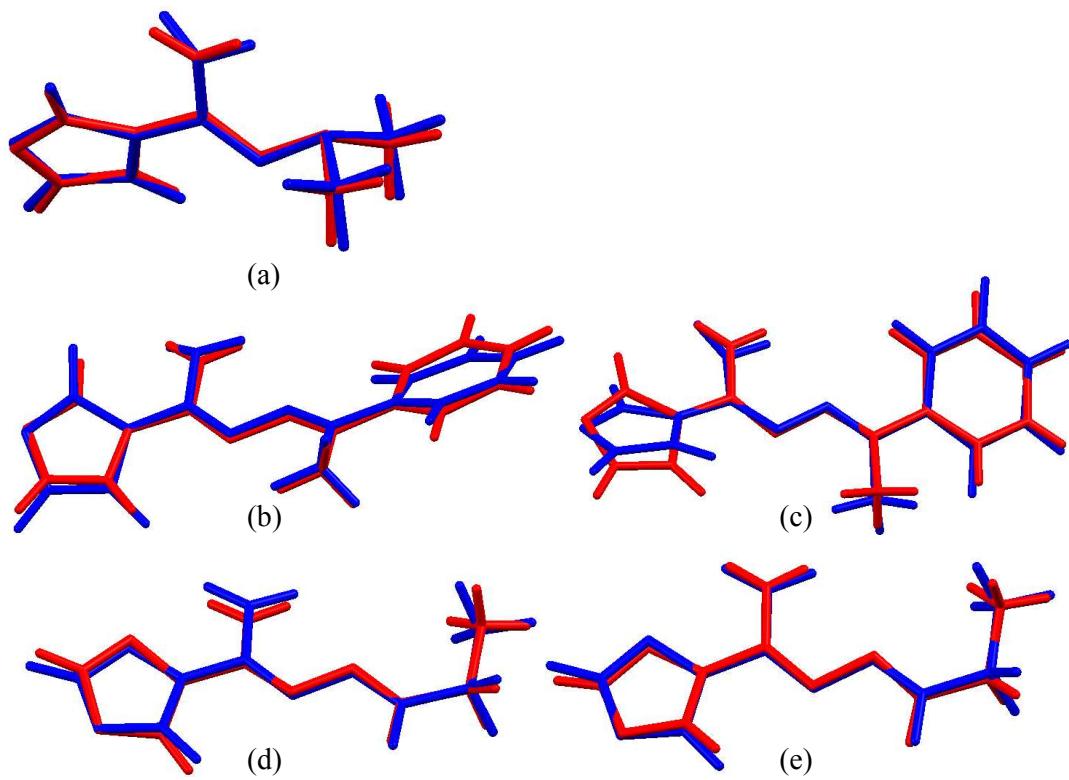


Figure S3. Comparison of calculated (blue) and experimental (red) geometries for **1** (a), two independent molecules of **2** (b, c) and two independent molecules of **3** (d, e).

Possible Polymorphs

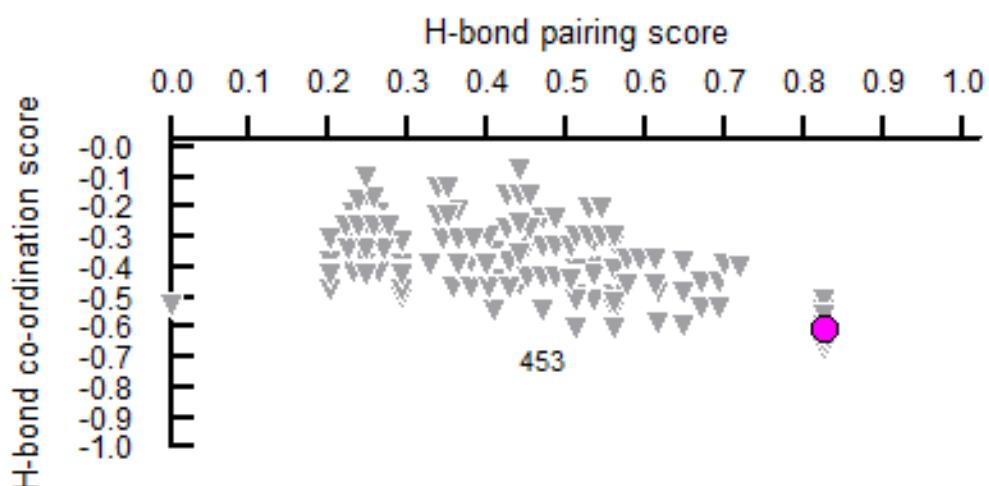


Figure S4. Putative structure landscape calculated for **2**.

Table S1. Probabilities of Realization of Underlying Topologies for a Particular Connection Type.^a

Connection Type	Periodicity	Topology	P, %
B ⁰¹	0D	1M2-1	100.0000%
B ²	0D	2M3-1	0.0648%
		2M4-1	0.4404%
		2M6-1	0.2655%
	1D	2C1	99.2293%
K ⁰²	0D	2M6-1	0.0410%
	1D	2C1	99.9590%
K ²¹	0D	3M4-1	0.0549%
	1D	SP 1-periodic net 4 ⁴ (0,2)	36.0242%
	2D	fes	0.1098%
		hcb	60.3515%
		KIa	0.9336%
	3D	bto /B2O3; 3/10/h1	0.2197%
		dia-f decorated diamond-f; 3/4/t1	0.2746%
		etb ; 3/8/h1; sqc327	0.1098%
		lig LiGe; 3/8/t1; sqc978	0.3844%
		pcu-h ; 3/6/h1; sqc328	0.1098%
		srs SrSi2; 3/10/c1	0.6041%
		ths ThSi2; 3/10/t4	0.8237%
K ⁴	1D	4C1	0.0319%
		4C2	0.0319%
		4C3	0.0319%
		SP 1-periodic net 3 ⁶ (1,2)	15.4435%
		SP 1-periodic net 4 ⁴ (0,3)	0.0319%
		SP 1-periodic net 4 ⁴ (0,4); CrF4	0.0319%
		SP 1-periodic net 4 ⁴ (0,6)	0.0319%
		SP 1-periodic net 4 ⁴ (1,3)	0.0638%
		SP 1-periodic net 4 ⁴ (2,2)	0.3829%
		SP 1-periodic net 4 ⁴ (2,3)	0.0638%
		SP 1-periodic net 4 ⁴ (3,3)	0.0319%

2D	4L1	0.6063%
	4L12	0.0319%
	4L2	1.5316%
	4L7	0.0319%
	kgm	0.0638%
	sql	63.0185%
3D	4/4/t16	0.0319%
	bcu-x-4-P3212	0.0319%
	cds CdSO4; 4/6/t4; sqc5	1.4040%
	crb /BCT; 4/4/t5; sqc184	0.0319%
	dia Diamond; 4/6/c1; sqc6	13.7524%
	dmp	0.5743%
	gis Gismondine GIS; 4/4/t3; sqc2200	0.3191%
	lvt , Net #97; 4/4/t1; sqc176	0.6063%
	nbo NbO; 4/6/c2; sqc35	0.3510%
	neb ; 4/6/o1; sqc182	0.0638%
	qtz Quartz; 4/6/h1	0.4148%
	qzd quartz-dual, "dense" net	0.1914%
	snw -4-I4122	0.1276%
	sod /SOD; 4/4/c1; sqc970	0.0638%
	svi-x-4-P42/nbc	0.0319%
	tcb	0.1595%
	unc ; 4/6/t1	0.0319%
	unh ; 4/5/h4	0.0319%
	unj ; 4/5/h3	0.0638%
	uny ; 4/3/h2	0.0319%
	uoc ; 4/4/t2	0.1276%
	usf ; 4/6/h7; sqc906	0.0319%
	zst	0.0638%

a Underlying topologies for discrete, 1-periodic, 2- and 3-periodic networks are denoted in terms of notations described at Refs. [Alexandrov, E. V.; Blatov, V. A.; Kochetkov, A. V.; Proserpio, D.M. CrystEngComm 2011, 13, 3947], [Koch, E.; Fischer, W. Z. Kristallogr. 1978, 148, 107] and [O'Keeffe, M.; Peskov, M. A.; Ramsden, S. J.; Yaghi, O. M. Acc.Chem. Res. 2008, 41, 1782].