Supplementary Information *for*

The non-adiabatic exciton transfer in tetrathiafulvalene chains: a theoretical study of signal transmission in a molecular logic system

Arthur I. Martynov,*[1] Aleksandr S. Belov[2], Vladimir K. Nevolin[1]

[1]National Research University of Electronic Technology, 1 Shokin Square, Zelenograd, Moscow, Russia. E-mail: i.martinov2@rambler.ru

[2]Department of Chemistry, Lomonosov Moscow State University, 1-3 Leninskie gory, Moscow, Russia

Table 1. Parameters of TTF2CN and TTF2F are required for evaluating the rate of $S_2 \rightarrow S_1$transfer.

TTF_2CN			**TTF_2F**		
Vibration frequency of mode ω_j (cm^{-1})	Huang-Rhys factor (y_j)	ΔQ	Vibration frequency of mode ω_j (cm^{-1})	Huang-Rhys factor (y_j)	ΔQ
3283.2	0.0000	0.06	3291.3	0.0000	0.03
3276.9	0.0005	-0.26	3282.9	0.0000	-0.03
3267.2	0.0000	-0.05	3266.5	0.0000	-0.04
3264.1	0.0000	-0.03	3264.5	0.0000	0.08
3263.7	0.0002	-0.15	3263.7	0.0000	0.00
2408.1	0.0012	-0.47	1756.3	0.0201	2.24
1710.4	0.0035	0.95	1708.9	0.0172	2.10
1693.8	0.8462	14.81	1690.1	0.1414	6.06
1680.3	0.0807	4.59	1671.5	0.0636	-4.09
1660.9	0.0739	4.42	1657.6	0.0066	1.32
1653.5	0.0010	-0.51	1642.3	0.0071	1.38
1641.5	0.0359	-3.10	1315.8	0.0000	0.04
1315.5	0.0000	-0.11	1309.2	0.0003	-0.34
1309.3	0.0057	-1.38	1271.5	0.0002	0.23
1271.1	0.0023	0.89	1265.6	0.0023	0.89
1266.0	0.0115	2.00	1236.6	0.0008	0.53
1236.7	0.0238	2.90	1210.5	0.0065	1.54
1145.3	0.2911	-10.56	1143.9	0.0022	0.92
1143.7	0.0067	1.61	1042.8	0.0051	-1.46
1042.4	0.0004	0.43	1039.8	0.0010	0.64
1039.6	0.0013	0.73	906.1	0.0000	0.00
906.2	0.0000	0.00	898.5	0.0460	-4.74
897.2	0.0091	2.11	894.7	0.0238	-3.42
893.5	0.0011	0.75	887.3	0.0017	-0.92
886.9	0.0106	-2.29	878.7	0.0027	1.16
877.8	0.0032	-1.27	869.4	0.0008	0.64
868.0	0.0775	6.26	830.3	0.0000	-0.06
840.5	0.0000	0.00	814.4	0.0000	0.00
830.2	0.0000	0.10	800.8	0.0011	0.78
814.7	0.0000	0.00	798.5	0.0007	-0.63
800.8	0.0109	2.45	784.5	0.0000	0.00
799.4	0.0474	5.10	771.4	0.0000	0.00
784.9	0.0000	0.00	770.1	0.2574	-12.11
770.1	0.7904	21.23			

763.1	0.0630	6.02	763.2	0.0199	-3.38
701.6	0.3121	13.97	705.4	0.0456	5.33
696.4	0.5953	-19.37	700.8	0.0050	-1.77
669.7	0.0000	0.00	669.9	0.0000	0.00
637.7	0.0168	-3.40	637.6	0.0037	-1.60
626.4	0.0472	-5.75	626.3	0.0086	-2.45
567.7	0.0000	0.00	549.9	0.0000	0.00
549.5	0.0000	0.00	538.9	0.0000	0.00
538.9	0.0000	0.00	536.8	0.0000	0.00
536.2	0.0000	0.00	522.4	0.0126	-3.26
524.9	0.1683	-11.86	494.0	0.0029	1.60
492.8	0.0056	-2.23	492.7	0.0016	-1.20
491.5	0.0832	8.62	468.2	0.0000	0.00
480.3	0.2985	16.52	454.7	0.0069	2.57
454.3	0.0283	5.23	449.9	0.0009	0.93
442.2	0.0000	0.00	442.3	0.0000	0.00
438.5	0.0720	8.49	427.1	0.0000	0.00
427.0	0.0000	0.00	385.1	0.0156	4.21
397.0	0.0000	0.00	363.0	0.0019	-1.52
373.5	0.1170	-11.73	332.0	0.0003	-0.60
331.6	0.0225	5.46	315.4	0.0174	-4.92
326.3	0.0674	9.52	281.6	0.0004	0.79
289.7	0.0183	-5.27	258.1	0.0000	0.00
258.1	0.0000	0.00	251.2	0.8836	39.30
250.7	3.0090	-72.59	247.6	0.0000	0.00
247.4	0.0000	0.00	246.0	0.0000	0.00
241.8	0.0000	0.00	239.6	0.0000	0.00
169.2	0.0598	12.46	145.9	0.0093	-5.29
153.1	0.0000	0.00	135.7	0.0377	11.05
144.7	0.0182	-7.44	107.2	0.0000	0.00
116.3	0.2269	29.26	86.7	0.0000	0.00
107.4	0.0000	0.00	79.9	0.0540	17.22
85.8	0.0000	0.00	71.9	0.0000	0.00
74.3	0.0000	0.29	57.4	0.0000	0.00
70.1	0.0000	0.00	39.7	0.0000	0.55
57.4	0.0000	0.00	38.9	0.0000	0.00
35.9	0.1903	48.21			
35.9	0.0000	0.00			

Table 2. Non-adiabatic matrix elements (NACME) of TTF_2CN optimized at S_2-state

ATOM	D/DX	D/DY	D/DZ
H	-0.0000482	0.0001060	0.0000000
C	0.0005460	0.0003236	0.0000000
C	-0.0002571	0.0005406	0.0000000
H	-0.0002503	-0.0000940	0.0000000
S	-0.0008720	-0.0026407	0.0000000
C	0.0066516	0.0007314	0.0000000
S	-0.0030373	-0.0018780	0.0000000
C	-0.0037041	0.0091925	0.0000000
S	-0.0083810	-0.0010729	0.0000000
S	0.0072023	-0.0018737	0.0000000
C	-0.0090075	0.0012745	0.0000000
H	0.0018164	-0.0006127	0.0000000
C	0.0104612	0.0069042	0.0000000
C	-0.0116452	-0.0065613	0.0000000
C	0.0076524	-0.0031057	0.0000000
S	0.0124518	0.0029841	0.0000000
H	-0.0016599	0.0005241	0.0000000
S	-0.0036147	0.0051922	0.0000000
C	-0.0058532	-0.0121247	0.0000000
C	-0.0003400	-0.0106863	0.0000000
S	0.0031307	0.0082404	0.0000000
S	-0.0011064	0.0083247	0.0000000
C	-0.0020849	-0.0025673	0.0000000
C	0.0018410	-0.0011613	0.0000000
H	-0.0000017	-0.0001506	0.0000000
C	0.0002697	0.0003318	0.0000000
N	-0.0002512	-0.0001923	0.0000000

Table 3. Non-adiabatic matrix elements (NACME) of TTF_2F optimized at S_2-state

ATOM	D/DX	D/DY	D/DZ
H	-0.0042662	0.0086480	0.0000000
C	0.0065450	0.0150792	0.0000000
C	0.0021913	0.0106624	0.0000000
H	-0.0086672	-0.0032553	0.0000000
S	-0.0575443	-0.0552413	0.0000000
C	0.1717821	-0.0080935	0.0000000
S	-0.0342042	0.0066427	0.0000000
C	-0.1216084	0.0304310	0.0000000
S	0.0124307	-0.0045626	0.0000000
S	0.0459140	0.0001636	0.0000000
C	-0.0491825	-0.0204819	0.0000000
H	0.0049204	0.0006581	0.0000000
C	0.0351556	0.0524981	0.0000000
C	-0.0423362	-0.0172150	0.0000000
C	0.0164430	-0.0153402	0.0000000
S	0.0681906	0.0064810	0.0000000
H	0.0011259	0.0036897	0.0000000
S	0.0215101	-0.0077360	0.0000000
C	-0.1645730	0.0123668	0.0000000
C	0.1520673	-0.1036082	0.0000000
S	-0.0022129	0.0712673	0.0000000
S	-0.0452881	0.0332962	0.0000000
C	-0.0092898	-0.0136097	0.0000000
C	0.0170003	-0.0006293	0.0000000
H	-0.0065852	-0.0056398	0.0000000
F	-0.0095225	0.0034940	0.0000000

Table 4. Coordinates of TTF_2CN optimized at S_0

ATOM	X	Y	Z
H	-8.7542582642	-0.3513168130	0.0000000000
C	-7.7384614449	0.0232370044	0.0000000000
C	-7.4062761109	1.3108417205	0.0000000000
H	-8.1138464976	2.1302689336	0.0000000000
S	-5.7001796422	1.7225532991	0.0000000000
C	-5.1370554296	0.0381946330	0.0000000000
S	-6.4456769689	-1.1633224710	0.0000000000
C	-3.8385024425	-0.2965109253	0.0000000000
S	-2.5352917408	0.9071249029	0.0000000000
S	-3.2718610046	-1.9789947822	0.0000000000
C	-1.5776489173	-1.5676541315	0.0000000000
H	-0.8804491684	-2.3967857412	0.0000000000
C	-1.2150573458	-0.2780955926	0.0000000000
C	0.1535375937	0.2211084702	0.0000000000
C	0.5190106676	1.5094434776	0.0000000000
S	1.4748043221	-0.9641585161	0.0000000000
H	-0.1758728668	2.3402394433	0.0000000000
S	2.2159841189	1.9168290124	0.0000000000
C	2.7779006011	0.2357920910	0.0000000000
C	4.0763453166	-0.0985432078	0.0000000000
S	5.3837911629	1.1062140517	0.0000000000
S	4.6336297496	-1.7884533599	0.0000000000
C	6.6773181153	-0.1013356482	0.0000000000
C	6.3246982779	-1.3941142459	0.0000000000
H	7.0357051630	-2.2108264448	0.0000000000
C	8.0275059622	0.3470362939	0.0000000000
N	9.1228015512	0.7204344046	0.0000000000

Table 5. Coordinates of TTF_2CN optimized at S_1

ATOM	X	Y	Z
H	-8.7359548399	-0.3634942081	0.0000000000
C	-7.7213893265	0.0143671128	0.0000000000
C	-7.3930612552	1.3029343843	0.0000000000
H	-8.1029712147	2.1203270211	0.0000000000
S	-5.6881432302	1.7195203224	0.0000000000
C	-5.1200077809	0.0371467934	0.0000000000
S	-6.4248906499	-1.1681764899	0.0000000000
C	-3.8202468978	-0.2925846005	0.0000000000
S	-2.5194682128	0.9139582774	0.0000000000
S	-3.2475673559	-1.9737727830	0.0000000000
C	-1.5569962373	-1.5596974047	0.0000000000
H	-0.8560313476	-2.3858202856	0.0000000000
C	-1.1962826304	-0.2691724835	0.0000000000
C	0.1688558660	0.2376341107	0.0000000000
C	0.5349162111	1.5251364078	0.0000000000
S	1.5076264474	-0.9615795156	0.0000000000
H	-0.1439289092	2.3684104334	0.0000000000
S	2.2545287517	1.9299053153	0.0000000000
C	2.7508111524	0.2675682221	0.0000000000
C	4.0902360547	-0.0795094146	0.0000000000
S	5.3089898096	1.1440321579	0.0000000000
S	4.5301500756	-1.7879658125	0.0000000000
C	6.6665446400	-0.1499410442	0.0000000000
C	6.2790281957	-1.4196944447	0.0000000000
H	6.9327236627	-2.2822957097	0.0000000000
C	7.9985016842	0.3170467961	0.0000000000
N	9.0757338804	0.7453777728	0.0000000000

Table 6. Coordinates of TTF_2CN optimized at S_2

ATOM	X	Y	Z
H	-8.7132572237	-0.3250348743	0.0000000000
C	-7.7010423389	0.0577137288	0.0000000000
C	-7.3517714082	1.3394677682	0.0000000000
H	-8.0337813256	2.1797467082	0.0000000000
S	-5.6165167757	1.7367075099	0.0000000000
C	-5.1448238898	0.0529409365	0.0000000000
S	-6.4037770203	-1.1552145644	0.0000000000
C	-3.8080192647	-0.3032597070	0.0000000000
S	-2.5852762943	0.9436314783	0.0000000000
S	-3.3428180345	-1.9852353222	0.0000000000
C	-1.5977635113	-1.5839910279	0.0000000000
H	-0.9408046953	-2.4445434968	0.0000000000
C	-1.2236794296	-0.3075837802	0.0000000000
C	0.1375285817	0.1999358671	0.0000000000
C	0.5020871872	1.4886235014	0.0000000000
S	1.4667421077	-0.9819439780	0.0000000000
H	-0.2001332468	2.3134137026	0.0000000000
S	2.1957743690	1.8998802640	0.0000000000
C	2.7664150112	0.2206840649	0.0000000000
C	4.0666813610	-0.1056150506	0.0000000000
S	5.3690155253	1.1059497423	0.0000000000
S	4.6330445151	-1.7929335385	0.0000000000
C	6.6683081254	-0.0954577544	0.0000000000
C	6.3219245024	-1.3900348752	0.0000000000
H	7.0372836819	-2.2029505870	0.0000000000
C	8.0165011477	0.3587971647	0.0000000000
N	9.1102767899	0.7367691906	0.0000000000

Table 7. Coordinates of TTF_2F optimized at S_0

ATOM	X	Y	Z
H	-8.5785037546	-0.4029041564	0.0000000000
C	-7.5652266379	-0.0215414999	0.0000000000
C	-7.2418115906	1.2683335116	0.0000000000
H	-7.9550682909	2.0828264309	0.0000000000
S	-5.5386020203	1.6917391078	0.0000000000
C	-4.9638691024	0.0109769333	0.0000000000
S	-6.2645659755	-1.1994842708	0.0000000000
C	-3.6629850259	-0.3145752799	0.0000000000
S	-2.3689547478	0.8983321010	0.0000000000
S	-3.0838281524	-1.9924962575	0.0000000000
C	-1.3920130027	-1.5685680590	0.0000000000
H	-0.6882730954	-2.3920684928	0.0000000000
C	-1.0390207980	-0.2764651049	0.0000000000
C	0.3255096236	0.2338979590	0.0000000000
C	0.6772482543	1.5261808944	0.0000000000
S	1.6572189621	-0.9395124373	0.0000000000
H	-0.0266070784	2.3493906911	0.0000000000
S	2.3693864619	1.9507176227	0.0000000000
C	2.9486561411	0.2743461954	0.0000000000
C	4.2494727628	-0.0505697773	0.0000000000
S	5.5382546934	1.1718384706	0.0000000000
S	4.8201778431	-1.7380518906	0.0000000000
C	6.8242078113	-0.0318411790	0.0000000000
C	6.5266872841	-1.3237633951	0.0000000000
H	7.2613551159	-2.1172130008	0.0000000000
F	8.0550305122	0.4699329978	0.0000000000

Table 8. Coordinates of TTF_2F optimized at S_1

ATOM	X	Y	Z
H	-8.5741102753	-0.3823763385	0.0000000000
C	-7.5600133511	-0.0032040229	0.0000000000
C	-7.2336886064	1.2859391646	0.0000000000
H	-7.9452622074	2.1019104909	0.0000000000
S	-5.5295915403	1.7057594147	0.0000000000
C	-4.9582745812	0.0238605674	0.0000000000
S	-6.2618195994	-1.1839221292	0.0000000000
C	-3.6580616903	-0.3039021657	0.0000000000
S	-2.3585281997	0.9029439086	0.0000000000
S	-3.0842144362	-1.9846122461	0.0000000000
C	-1.3926596605	-1.5689686206	0.0000000000
H	-0.6909876156	-2.3944805660	0.0000000000
C	-1.0318044233	-0.2786276763	0.0000000000
C	0.3311792413	0.2270792911	0.0000000000
C	0.7088490026	1.5080235713	0.0000000000
S	1.6827321024	-0.9842561998	0.0000000000
H	0.0364541104	2.3569152113	0.0000000000
S	2.4342294982	1.9195166675	0.0000000000
C	2.916430052	0.2226507010	0.0000000000
C	4.2538841029	-0.1150622957	0.0000000000
S	5.4724480371	1.1931094785	0.0000000000
S	4.7866661704	-1.7595368512	0.0000000000
C	6.7827986589	-0.0137883113	0.0000000000
C	6.5238798414	-1.3116043991	0.0000000000
H	7.2457497279	-2.1152408849	0.0000000000
F	7.9902135837	0.5411477870	0.0000000000

Table 9. Coordinates of TTF_2F optimized at S_2

ATOM	X	Y	Z
H	-8.5346869326	-0.3801125706	0.0000000000
C	-7.5257295826	0.0111301212	0.0000000000
C	-7.1866289632	1.2952219779	0.0000000000
H	-7.8745851973	2.1306160643	0.0000000000
S	-5.4530141223	1.7068969768	0.0000000000
C	-4.9696355541	0.0257871731	0.0000000000
S	-6.2184336021	-1.1937380079	0.0000000000
C	-3.6302799774	-0.3198559761	0.0000000000
S	-2.4158749949	0.9349215538	0.0000000000
S	-3.1498881537	-1.9971958375	0.0000000000
C	-1.4094979720	-1.5814224152	0.0000000000
H	-0.7436424060	-2.4350344427	0.0000000000
C	-1.0459526722	-0.3013105953	0.0000000000
C	0.3115269990	0.2170001784	0.0000000000
C	0.6626029472	1.5096166869	0.0000000000
S	1.6505690210	-0.9532789937	0.0000000000
H	-0.0479957516	2.327178145	0.0000000000
S	2.3514986348	1.9375347222	0.0000000000
C	2.9388955941	0.2629530894	0.0000000000
C	4.2413470009	-0.0545023945	0.0000000000
S	5.5253656855	1.174099531	0.0000000000
S	4.8203080418	-1.7395706117	0.0000000000
C	6.8164755822	-0.0238778907	0.0000000000
C	6.5248974815	-1.3171521406	0.0000000000
H	7.2635119159	-2.1069410304	0.0000000000
F	8.0455163270	0.4831404745	0.0000000000