STRUCTURAL CHEMISTRY

Volume 76 (2020)

Supporting information for article:

When solvent becomes reactant: a study of 6-aminothiocytosine derivatives

Anita M. Grześkiewicz, Agata Ostrowska, Dmytro Borzylo and Maciej Kubicki

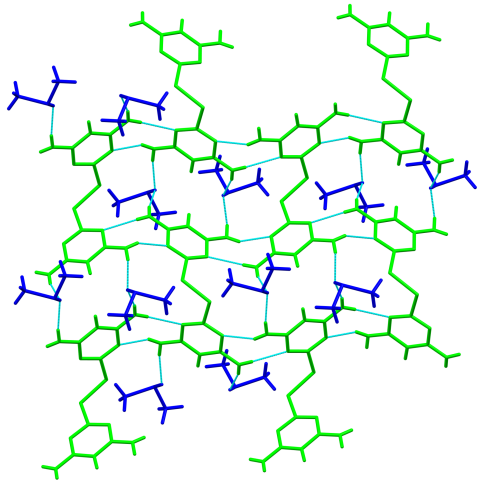
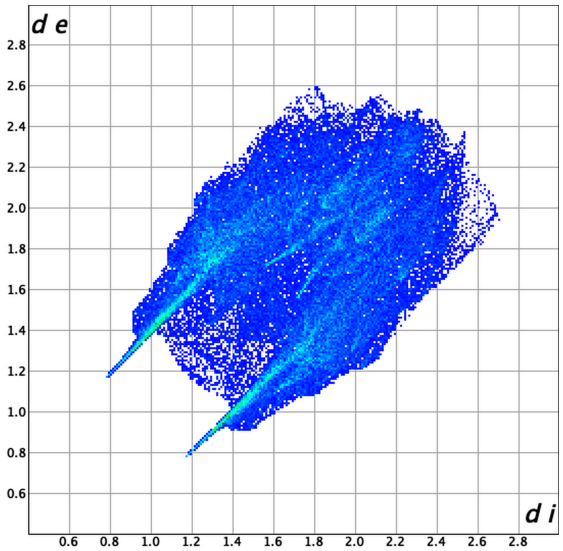
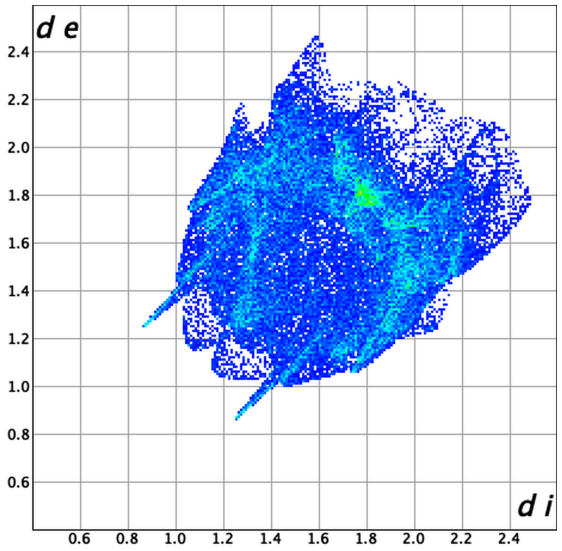


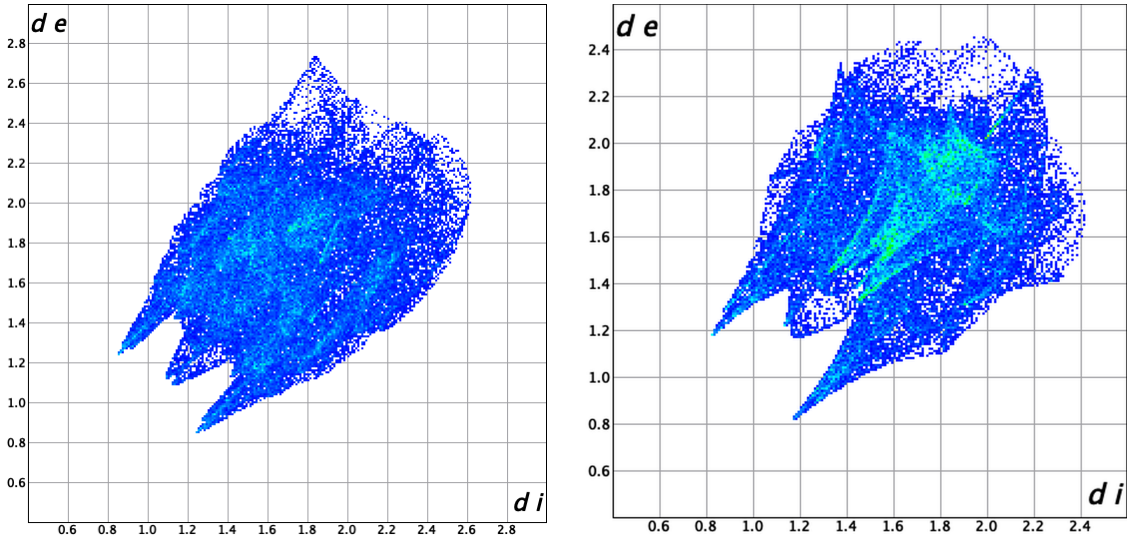
Fig. S1. Crystal packing of the DMSO solvate of **1** (Papastavrou et al., 2008).



(a)



(b)



(c) (d)

Fig. S2. Fingerprint plots for (a) **1**, (b) **2**, (c) **3** and (d) DAPMT anion in **4**.

Table Suppl. 1. (3,-1) Critical points data; Gcp, Vcp – kinetic and potential energy dnsity, DIST_12 – distance atom1-atom2. DCP1, DCP2 – distance atom1(2)…CP, DEN – electron density at CP, LAPL – Laplacian at CP,

Atom1	Atom2	sym2	Gcp	Vcp	DIST_12	DCP1	DCP2	DEN	LAPL	3_HESSIAN_EIGEN-VALUES		
			kJ/mol/Bohr^3		Å	Å	Å	e·Å^{-3}	e·Å^{-5}	e·Å^{-5}		
1												
C2	H6B	x,1-y,-1/2+z	7.90	-5.61	3.1595	1.8351	1.3425	0.03388	0.374	-0.056	-0.023	0.453
N1	H12	x,y,1+z	30.37	-28.47	2.3886	1.4329	0.9805	0.11782	1.185	-0.336	-0.160	1.682
N1	H11A	-1/2+x,1/2-y,1/2+z	43.44	-43.04	2.1622	1.2689	0.8934	0.15649	1.609	-0.589	-0.557	2.755
N3	H13B	1/2+x,1/2-y,1/2+z	26.72	-23.64	2.3748	1.3680	1.0071	0.10101	1.094	-0.322	-0.322	1.738
N3	H5	x,1-y,-1/2+z	7.87	-5.52	3.0324	1.7108	1.3448	0.03294	0.375	-0.063	-0.038	0.476
N3	H11B	x,y,1+z	27.27	-24.62	2.3865	1.3977	0.9928	0.10510	1.098	-0.317	-0.262	1.677
H4B	S7	1/2+x,1/2-y,1/2+z	10.63	-8.19	3.1366	1.3058	1.8329	0.04707	0.480	-0.100	-0.045	0.625
H4A	N13	1/2+x,1/2+y,1+z	27.40	-24.66	2.3825	0.9976	1.3851	0.10500	1.106	-0.329	-0.324	1.760
H4B	N14	1/2+x,1/2-y,1/2+z	39.30	-38.46	2.1900	0.9019	1.2882	0.14514	1.474	-0.530	-0.517	2.521
H5	C9	x,1-y,1/2+z	12.79	-10.21	2.8275	1.2130	1.6199	0.05573	0.565	-0.103	-0.103	0.770
H6A	S8	-1/2+x,1/2+y, z	6.13	-4.31	3.3699	1.4192	1.9543	0.02852	0.292	-0.058	-0.045	0.395
H6A	N10	-1/2+x,1/2-y,1/2+z	16.11	-12.77	2.6042	1.1291	1.4758	0.06331	0.714	-0.182	-0.174	1.070
H6B	N11	-1/2+x,1/2+y,1+z	5.55	-3.73	3.2870	1.4382	1.8552	0.02423	0.271	-0.046	-0.027	0.343
H6B	N14	x,1-y, 1/2+z	12.31	-9.10	2.8097	1.2568	1.5715	0.04770	0.570	-0.107	-0.076	0.753
S8	C11	x, -y, 1/2+z	16.33	-13.47	3.2851	1.7188	1.5664	0.06792	0.705	-0.121	-0.114	0.939
S8	N13	1/2+x,1/2-y,1/2+z	19.68	-16.94	3.2895	1.6778	1.6212	0.08092	0.823	-0.194	-0.085	1.103
N10	H13A	1/2+x,1/2-y,1/2+z	23.10	-19.61	2.4669	1.4085	1.0624	0.08729	0.976	-0.268	-0.225	1.470
2												
N3	C6	x,y,1+z	9.63	-6.73	3.4058	1.6892	1.7285	0.03679	0.460	-0.047	-0.020	0.528
N1	H6B	3/4-x,-1/4+y,1/4+z	35.25	-33.31	2.2486	1.3101	0.9390	0.13016	1.366	-0.456	-0.441	2.263
S7	H4A	x,-1/2+y,-1/2+z	12.57	-10.21	2.9887	1.7648	1.2289	0.05671	0.548	-0.134	-0.113	0.795
S7	H4A	x,-1/2+y,1/2+z	13.76	-11.46	2.9396	1.7564	1.1876	0.06218	0.590	-0.143	-0.118	0.851
N4	H4B	½-x,1-y,-1/2+z	17.60	-14.43	2.6228	1.5189	1.1112	0.07042	0.762	-0.185	-0.135	1.082
S7	C8	x,y,-1+z	12.32	-9.85	3.5956	1.8267	1.8027	0.05460	0.543	-0.093	-0.017	0.653
H5	N6	3/4-x,1/4+y,-1/4+z	11.29	-8.75	2.9223	1.2352	1.7111	0.04926	0.508	-0.103	-0.064	0.676
C5	H6A	3/4-x,1/4+y,3/4+z	15.51	-13.46	2.7845	1.6873	1.1275	0.07094	0.644	-0.188	-0.133	0.966
3												

N3	H4B	1-x,1/2+y,1/2-z	8.45	-6.11	3.0156	1.8069	1.2957	0.03647	0.396	-0.075	-0.039	0.510
N1	C10	2-x,-1/2+y,1/2-z	7.95	-5.45	3.6033	1.6565	1.9514	0.03155	0.384	-0.054	-0.024	0.462
C6	H10A	x,3/2-y,1/2+z	17.13	-14.25	2.7531	1.6134	1.1484	0.07082	0.735	-0.149	-0.057	0.940
N3	H6B	x,1/2-y,-1/2+z	31.21	-28.83	2.3161	1.3514	0.9652	0.11748	1.233	-0.375	-0.366	1.974
H4A	O9	1-x,1-y,-z	27.75	-23.76	2.3496	1.0054	1.3464	0.09867	1.165	-0.320	-0.285	1.770
H5	H8B	x,1/2-y,1/2+z	10.77	-8.91	2.4386	1.2448	1.1987	0.05309	0.464	-0.140	-0.133	0.737
N4	H10C	x,-1+y,z	4.17	-2.68	3.3348	1.8430	1.4919	0.01823	0.208	-0.034	-0.031	0.273
H4B	O9	1-x,-1/2+y,1/2-z	13.86	-10.12	2.7240	1.2461	1.4969	0.05008	0.646	-0.106	-0.084	0.836
C6	S7	2-x,-1/2+y,1/2-z	9.28	-6.86	3.5791	1.7112	1.8681	0.04026	0.429	-0.060	-0.055	0.544
H5	O9	1-x,-1/2+y,1/2-z	15.66	-11.77	2.6599	1.2234	1.4557	0.05677	0.718	-0.142	-0.107	0.967
H6A	N1	2-x,1-y,1-z	34.74	-32.81	2.2521	0.9388	1.3134	0.12892	1.346	-0.449	-0.444	2.239
N6	H8A	2-x,-1/2+y,1/2-z	10.73	-8.03	2.8905	1.6333	1.2628	0.04491	0.493	-0.094	-0.084	0.670
H6A	H10A	2-x,-1/2+y,1/2-z	7.54	-5.55	2.7022	1.3613	1.3427	0.03528	0.350	-0.072	-0.032	0.454
S7	C6	2-x,1/2+y,1/2-z	9.27	-6.85	3.5791	1.8681	1.7112	0.04024	0.429	-0.059	-0.056	0.544
H8A	H10B	x,3/2-y,-1/2+z	1.04	-0.59	3.7225	1.8924	1.8461	0.00516	0.055	-0.007	-0.005	0.067
H10C	H10C	1-x,2-y,-z	3.13	-2.03	3.0950	1.5475	1.5475	0.01578	0.155	-0.031	-0.028	0.214

Table Suppl. 2 Interaction Energies (kJ/mol). R is the distance between molecular centroids (mean atomic position) in Å.

Total energies are the sum of the four energy components, scaled appropriately (see the scale factor table below)

1						
Symmetry operation	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
1/2+x,1/2-y,1/2+z	6.72	-75.1	-18.9	-34.1	81.9	-72.5
-1/2+x,1/2-y, 1/2+z	8.62	-59.0	-14.1	-19.9	59.1	-53.7
x, 1-y,1/2+z	6.71	-23.9	-5.8	-40.8	21.1	-52.1
x, y, -1+z	9.20	-20.8	-5.5	-30.8	45.7	-24.7
1/2+x,1/2+y,1+z	11.09	-15.6	-4.2	-10.9	20.1	-16.6
x, -y,1/2+z	7.48	3.1	-3.9	-19.9	25.2	-1.4
2						
1/2-x,1/2-y,-1+z	4.21	0.8	-8.7	-75.5	51.0	-39.8
1/2-x, -y, -1/2z	8.07	-26.6	-6.2	-26.2	27.6	-38.5
3/4-x,1/4+y,-1/4+z	10.09	-31.0	-8.7	-19.8	39.3	-32.2
-1/4+x, 3/4-y, -3/4+z	10.52	3.0	-2.2	-11.3	7.7	-3.6
3						
2-x,1-y,1-z	6.85	-64.5	-14.5	-20.7	61.1	-59.2

1-x,-1/2+y,1/2-z	6.54	-17.8	-4.5	-22.1	14.2	-32.6
1-x,1-y,-z	6.60	-21.5	-6.7	-20.6	23.5	-31.1
x,1/2-y,-1/2+z	7.04	-22.1	-4.8	-21.3	28.6	-27.8
2-x, y+1/2, -z+1/2	6.11	-0.2	-3.0	-20.3	15.0	-10.8
x,3/2-y,-1/2+z	7.64	-5.5	-1.2	-14.4	13.8	-10.6
4						
2-x, -y, 1-z	5.87	-40.6	-11.7	-14.4	32.4	-44.1
1-x, 1-y, 1-z	6.27	-37.0	-7.7	-19.7	42.7	-35.7
x, y, -1+z	8.09	-31.5	-6.2	-9.9	31.1	-27.3
2-x, 1-y, 1-z	3.93	-7.1	-2.4	-29.9	13.4	-27.1
-1+x, y,-1+z	8.51	-23.5	-5.6	-7.1	20.2	-22.7
1-x, -y, -z	6.56	-1.9	-3.8	-20.0	9.7	-16.3

Scale factors for benchmarked energy models; see Mackenzie et al. IUCrJ (2017)

Energy Model	k_{ele}	k_{pol}	k_{dis}	k_{rep}
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Table Suppl_3. Percentage of different kinds of contacts in the total Hirshfeld surface.

inside	outside	1	2	3
N	N	1.0	0.7	0.0
N	C	0.3	3.1	0.0
N	H	19.5	13.4	11.8
N	S	1.4	0.4	0.3
N	O	-	-	0.0
C	N	0.4	3.2	0.0
C	C	3.3	1.8	0.0
C	H	7.5	8.4	7.5
C	S	2.4	0.0	1.5
C	O	-	-	0.0
H	N	15.8	9.9	10.0
H	C	6.5	5.5	4.4
H	H	21.1	33.8	44.5
H	S	5.5	6.4	3.0
H	O	-	-	4.1
S	N	1.8	0.9	0.3
S	C	2.5	0.0	1.6
S	H	10.9	12.5	6.2
S	S	0.0	0.0	0.0
S	O	-	-	0.0
O	N	-	-	0.0
O	C	-	-	0.0
O	H	-	-	4.6
O	S	-	-	0.0
O	O	-	-	0.0