Electronic supplementary materials *Mendeleev Commun*., 2008, **18**, 312–314

The role of H-bonds in charge transfer in the crystal of 1,5-naphthalenedisulfonic acid tetrahydrate

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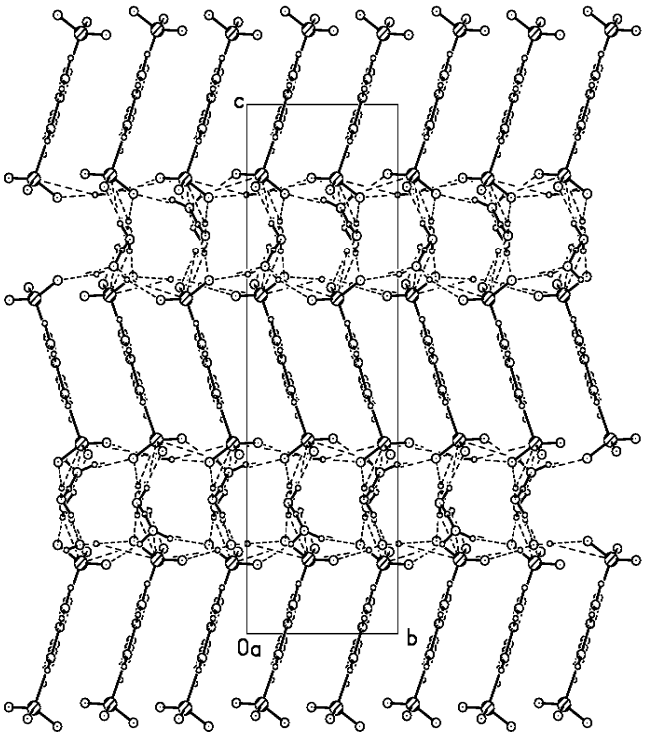
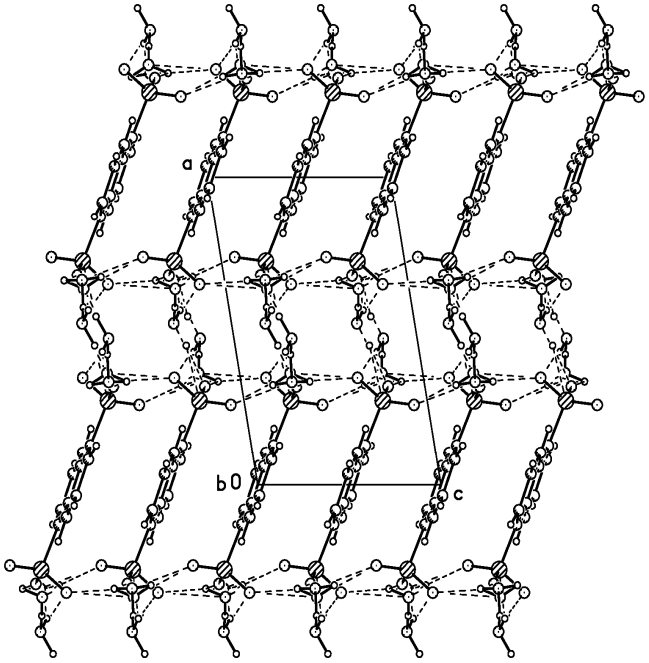


1A



1B

Figure S1 The projection of crystal packing in **1A** and **1B**.

Table S1 H-bond parameters in 1A.

Bond	Symm Code	D-H,Å	H…A,Å	D….A,Å	DHA,°
O(1W)-H(1WA)…O(4W)	[1_555]	0.955(15)	1.497(16)	2.4371(8)	167.4(15)
O(2W)-H(2WA)…O(3W)	[1_555]	0.991(14)	1.451(14)	2.4393(7)	174.6(14)
O(1W)-H(1WB)…O(5)	[2_655]	0.841(12)	1.817(12)	2.6461(5)	168.3(13)
O(1W)-H(1WC)…O(2)	[3_665]	0.794(12)	1.831(12)	2.6199(5)	172.2(12)
O(2W)-H(2WB)…O(6)	[1_455]	0.847(12)	1.755(12)	2.5983(5)	173.4(12)
O(2W)-H(2WC)…O(1)	[4_455]	0.838(14)	1.787(14)	2.6179(5)	171.4(13)
O(3W)-H(3WB)…O(2)	[3_665]	0.872(13)	1.853(13)	2.7052(6)	165.0(11)
O(3W)-H(3WA)…O(3)	[3_655]	0.862(12)	1.840(12)	2.6855(7)	166.5(12)
O(4W)-H(4WB)…O(6)	[1_565]	0.866(14)	1.861(14)	2.7162(6)	169.3(12)
O(4W)-H(4WA)…O(4)	[1_555]	0.827(12)	1.874(12)	2.6872(6)	167.7(12)

[3655.] = 1-x,-y,-z; [3665.] = 1-x,1-y,-z; [2655.] = 1-x,1/2+y,1/2-z; [1455.] = -1+x,y,z; [4455.] = -1+x,1/2-y,1/2+z; [1565.] = x,1+y,z

Table S2 H-bond parameters in 1B.

Bond	Symm Code	D-H,Å	H…A,Å	D….A,Å	DHA,°
O(1W)–H(1WC)…O2	[1_565]	0.928(18)	1.704(17)	2.6174(6)	167.1(14)
O(1W)-H(1WA)…O(2W')	[1_555]	1.008(19)	1.45(2)	2.4487(11)	170(2)
O(1W)-H(1WA)… O(2W)	[1_555]	1.006(18)	1.41(2)	2.414 (11)	173(2)
O(1W)-H(1WB)…O(3)	[2_655]	0.943(16)	1.675(16)	2.6150(7)	174.4(15)
O(2W')–H(2WB)…O(1)	[4_555]	0.85(2)	1.85(2)	2.6689(9)	160.1(17)
O(2W')–H(2WA)…O(2)	[4_554]	0.83(2)	1.92(2)	2.7215(9)	160.2(18)

[3756.] = 2-x,-y,1-z; [4554.] = x,1/2-y,-1/2+z; [4555.] = x,1/2-y,1/2+z; [2655.] = 1-x,1/2+y,1/2-z; [1565.] = x,1+y,z

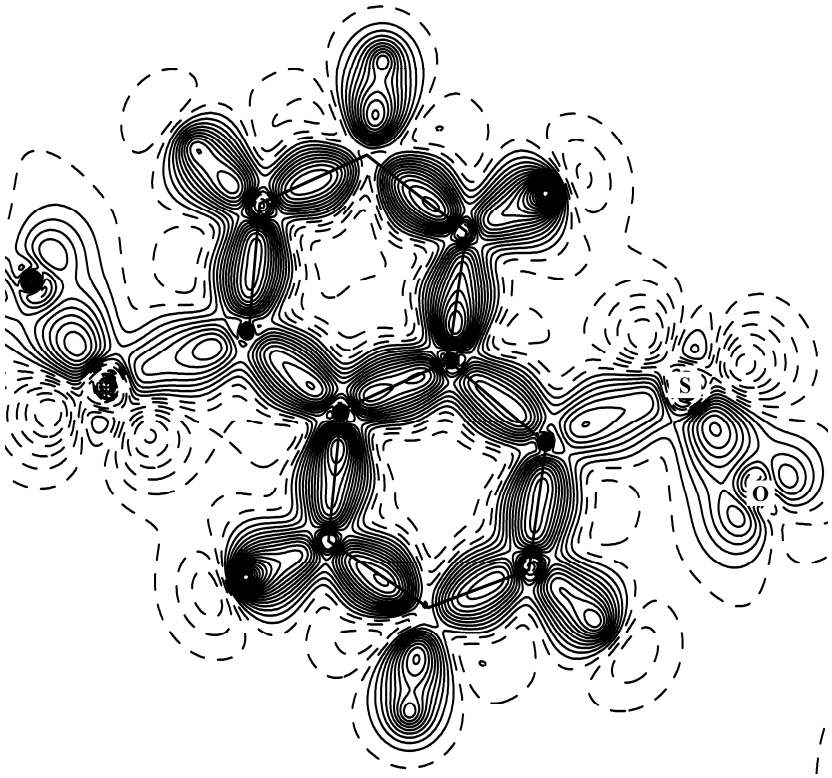


Figure S2 The deformation electron density map in the plane of dianion in **1A**. The contours are drawn with 0.05eÅ^{-3} step, the negative ones are dashed.

Table S3 Topological parameters for dianion at 1A in critical point (3,-1).

Bond	$\rho(r)$, eÅ^{-3}	$\nabla^2\rho(r)$,eÅ^{-5}	Rij	d1	d2	ellipticity
S(1)-O(1)	2.258	-9.991	1.4611	0.6239	0.8371	0.08
S(1)-O(2)	2.077	-4.909	1.4786	0.6219	0.8567	0.09
S(1)-O(3)	2.202	-5.792	1.4557	0.6138	0.8420	0.08
S(1)-C(1)	1.368	-5.189	1.7684	0.9277	0.8407	0.09
S(2)-O(4)	2.210	-5.950	1.4558	0.6149	0.8408	0.08
S(2)-O(5)	2.233	-8.903	1.4584	0.6224	0.8360	0.05
S(2)-O(6)	2.058	-6.238	1.4798	0.6288	0.8509	0.04
S(2)-C(5)	1.367	-5.221	1.7699	0.9413	0.8285	0.08
C(1)-C(2)	2.212	-19.347	1.3757	0.6868	0.6889	0.22
C(1)-C(9)	1.929	-14.368	1.4325	0.7046	0.7278	0.20
C(2)-C(3)	2.001	-18.030	1.4098	0.7146	0.6952	0.21
C(3)-C(4)	2.173	-21.012	1.3735	0.6773	0.6962	0.19
C(4)-C(10)	1.995	-15.693	1.4238	0.6802	0.7436	0.17
C(5)-C(6)	2.161	-17.372	1.3774	0.6913	0.6861	0.19
C(5)-C(10)	1.890	-13.807	1.4331	0.7224	0.7106	0.17
C(6)C(7)	1.977	-15.975	1.4109	0.7200	0.6909	0.18
C(7)C(8)	2.181	-20.480	1.3726	0.7090	0.6636	0.16
C(8)C(9)	2.025	-15.121	1.4237	0.6934	0.7303	0.19
C(9)C(10)	1.963	-14.556	1.4318	0.7199	0.7119	0.20

Table S4 The volumes ($Å^3$), population and charges (e) in 1A.

Atom	**V**	**Population**	**Charge, e**
S(1)	6.397665	13.57876	2.421245
S(2)	6.6212	13.6774	2.322604
O(1)	16.06719	9.016197	-1.0162
O(2)	14.9301	8.855214	-0.85521
O(3)	17.1908	9.007024	-1.00702
O(4)	17.07714	9.010587	-1.01059
O(5)	16.75967	8.973507	-0.97351
O(6)	14.66202	8.849023	-0.84902
C(1)	10.45951	6.121025	-0.12103
C(2)	11.19559	6.03465	-0.03465
C(3)	11.42843	5.964582	0.035418
C(4)	11.63605	6.023507	-0.02351
C(5)	10.53593	6.100895	-0.1009
C(6)	11.90583	6.121019	-0.12102
C(7)	11.54333	6.01473	-0.01473
C(8)	12.15123	6.036942	-0.03694
C(9)	10.68093	6.002234	-0.00223
C(10)	10.67046	5.976613	0.023387
H(4)	4.893366	0.804822	0.195178
H(8)	4.637044	0.785548	0.214452
H(2)	5.829278	0.798105	0.201895
H(6)	5.510348	0.789735	0.210265
H(3)	7.528789	0.86687	0.13313
H(7)	7.90299	0.890836	0.109164
O(1W)	21.0473	9.49168	-1.49168
O(2W)	20.39339	9.476128	-1.47613
H(1WA)	1.753867	0.558105	0.558105
H(1WB)	1.608357	0.406983	0.406983
H(1WC)	1.340412	0.345806	0.345806
H(2WA)	1.926379	0.577595	0.577595
H(2WB)	1.645823	0.40318	0.40318
H(2WC)	1.639471	0.430018	0.430018

Table S5 Topological parameters in critical points (3,-1) for interactions formed by SO_3 group in 1A and their energy estimated within Espinosa correlation scheme.

Contact	ρ(r), eÅ^{-3}	$\nabla^2\rho$(r),eÅ^{-5}	v(r), au	**Econt, kcal/mol**
O(1) 3 - O(2W) 51	0.038	0.52	-0.0028	**-0.88**
O(1) 3 - H(4) 50	0.031	0.34	-0.00191	**-0.60**
O(1) 3 - O(6) 48	0.026	0.37	-0.00183	**-0.57**
O(1) 3 - O(4W) 44	0.034	0.51	-0.0026	**-0.82**
O(1) 3 - H(2WC) 41	0.202	6.72	-0.03974	**-12.47**
Total				**-15.34**
O(2) 4 - H(3WB) 42	0.207	4.18	-0.03166	**-9.93**
O(2) 4 - H(1WC) 41	0.176	6.44	-0.03545	**-11.12**
Total				**-21.05**
O(3) 5 - H(6) 46	0.032	0.42	-0.00222	**-0.70**
O(3) 5 - H(3) 42	0.052	0.59	-0.00378	**-1.19**
O(3) 5 - H(3WA) 41	0.209	4.45	-0.03296	**-10.34**
O(3) 5 - H(8) 36	0.083	1.1	-0.00758	**-2.38**
				-14.60
O(4) 6 - O(2W) 46	0.024	0.34	-0.00168	**-0.53**
O(4) 6 - H(7) 45	0.024	0.27	-0.0014	**-0.44**
O(4) 6 - H(2) 41	0.042	0.55	-0.00311	**-0.98**
O(4) 6 - H(4) 35	0.083	1.08	-0.00753	**-2.36**
O(4) 6 - H(4WA) 34	0.145	4.69	-0.0258	**-8.09**
Total				**-12.40**
O(5) 7 - H(1WB) 41	0.192	5.85	-0.03541	**-11.11**
O(5) 7 - O(3W) 12	0.031	0.48	-0.0024	**-0.75**
O(5) 7 - O(1W) 9	0.043	0.6	-0.00335	**-1.05**
Total				**-12.91**
O(6) 8 - O(1) 47	0.026	0.37	-0.00183	**-0.57**
O(6) 8 - H(4WB) 42	0.226	4.22	-0.0345	**-10.82**
O(6) 8 - H(2WB) 41	0.246	6.89	-0.04684	**-14.70**
Total				**-26.10**