Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Dithienothiazine dimer, trimer and polymer – novel electron-rich donors with red-shifted luminescence

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4-(4-((Triisopropylsilyl)oxy)phenyl)-4*H*-dithieno[2,3-b:3',2'-e][1,4]thiazin **1b**

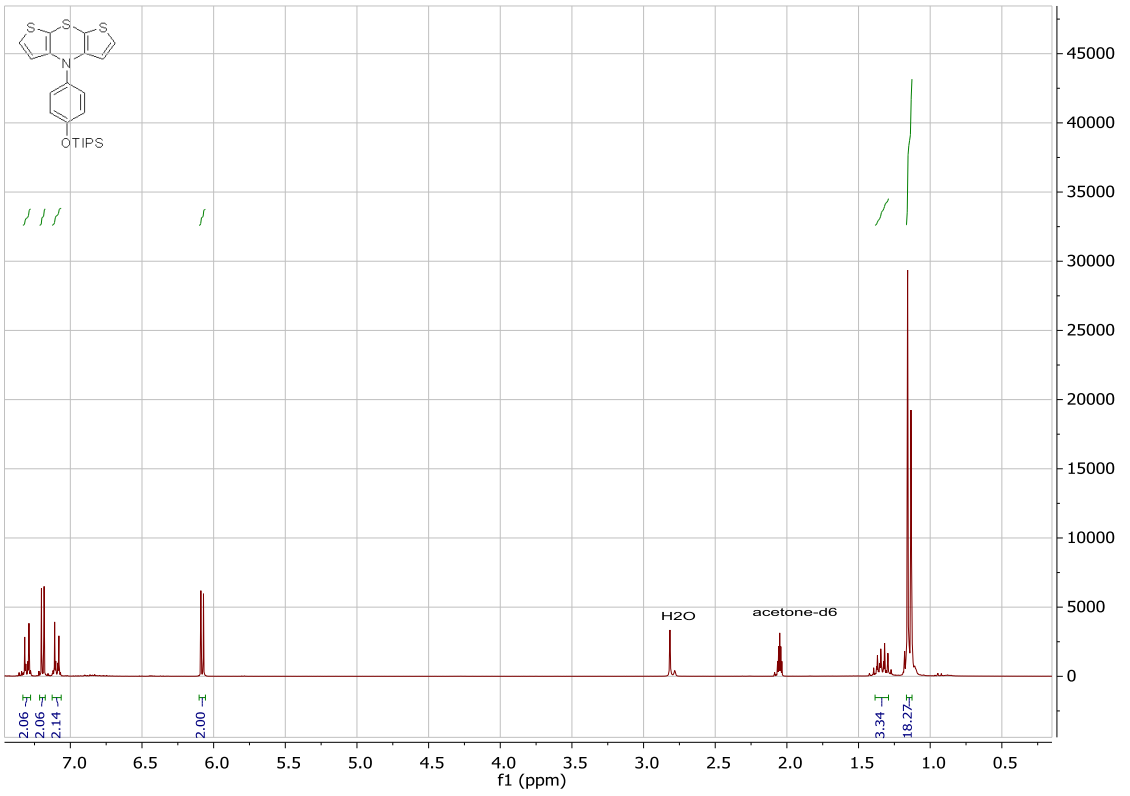


Figure 1. ^{1}H NMR spectrum (300 MHz) of **1b**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

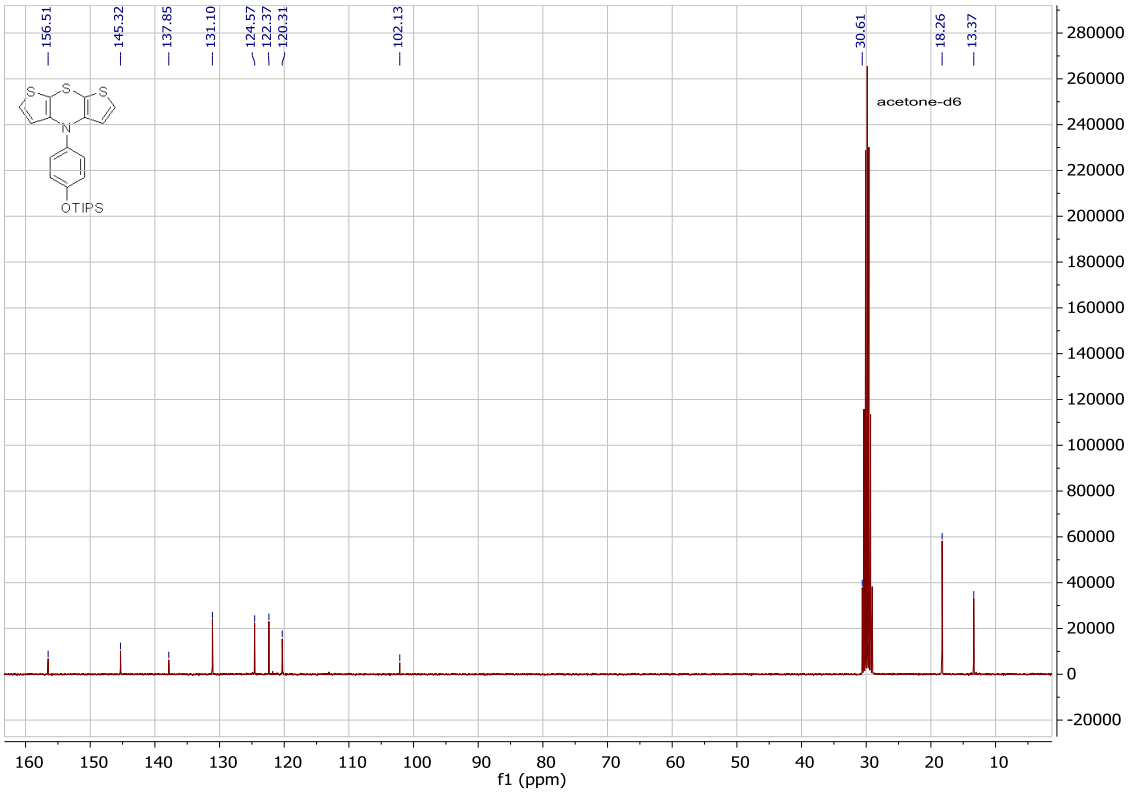


Figure 2. ^{13}C NMR spectrum (75 MHz) of **1b**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4-(4-((2-Decyltetradecyl)oxy)phenyl) 4*H*-dithieno[2,3-b:3',2'-e][1,4]thiazine **1c**

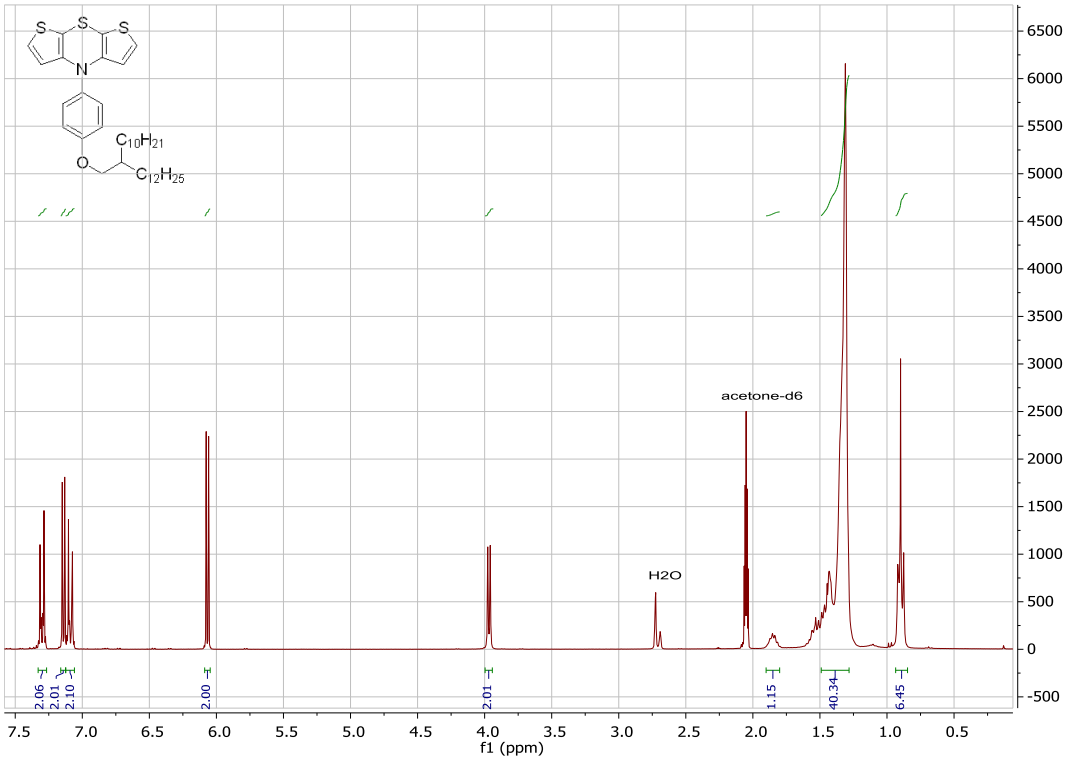


Figure 3. ^{1}H NMR spectrum (300 MHz) of **1c**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

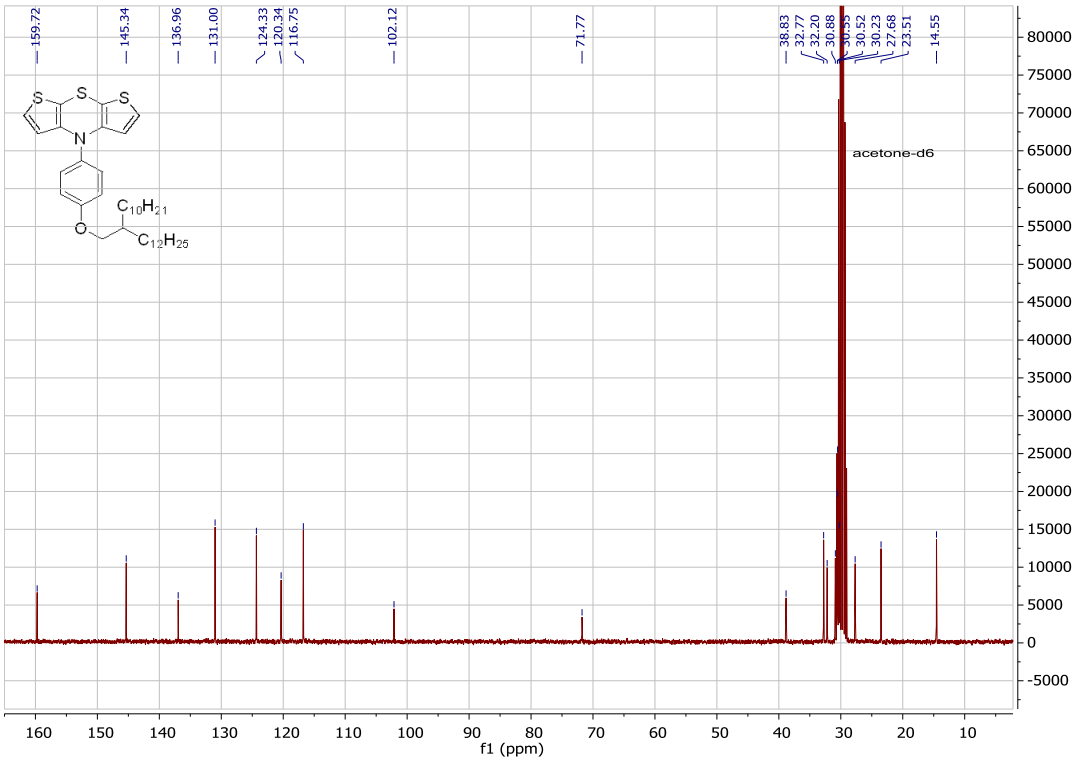


Figure 4. ^{13}C NMR spectrum (75 MHz) of **1c**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4-(4-Hexylphenyl)-2-iodo-*4H*-dithieno[2,3-b:3',2'-e][1,4]thiazin **2a**

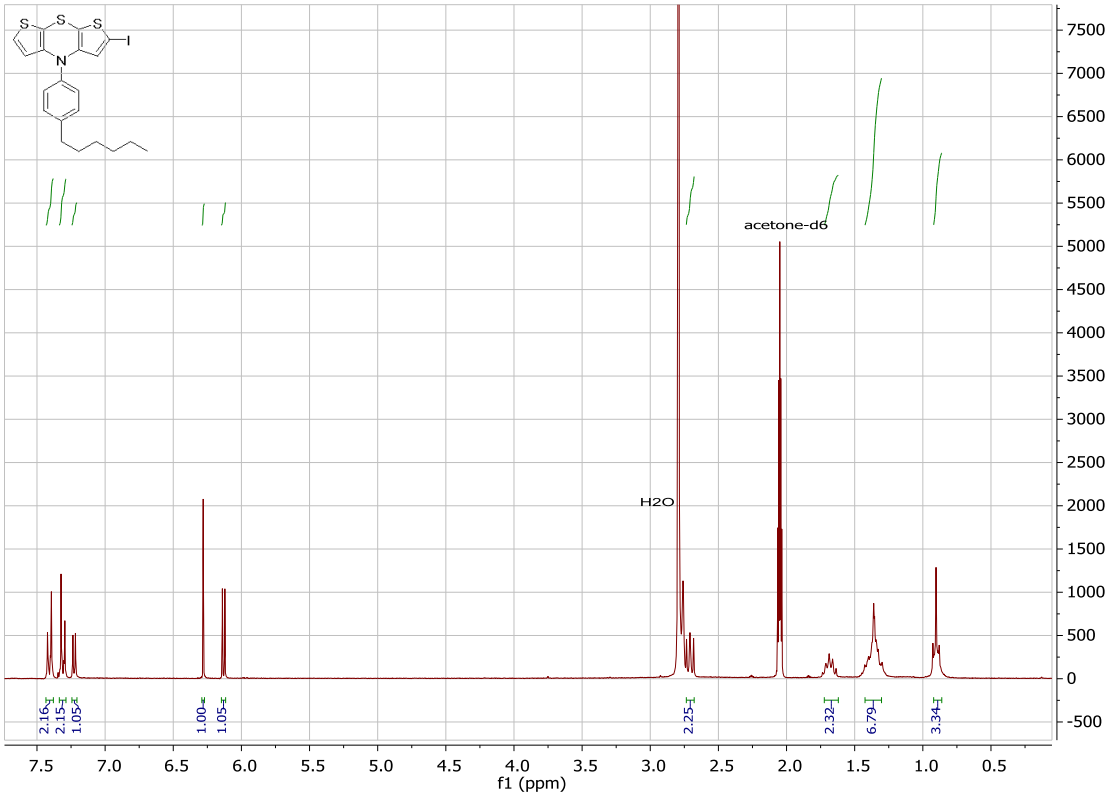


Figure 5. ^{1}H NMR spectrum (300 MHz) of **2a**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

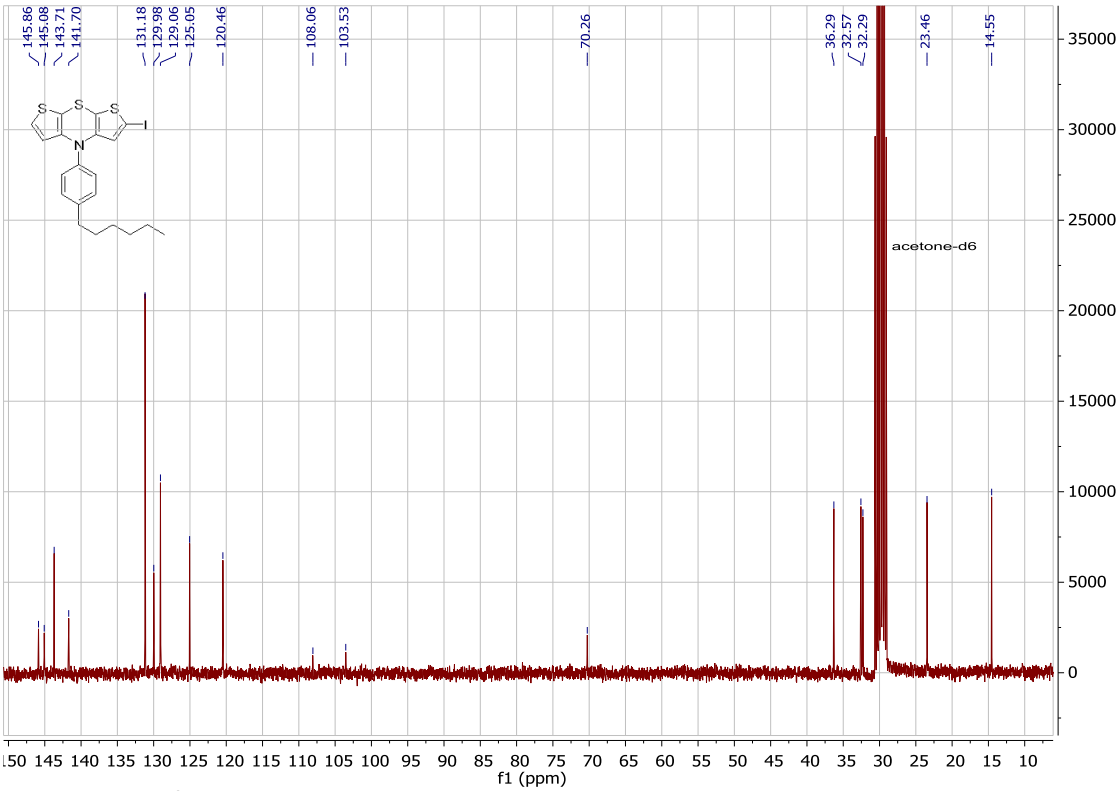


Figure 6. ^{13}C NMR spectrum (75 MHz) of **2a**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4-(4-((Triisopropylsilyl)oxy)phenyl)-2,6-diiodo-*4H*-dithieno[2,3-b:3',2'-e][1,4]thiazin **2b**

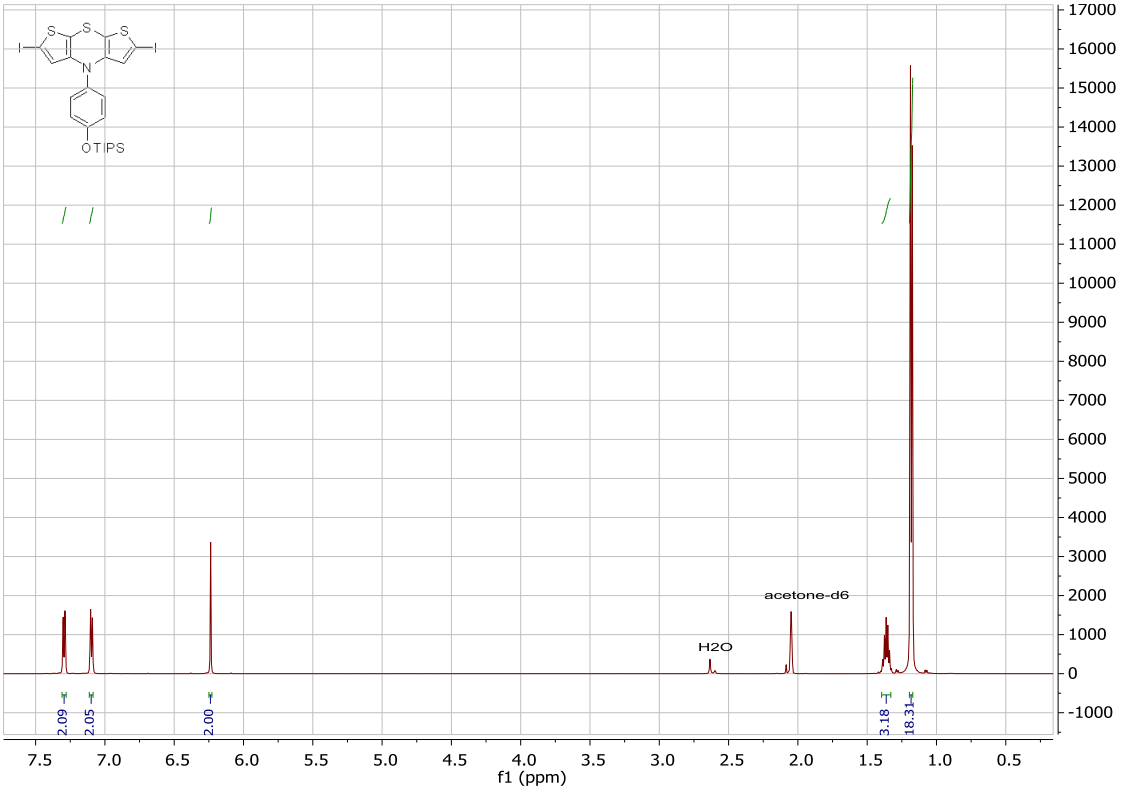


Figure 7. ^{1}H NMR spectrum (600 MHz) of **2b**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

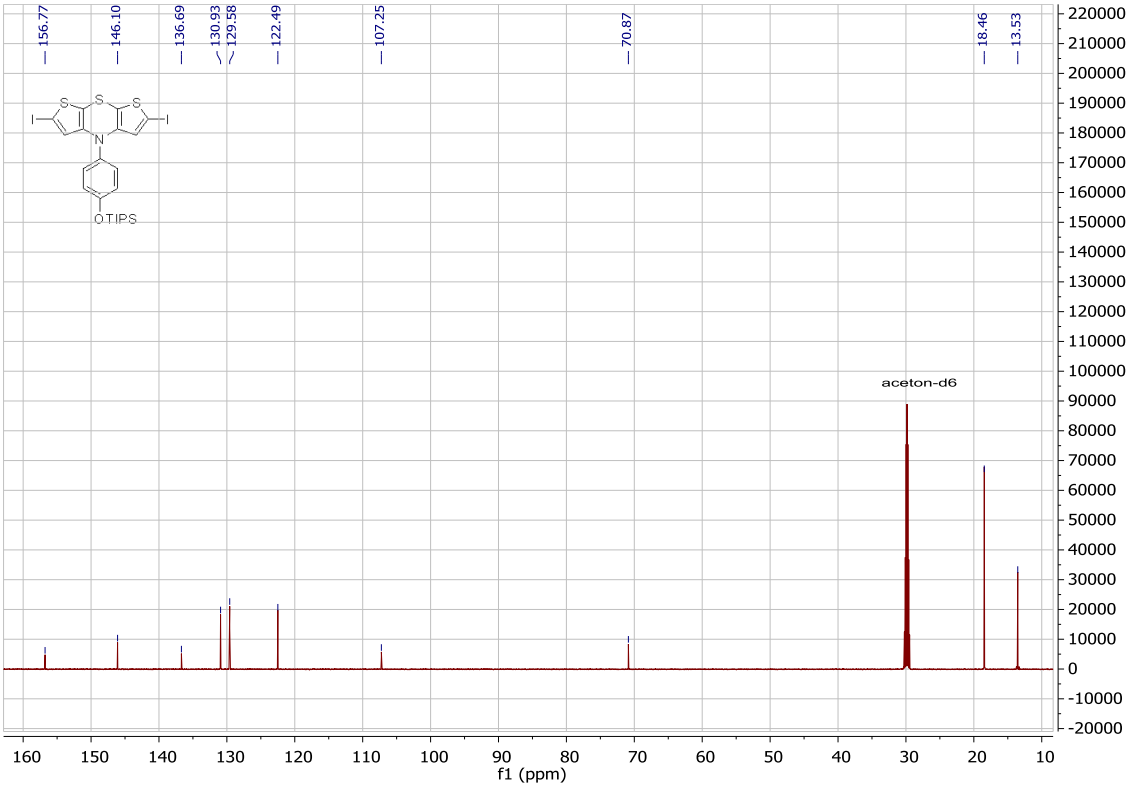


Figure 8. ^{13}C NMR spectrum (125 MHz) of **2b**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4-(4-((2-Decyltetradecyl)oxy)phenyl)-2,6-diiodo-*4H*-dithieno[2,3-b:3',2'-e][1,4]thiazin **2c**

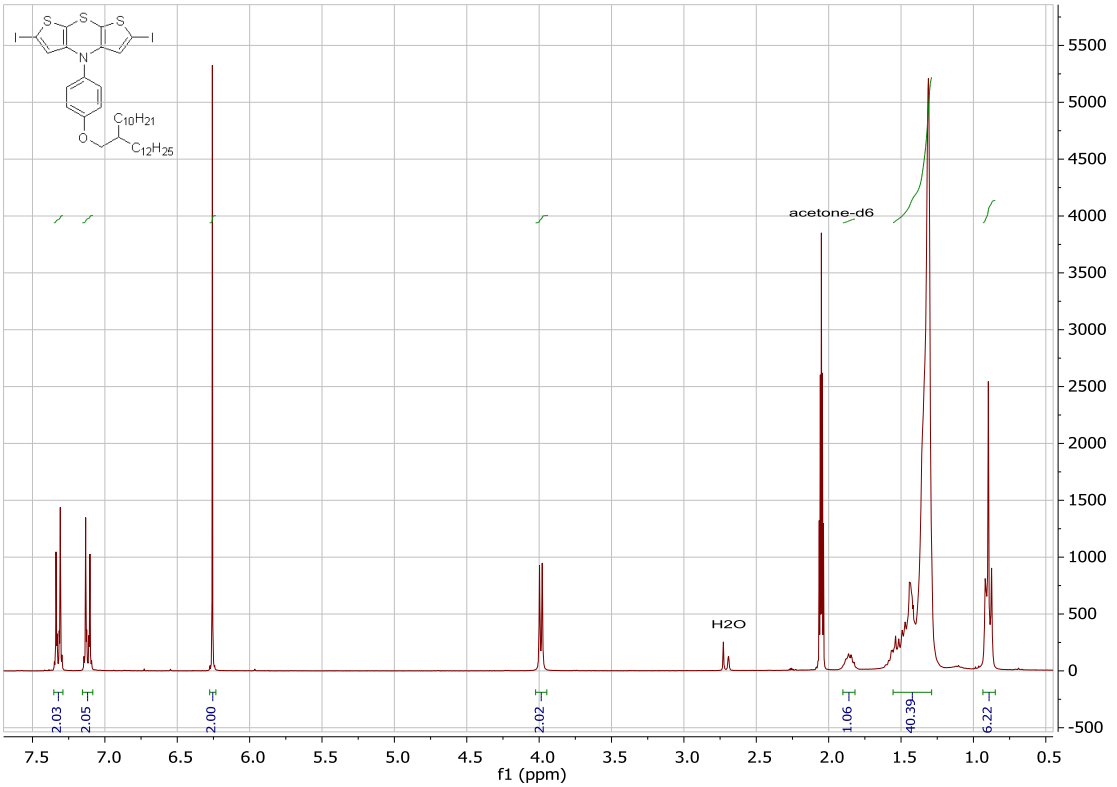


Figure 9. ^{1}H NMR spectrum (300 MHz) of **2c**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

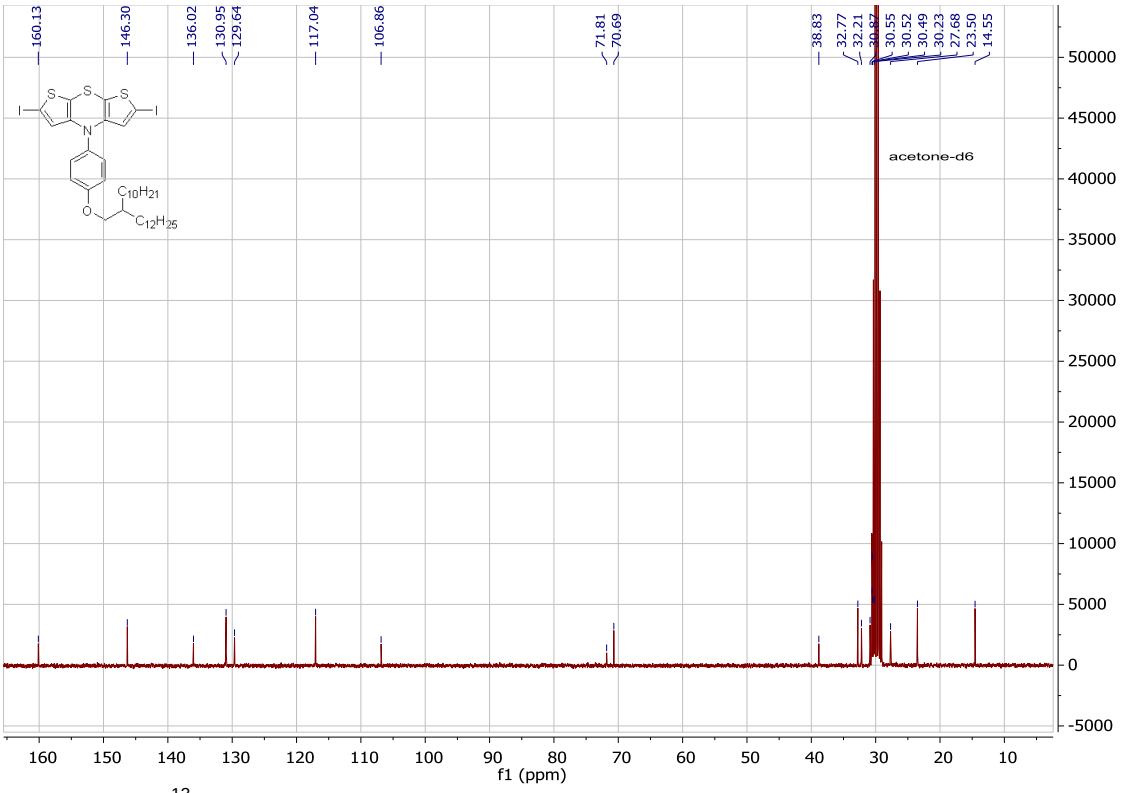


Figure 10. ^{13}C NMR spectrum (75 MHz) of **2c**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4-(4-Hexylphenyl)-2,6-bis(4,4,5,5-tetramethyl1,3,2-dioxaborolan-2-yl)-*4H*-dithieno[2,3-b:3',2'-e][1,4]thiazin **3a**

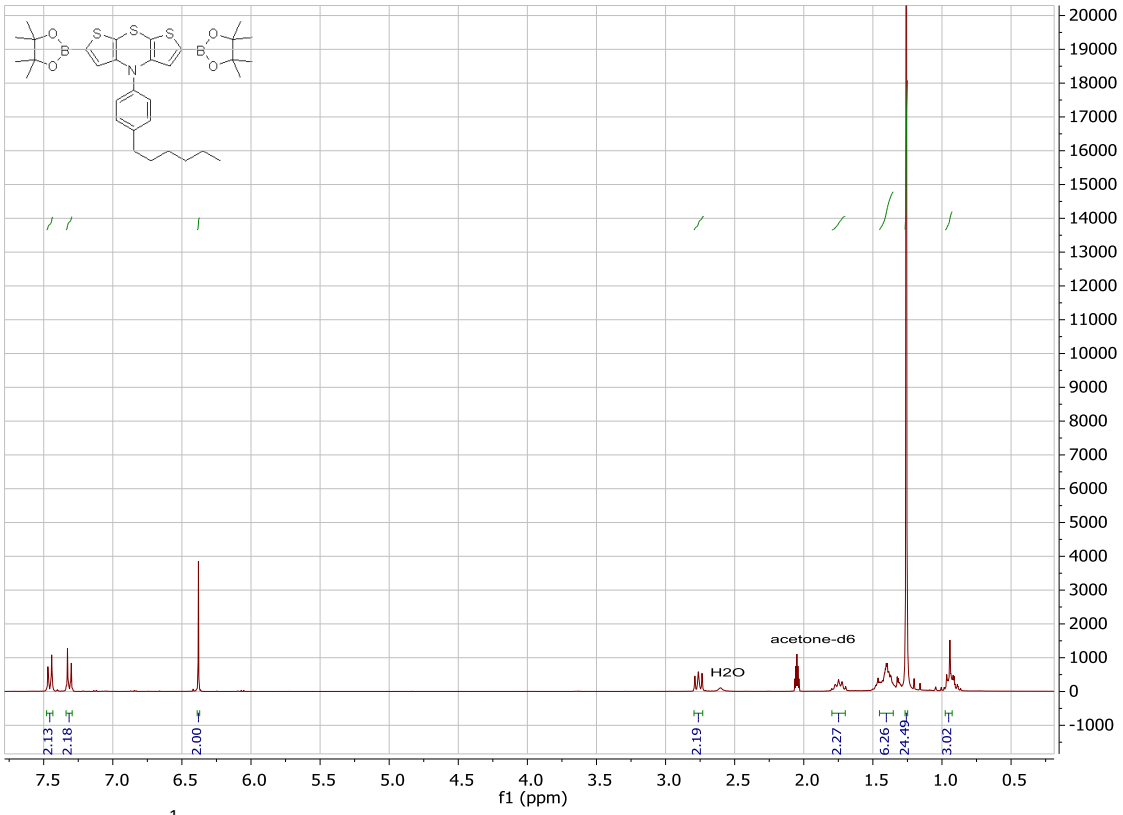


Figure 11. ^{1}H NMR spectrum (300 MHz) of **3a**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

Figure 12. ^{13}C NMR spectrum (75 MHz) of **3a**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4,4‘,-Bis(4-hexylphenyl)-4*H*,4’*H*-2,2-bidithieno[2,3-*b*:3’,2’-*e*][1,4]thiazin **4**

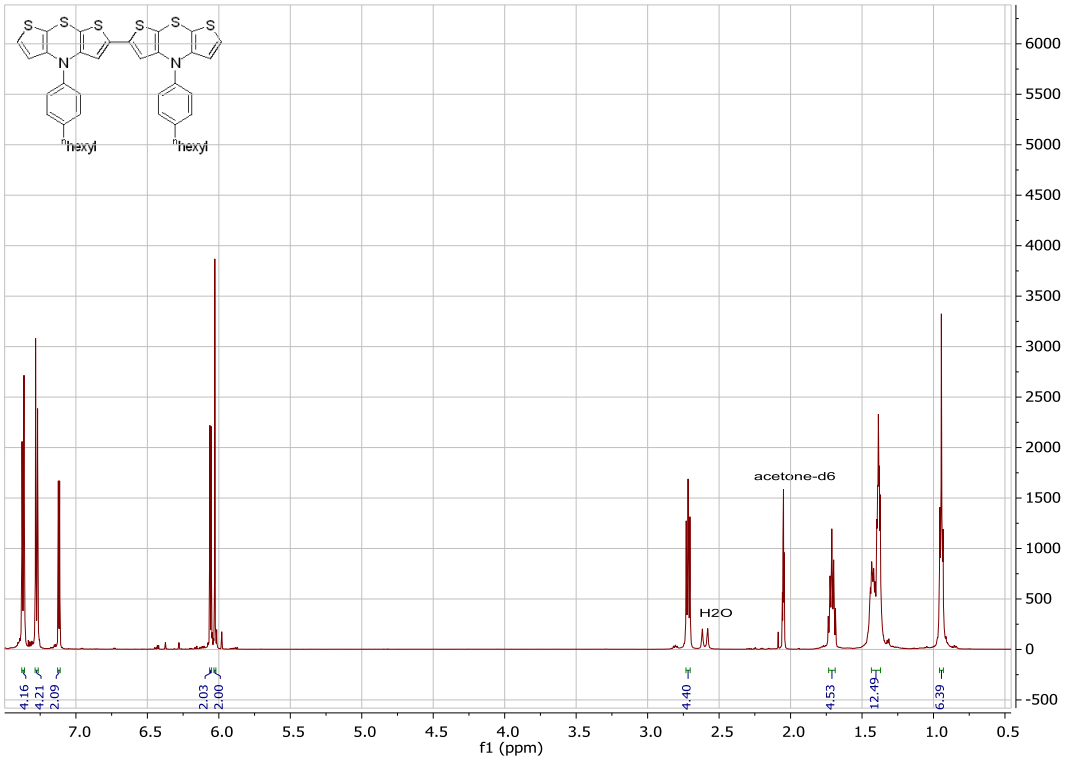


Figure 13. ^{1}H NMR spectrum (600 MHz) of **4**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

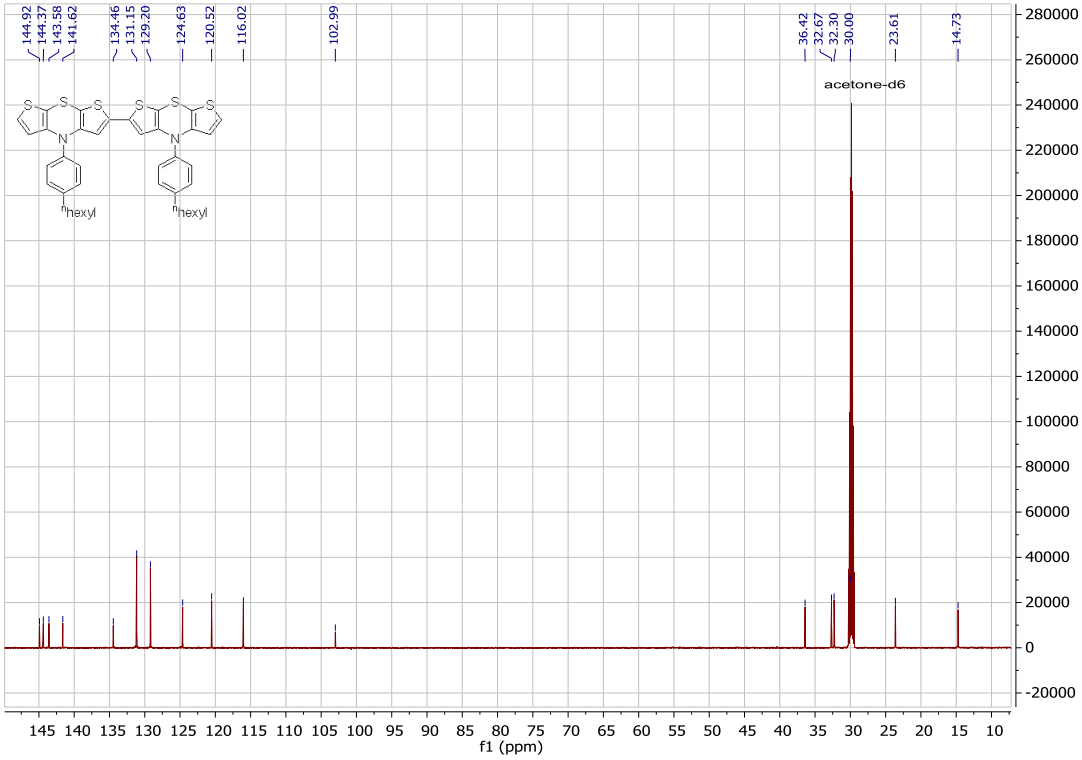


Figure 14. ^{13}C NMR spectrum (150 MHz) of **4**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

4,4‘,4‘‘-Tris(4-hexylphenyl)-4*H*,4’*H*,4‘‘*H*-2,2‘:6‘,2‘‘-terdithieno[2,3-*b*:3’,2’-*e*][1,4]thiazin **5**

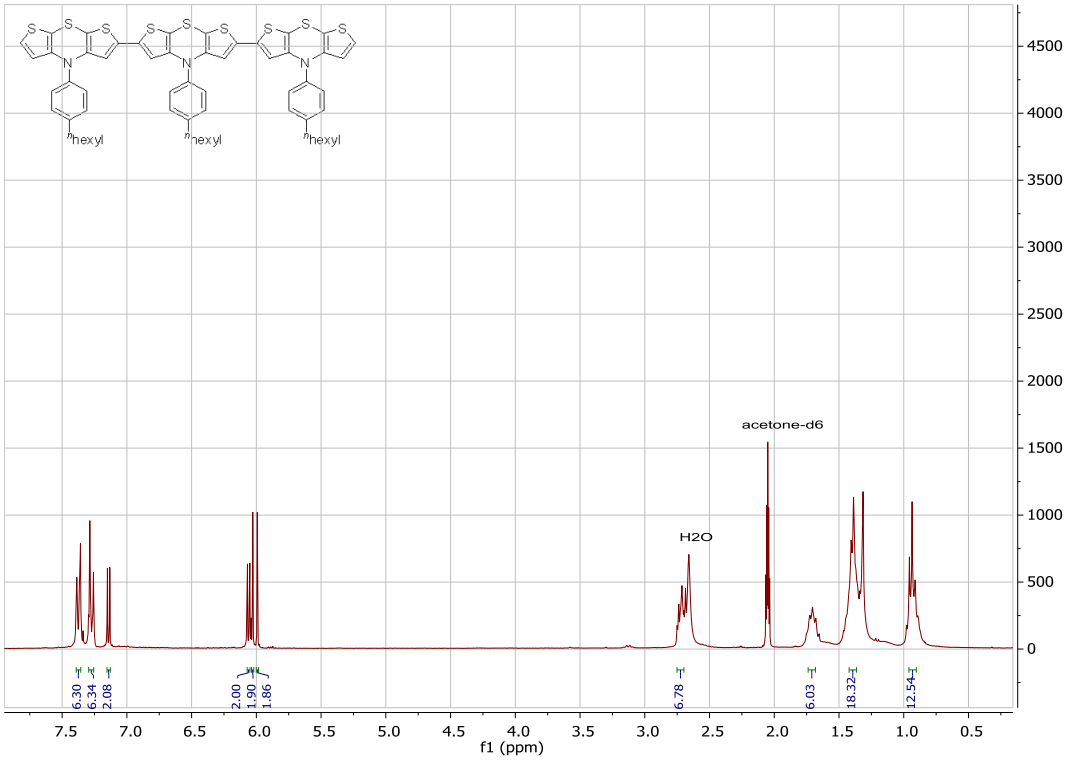


Figure 15. ^{1}H NMR spectrum (300 MHz) of **5**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

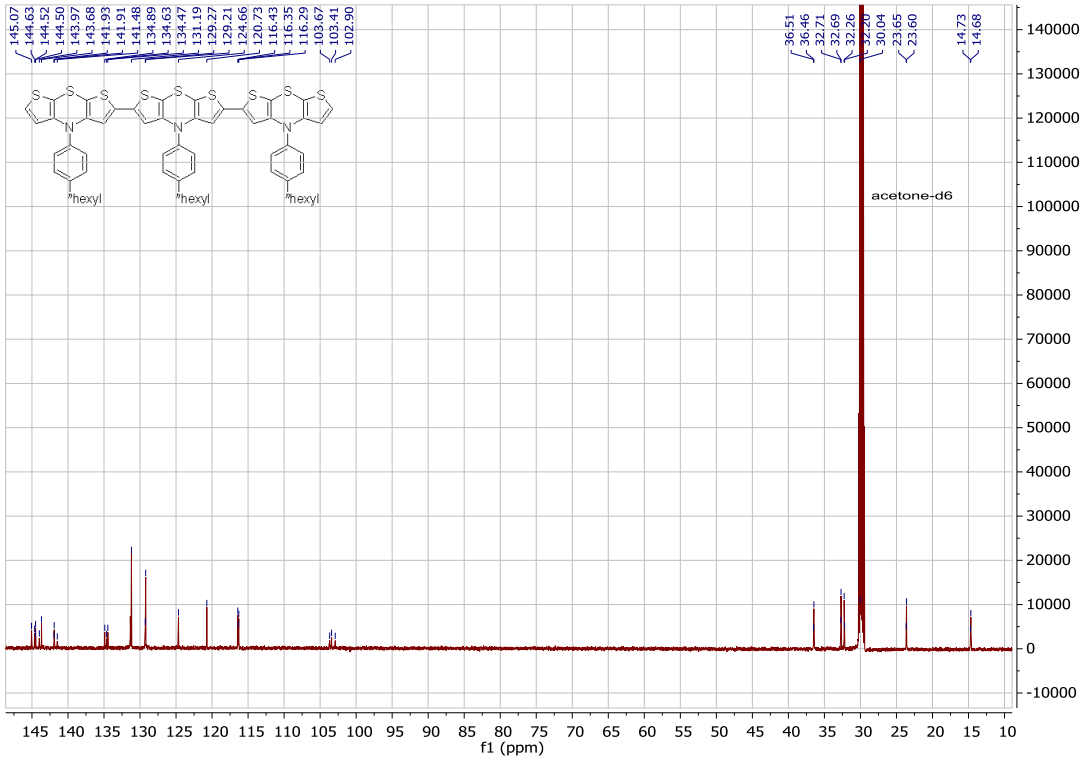


Figure 16. ^{13}C NMR spectrum (75 MHz) of **5**, recorded in acetone-d_6/CS_2 (5:1) at 298 K.

Poly(4-((2-decyltetradecyl)oxy)phenyl)-4H-dithieno[2,3-b:3',2'-e][1,4]thiazine (**6**)

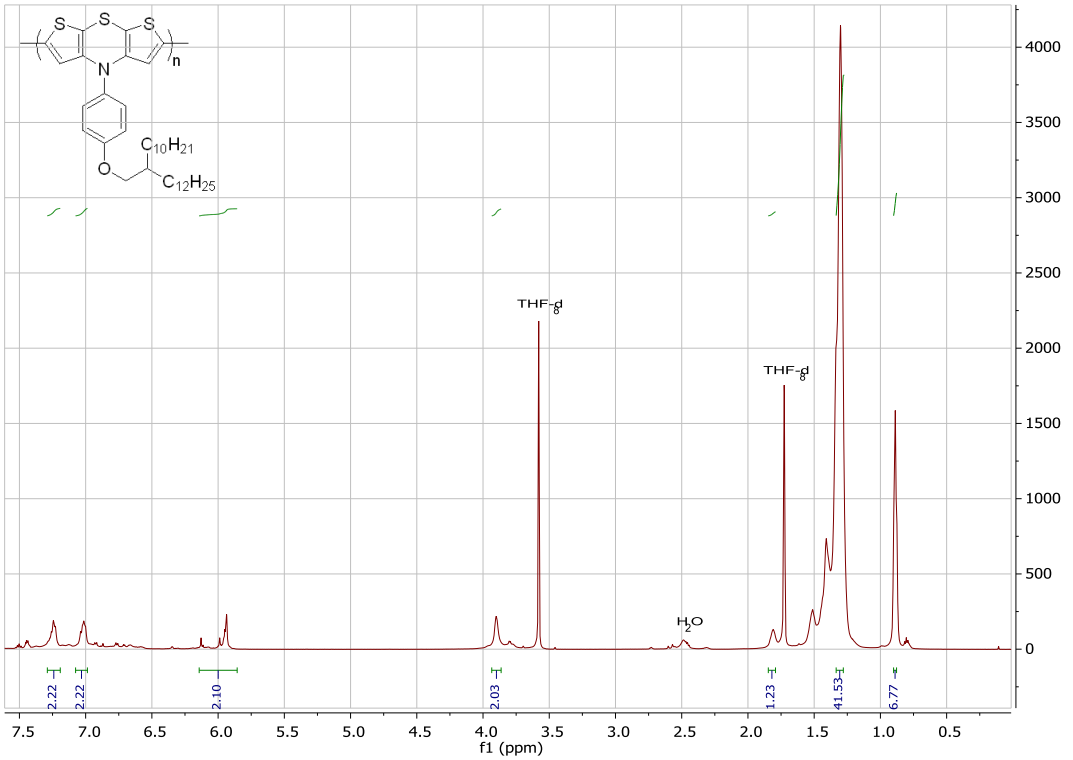


Figure 17. ^{1}H NMR spectrum (600 MHz) of polymer **6**, recorded in THF-d_8 at 298 K.

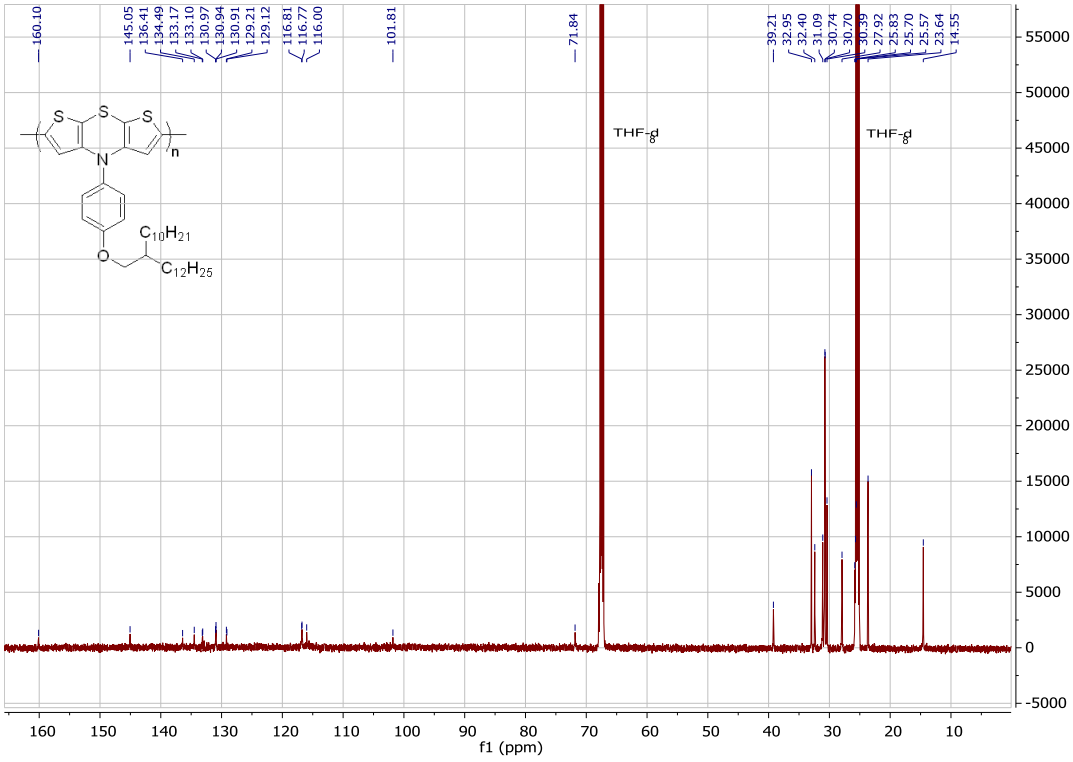


Figure 18. ^{13}C NMR spectrum (125 MHz) of polymer **6**, recorded in THF-d_8 at 298 K.

2 Solid state emission spectra of dimer **4**

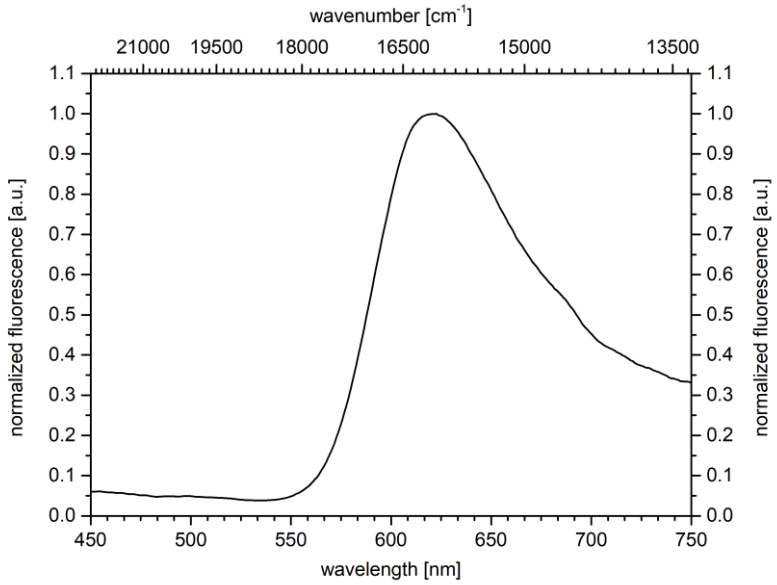


Figure 19. Emission spectrum in solid state of dimer **4** (293 K, λ_{exc} = 405 nm).

3 Experimental vs. calculated UV/Vis spectra of dimer **4** and trimer **5**

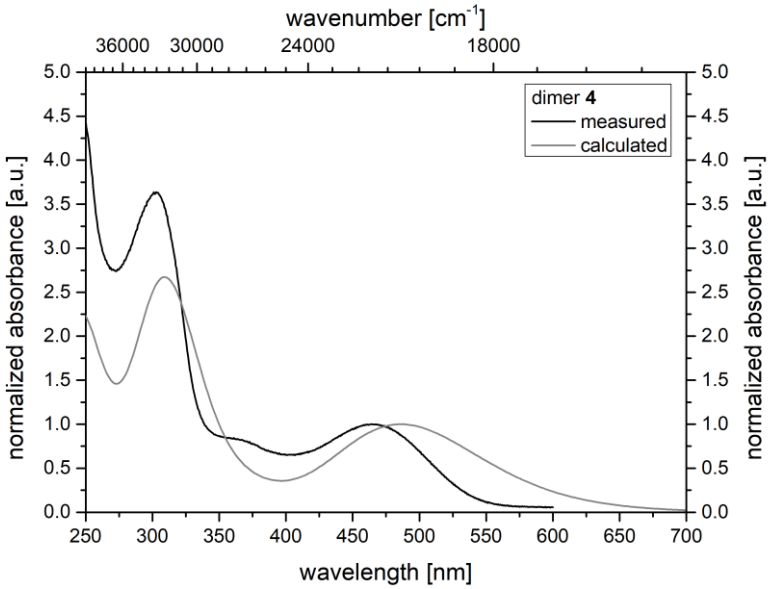


Figure 20. Experimental (black) and calculated (grey) absorption spectra of dimer **4** (Recorded in CH_2Cl_2, T = 293 K, c = 10^{-5} M).

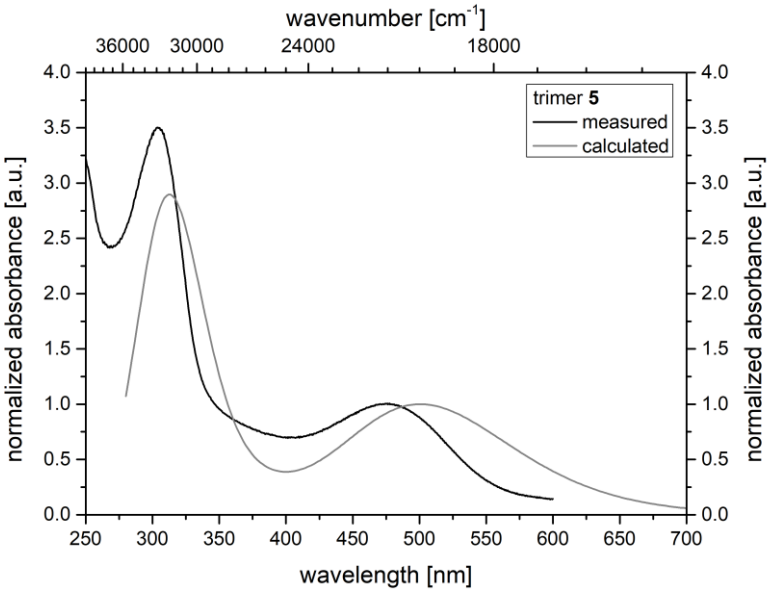
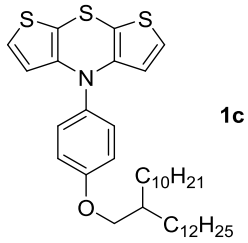


Figure 21. Experimental (black) and calculated (grey) absorption spectra of trimer **5** (Recorded in CH_2Cl_2, T = 293 K, c = 10^{-5} M).

4 Absorption, cyclic voltammetry and TD-DFT data of monomer **1c**



1c

$\lambda_{max(abs)}$ [nm][(a)] (ε [l·mol^{-1}·cm^{-1}])	$\lambda_{max(em)}$[(b)] [nm]	λ_{calc} [nm]	Most dominant contribution	Oscillator-strength *f*	E_{HOMO}[(d)] [eV]	E_0[(g)] [V]
400sh		397	HOMO → LUMO (95%)	0.0044	-4.63	-0.17,
313 (5000)		326	HOMO → LUMO+1 (92%)	0.0847		0.73

Absorption spectrum of **1c**

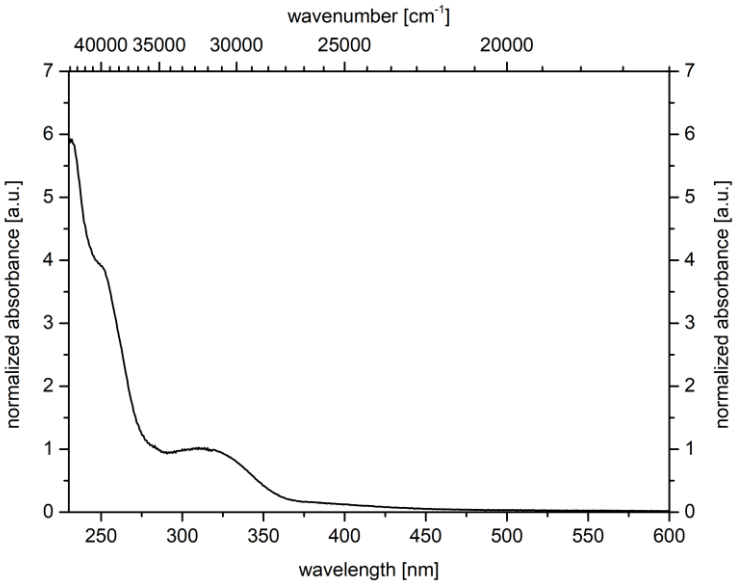


Figure 22. Recorded in CH_2Cl_2, T = 293 K, c = 10^{-5} M.

Cyclic voltammogram of **1c**

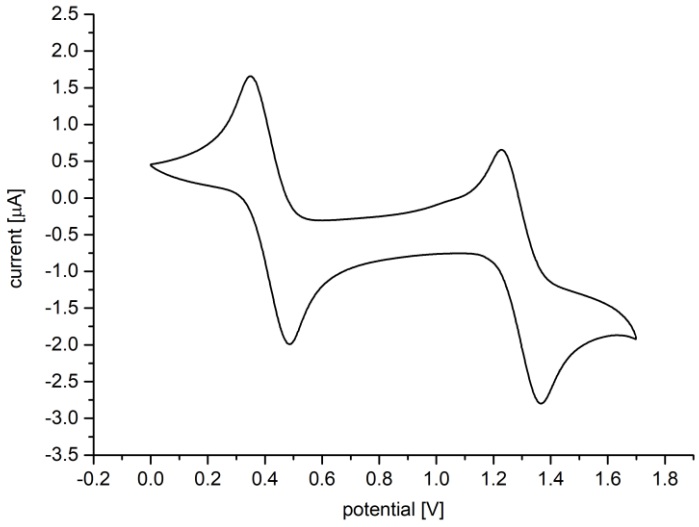


Figure 23. Recorded in CH_2Cl_2, *T* = 293 K, 0.1 M electrolyte [$^{n}Bu_4N$][PF_6]; *v* = 100 mV/s; Pt-working, Ag/AgCl-reference and Pt-counter electrode.

5 Cyclic voltammogram of trimer **5**

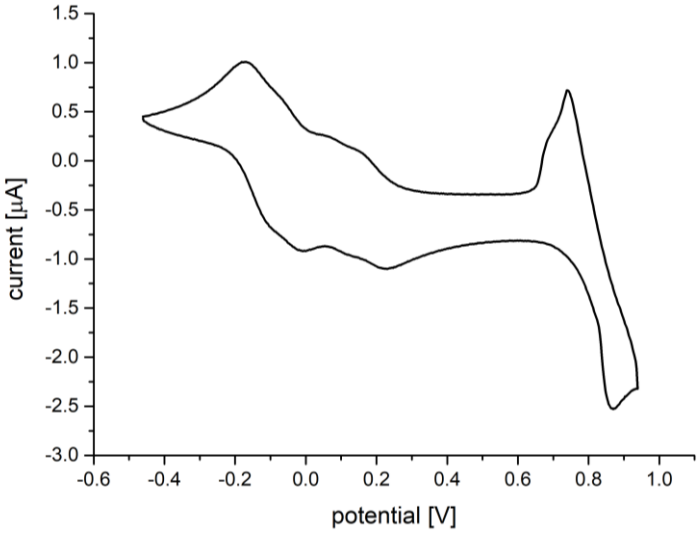


Figure 24. Recorded in CH_2Cl_2, *T* = 293 K, 0.1 M electrolyte [$^{n}Bu_4N$][PF_6]; *v* = 100 mV/s; Pt-working, Ag/AgCl-reference and Pt-counter electrode

6 Cyclic voltammogram of polymer **6**

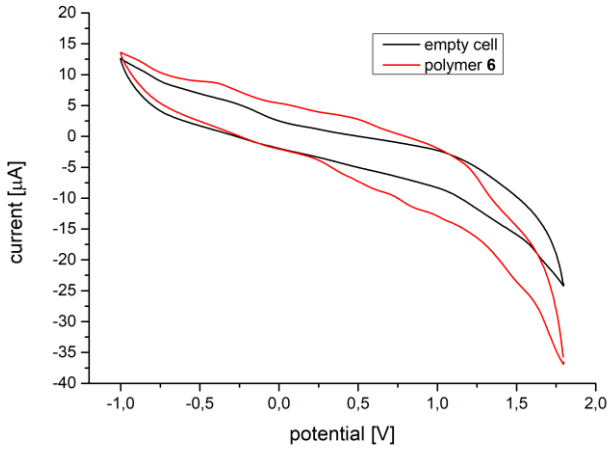


Figure 25. Recorded in CH_2Cl_2, T = 293 K, 0.1 M electrolyte [$^{n}Bu_4N$][PF_6]; v = 100 mV/s; Pt-working, Ag/AgCl-reference and Pt-counter electrode

7 Nernstian reversibility

The electrochemical reversibility of the dimer **4** was determined by the reversibility of the redox standards ferrocene and decamethylferrocene. Both standards are well known to be Nernstian reversible, that means that their difference of the peak potential has to be 57 mV. This main criterion for Nernstian reversibility is called peak-to-peak separation (ΔE_p).[1] The value of these peak-to-peak separation can be used as a guideline for determining the reversibility dimer **4**. However in some case the reversibility of ferrocene changes because of ohmic loss (iR) towards quasi-reversibility.[2] By plotting the peak separation of ferrocene or decamethylferrocene against the square rate of the scan rate, an adjusted peak-to-peak separation value can be determined (Figure). So the y-intercept gave in this case a peak separation of ferrocene of 115.3 mV and for decamethylferrocene of 80.8 mV at a scan rate of 0 mV/s. Based on this values the Nernstian reversibility of the oxidation of dimer **4** was determined by comparing their peak separation at 0 mV/s (Figure).

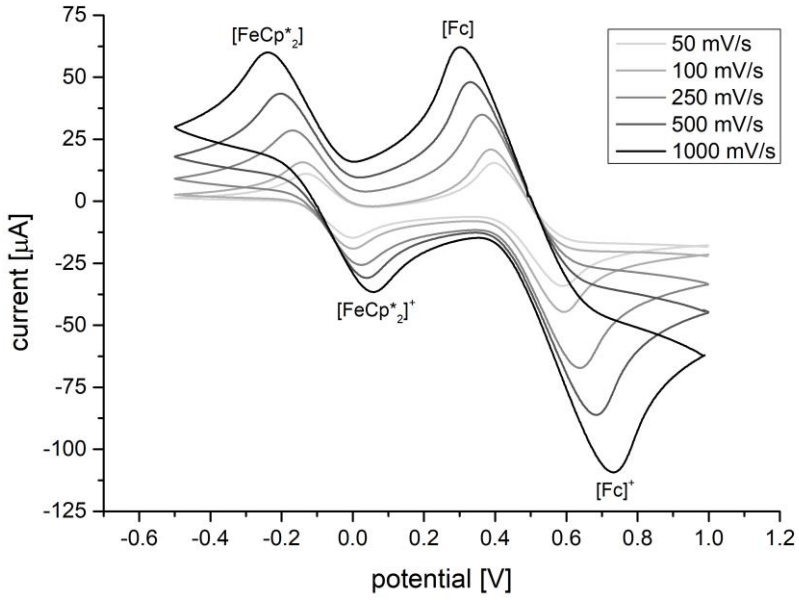


Figure 26: CVs of decamethylferrocene and ferrocene at different scan rates.

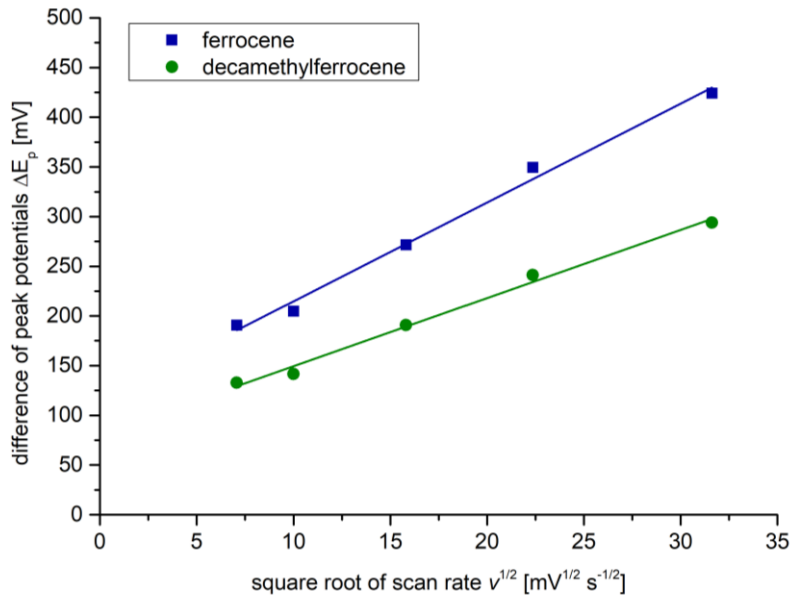


Figure 27. Peak separation vs. Square root of scan rate (Ferrocene: ΔE_p = 9.9 $mV^{-1/2}s^{1/2}v^{1/2}$ + **115.3 mV** (R^2 = 0.99); Decamethylferrocene: ΔE_p = 6.9 $mV^{-1/2}s^{1/2}v^{1/2}$ + **80.8 mV** (R^2 = 0.99)).

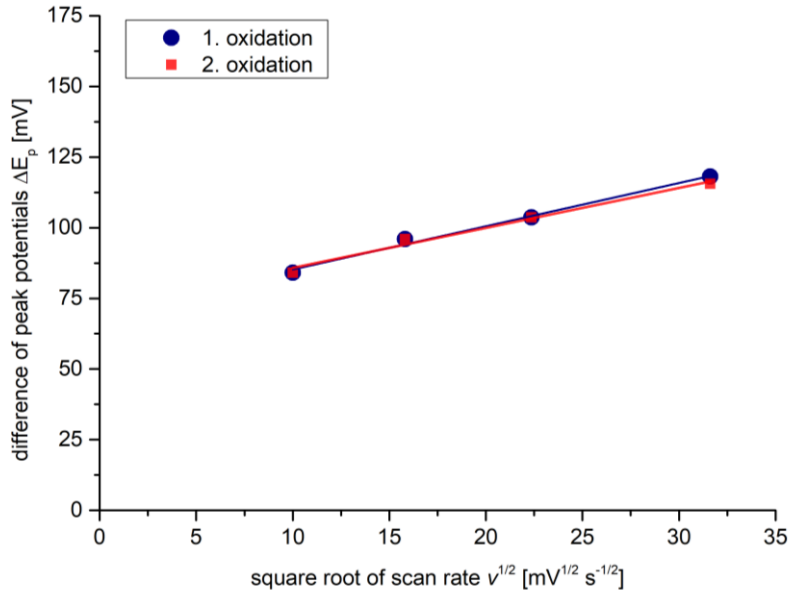


Figure 28. Peak separation vs. Square root of scan rate of dimer **4** (1. oxidation: ΔE_p = 1.5 $mV^{-1/2}s^{1/2}v^{1/2}$ + **70.0 mV** (R^2 = 0.99); 2. oxidation: ΔE_p = 1.4 $mV^{-1/2}s^{1/2}v^{1/2}$ + **71.6 mV** (R^2 = 0.99)).

8 Molecular weight distribution of polymer **6**

Gel permeation chromatography (GPC) was performed using a system equipped with an intelligent pump AI-12 and three Mz-columns from MZ-ANALYSENTECHNIK GmbH, Mainz, Germany (8 mm diameter, 10 µm particle size, precolumn of 50 mm, 3×100 Å of 300 mm). Tetrahydrofuran (unstabilized) HPLC was used as GPC eluent with a flow rate of 1 mL/min. The GPC system was calibrated with ten polystyrene standards from Agilent Technologies (MW 575 - 3039000 g mol-1). Differential refractive index spectra were recorded using a Viscotek V E3580 from Malvern Instruments GmbH, Herrenberg, Germany. Data analysis was performed using the NTeqGPC V6.0 software.

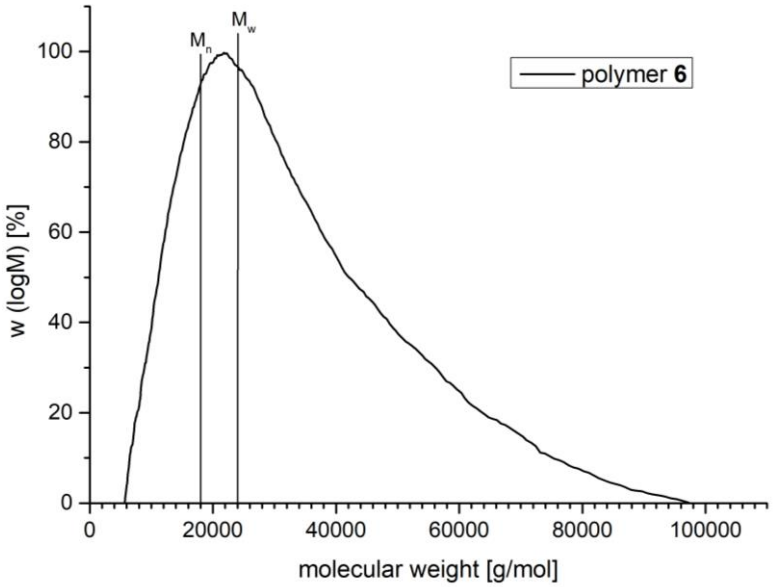


Figure 29. THF-GPC analysis of the dithienothiazine polymer **6** (*T* = 293 K, THF, flow rate 1mL/min, standard: polystyrene)

9 Effective conjugation length (ECL)

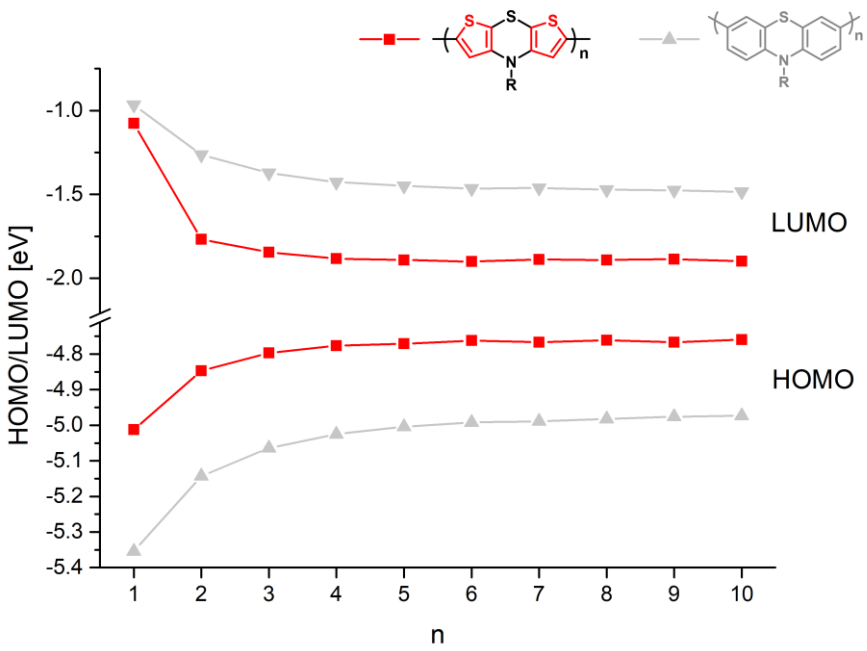


Figure 30. Comparison of the calculated HOMO and LUMO energies of oligo dithienothiazine and oligo phenothiazines (B3LYP/6-311G(d,p) IEPCM CH_2Cl_2, n = 1-10).

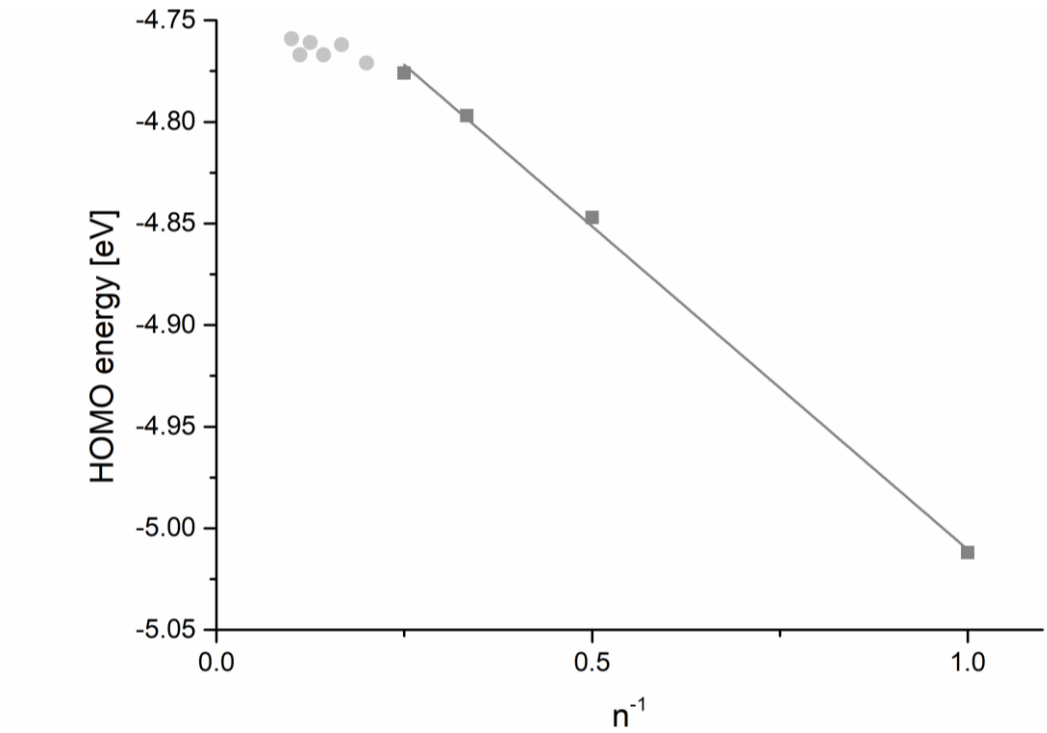


Figure 31. Determination of the effective conjugation length for oligo dithienothiazine (B3LYP/6-311G(d,p) IEFPCM CH_2Cl_2, $\mathbf{n_{ECL} = 4}$; E = -0.31803 eV n^{-1} – 4.69236 eV (R^2 = 0.998)).

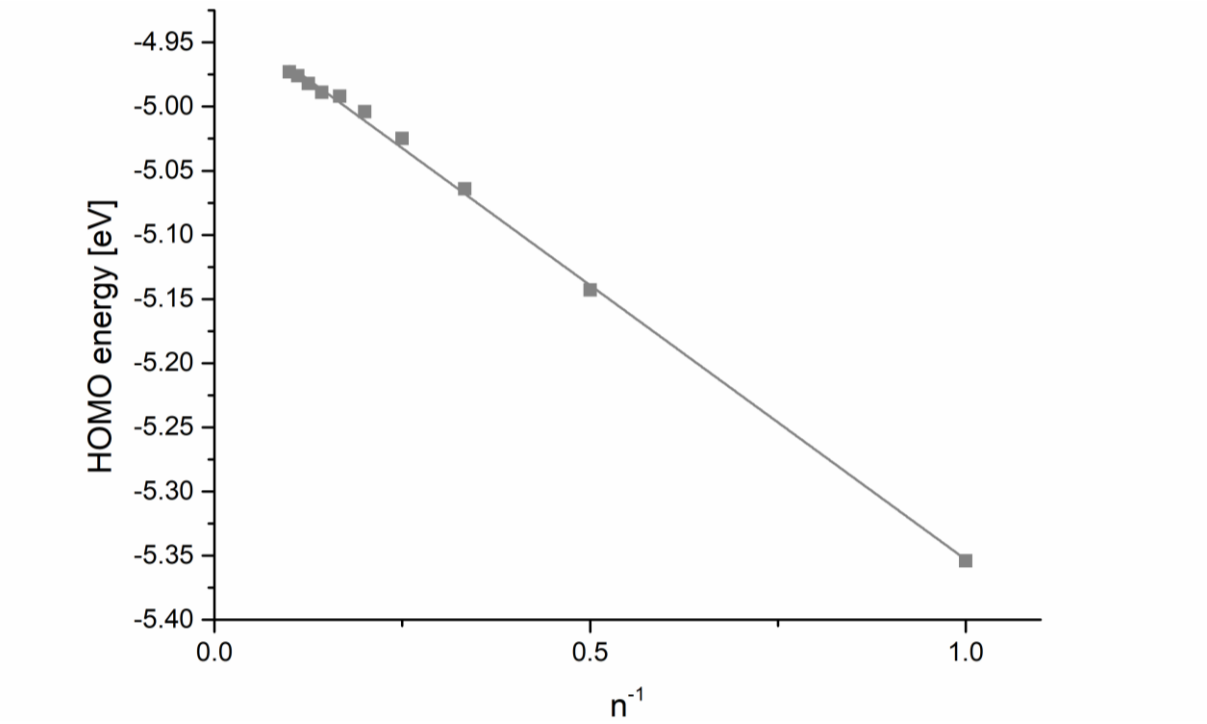


Figure 32. Determination of the effective conjugation length for oligo phenothiazine (B3LYP/6-311G(d,p) IEFPCM CH_2Cl_2, $\mathbf{n_{ECL} \geq 10}$; E = -0.42743 eV n^{-1} – 4.92548 eV (R^2 = 0.998)).

10 Results of quantum chemical calculations

10.1 Results of Conformational analysis

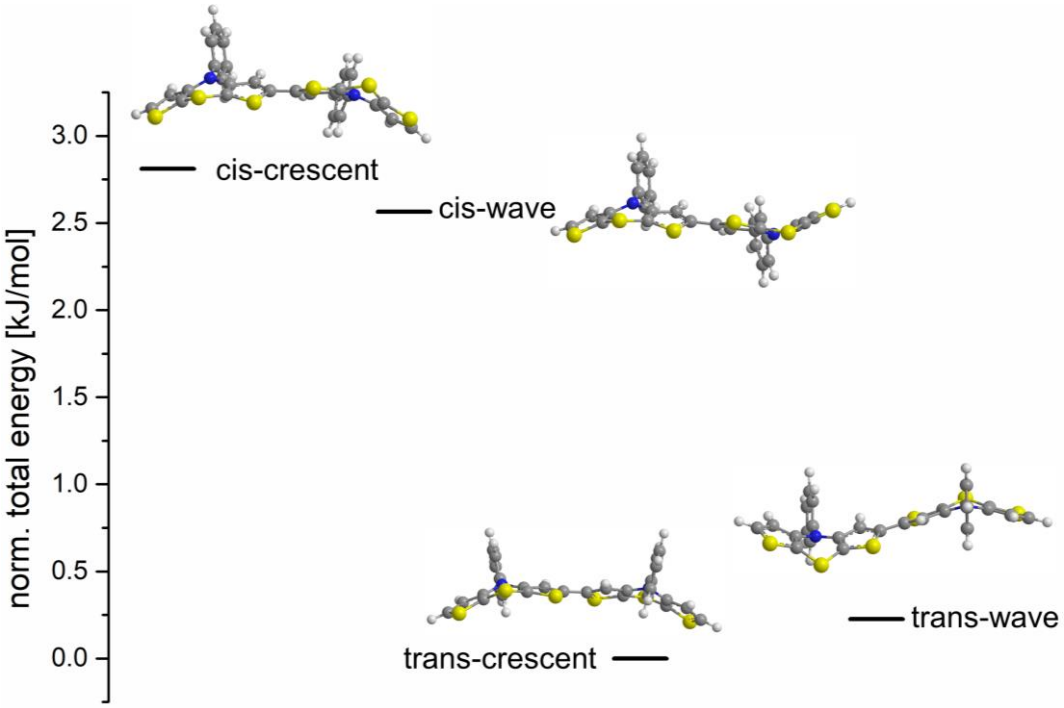


Figure 33. Normalized total energy of four minimum structures of the dithienothiazine dimer (B3LYP/6-311G(d,p) IEFPCM CH_2Cl_2).

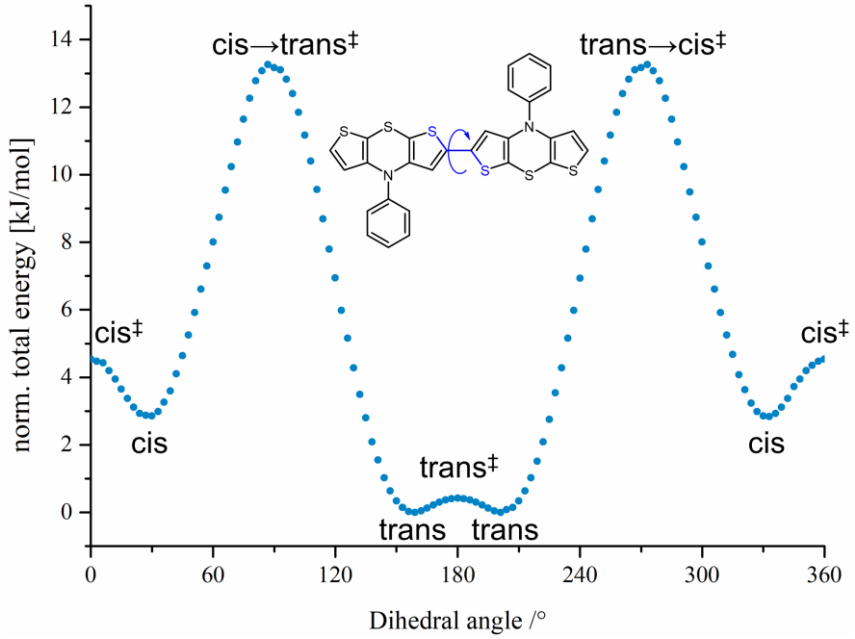


Figure 34. Dihedral scan of dithienothiazine dimer (B3LYP/6-31G(d) IEFPCM CH_2Cl_2).

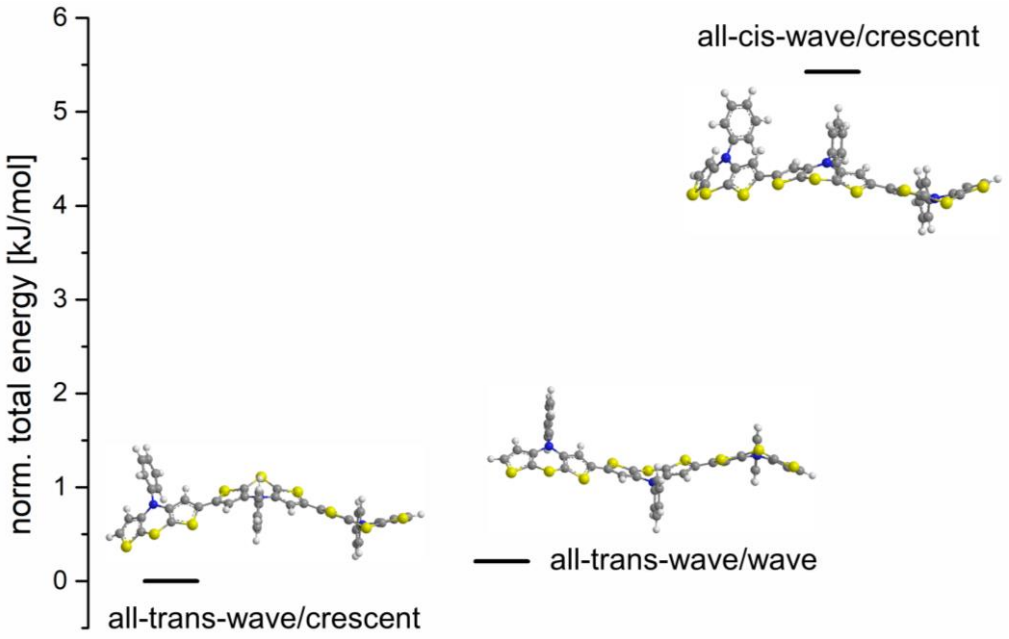


Figure 35. Normalized total energy of three minimum structures of the dithienothiazine trimer (B3LYP/6-311G(d,p) IEFPCM CH_2Cl_2).

10.2 Oxidation states of dithienothiazine dimer and trimer

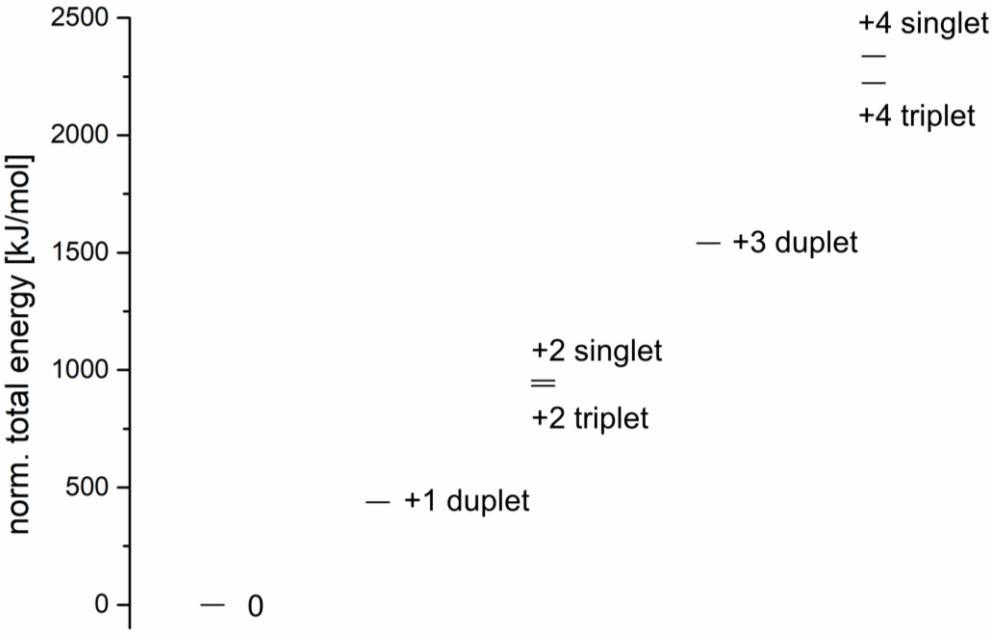


Figure 36. Normalized total energy of four oxidation states of the dithienothiazine dimer (UB3LYP/6-311G(d,p) IEFPCM CH_2Cl_2).

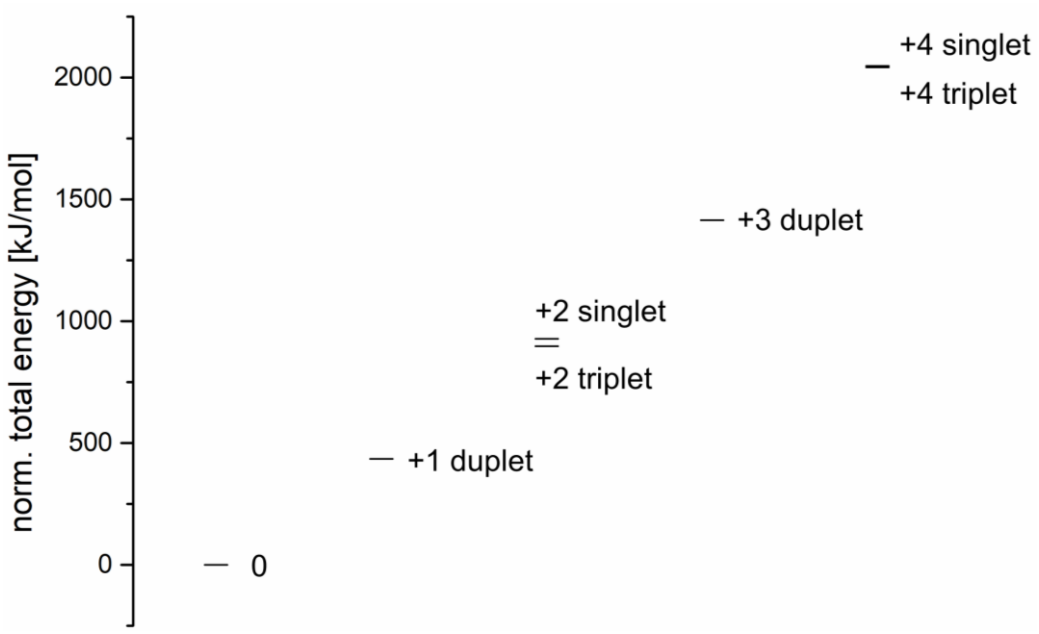
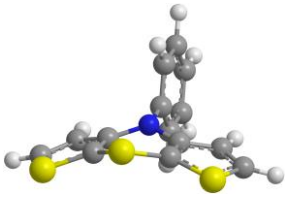


Figure 37. Normalized total energy of four oxidation states of the dithienothiazine trimer (UB3LYP/6-311G(d,p) IEFPCM CH_2Cl_2).

11 Data of quantum chemical calculations (B3LYP/6-311G(d,p) IEFPCM CH_2Cl_2)

11.1 Computed xyz-coordinates of dithienothiazine monomer



C	-1.635318	1.302026	0.189327
C	-0.275045	1.207128	0.019346
N	0.429033	-0.000015	0.223917
C	-0.275093	-1.207133	0.019345
C	-1.635371	-1.301969	0.189322
S	-2.649755	0.000047	0.847223
C	0.298406	-2.439277	-0.433978
C	-0.630304	-3.423078	-0.601707
S	-2.238071	-2.876077	-0.246005
S	-2.237951	2.876148	-0.246032
C	-0.630159	3.423086	-0.601712
C	0.298506	2.439240	-0.433999
C	1.866504	-0.000035	0.171312
C	2.539507	-0.000069	-1.053269
C	3.932765	-0.000084	-1.079765
C	4.655336	-0.000059	0.113127
C	3.982822	-0.000016	1.334083
C	2.589131	-0.000004	1.364342
H	1.353509	-2.580076	-0.618835
H	-0.472939	-4.441936	-0.919633
H	-0.472741	4.441939	-0.919630
H	1.353615	2.579988	-0.618864
H	1.971872	-0.000083	-1.976688
H	4.452503	-0.000113	-2.030940
H	5.739013	-0.000070	0.090375
H	4.541048	0.000006	2.263135

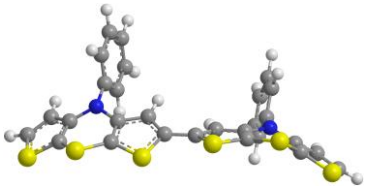
H 2.053193 0.000027 2.306041

SCF Done: E(RB3LYP) = -1788.39791194 A.U. after 1 cycles

E(HOMO) = -5.012 eV

E(LUMO) = -1.077 eV

11.2 Computed xyz-coordinates of dithienothiazine dimer (crescent cis conformer)



C 5.657238 -1.248963 0.158656

C 5.250781 -0.015320 -0.289633

N 3.997071 0.538009 0.053796

C 2.946558 -0.358292 0.345205

C 3.173674 -1.618659 0.846746

S 4.764084 -2.224277 1.345667

S 7.191934 -1.715542 -0.516840

C 7.308392 -0.205507 -1.362655

C 6.214003 0.583035 -1.165046

C 1.562985 -0.115281 0.099275

C 0.753209 -1.179232 0.417513

S 1.702643 -2.534274 1.005132

C 3.685670 1.889113 -0.330808

C 3.752694 2.899588 0.628207

C 3.450724 4.214096 0.275757

C 3.082860 4.519585 -1.033565

C 3.015935 3.508868 -1.992291

C 3.315679 2.193515 -1.643454

C -3.072490 -1.947645 0.078526

C -2.945697 -0.601304 0.331368

N -4.059377 0.261912 0.400974

C -5.212128 -0.100347 -0.331306

C -5.515802 -1.406654 -0.630129

S -4.620486 -2.809819 -0.008820

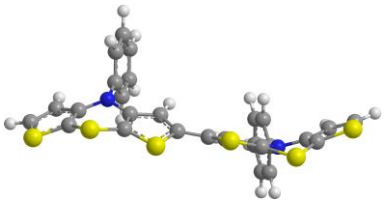
S	-1.527766	-2.736542	-0.048021
C	-0.691960	-1.241752	0.335861
C	-1.584012	-0.206871	0.486704
C	-6.160729	0.814466	-0.892879
C	-7.142984	0.187455	-1.600351
S	-6.931028	-1.533787	-1.634967
C	-3.862807	1.637110	0.776795
C	-4.154420	2.032379	2.082005
C	-3.967015	3.359868	2.464302
C	-3.489247	4.291480	1.544176
C	-3.197791	3.895535	0.238980
C	-3.383514	2.569603	-0.146797
H	8.181784	0.003358	-1.960540
H	6.093914	1.556618	-1.617476
H	1.181268	0.805412	-0.317068
H	4.041309	2.647342	1.641622
H	3.503965	4.997136	1.023201
H	2.848916	5.542036	-1.306959
H	2.729702	3.743048	-3.011135
H	3.264053	1.402675	-2.382915
H	-1.276004	0.798353	0.734758
H	-6.110753	1.886195	-0.766820
H	-7.983151	0.630596	-2.111816
H	-4.524928	1.297121	2.786318
H	-4.194099	3.664393	3.479370
H	-3.344047	5.323303	1.842658
H	-2.825903	4.617511	-0.478803
H	-3.158804	2.254104	-1.159189

SCF Done: E(RB3LYP) = -3575.59825206 A.U. after 1 cycles

E(HOMO) = -4.872 eV

E(LUMO) = -1.728 eV

11.3 Computed xyz-coordinates of dithienothiazine dimer (wave cis conformer)



C	-5.632430	-1.224770	-0.397323
C	-5.237070	0.042034	-0.039074
N	-3.994600	0.305285	0.580691
C	-2.935420	-0.589625	0.317810
C	-3.149600	-1.906000	-0.021532
S	-4.733550	-2.705730	-0.005040
S	-7.163390	-1.218490	-1.225720
C	-7.292080	0.500426	-1.036340
C	-6.204340	1.032720	-0.407877
C	-1.547570	-0.260832	0.358265
C	-0.723432	-1.313500	0.036319
S	-1.662720	-2.740750	-0.365240
C	-3.695870	1.647740	1.006640
C	-3.251960	2.606560	0.092443
C	-2.973340	3.901910	0.525279
C	-3.138880	4.241590	1.868560
C	-3.582450	3.283450	2.779420
C	-3.860890	1.985900	2.349700
C	3.149590	-1.906000	0.021523
C	2.935410	-0.589621	-0.317794
N	3.994590	0.305290	-0.580661
C	5.237060	0.042027	0.039092
C	5.632420	-1.224780	0.397310
S	4.733540	-2.705730	0.004998
S	1.662710	-2.740760	0.365223
C	0.723421	-1.313500	-0.036308
C	1.547560	-0.260826	-0.358238
C	6.204320	1.032710	0.407926

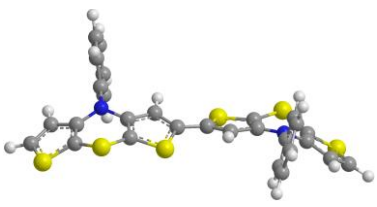
C	7.292050	0.500404	1.036390
S	7.163380	-1.218520	1.225720
C	3.695880	1.647740	-1.006630
C	3.860990	1.985910	-2.349670
C	3.582590	3.283460	-2.779410
C	3.138940	4.241590	-1.868580
C	2.973290	3.901910	-0.525320
C	3.251890	2.606560	-0.092466
H	-8.166310	1.013620	-1.406190
H	-6.091190	2.088620	-0.208618
H	-1.169290	0.709185	0.646596
H	-3.128980	2.336910	-0.950336
H	-2.629720	4.644450	-0.185750
H	-2.922950	5.249720	2.203470
H	-3.711750	3.543420	3.823740
H	-4.205590	1.231370	3.047000
H	1.169280	0.709196	-0.646552
H	6.091170	2.088620	0.208691
H	8.166280	1.013590	1.406250
H	4.205760	1.231380	-3.046950
H	3.711970	3.543430	-3.823720
H	2.923020	5.249720	-2.203510
H	2.629610	4.644440	0.185685
H	3.128830	2.336900	0.950303

SCF Done: E(RB3LYP) = -3575.59834598 A.U. after 1 cycles

E(HOMO) = -4.845 eV

E(LUMO) = -1.733 eV

11.4 Computed xyz-coordinates of dithienothiazine dimer (crescent trans conformer)



C	-5.312173	-1.787502	-0.631956

C	-5.381088	-0.451302	-0.319569
N	-4.333354	0.227885	0.340722
C	-3.024974	-0.271107	0.172872
C	-2.771696	-1.594163	-0.105440
S	-4.004083	-2.870634	-0.109754
S	-6.698213	-2.316527	-1.541932
C	-7.399155	-0.732675	-1.445998
C	-6.593090	0.149817	-0.790377
C	-1.830151	0.504156	0.241061
C	-0.687752	-0.224308	0.006727
S	-1.076925	-1.896734	-0.357546
C	-4.524049	1.592269	0.756310
C	-4.401910	2.642509	-0.157079
C	-4.590170	3.956266	0.267692
C	-4.900653	4.222718	1.600999
C	-5.022776	3.173661	2.510712
C	-4.834660	1.858103	2.089709
C	2.771696	1.594163	-0.105451
C	3.024975	0.271107	0.172863
N	4.333356	-0.227884	0.340710
C	5.381087	0.451301	-0.319585
C	5.312172	1.787500	-0.631975
S	4.004083	2.870634	-0.109771
S	1.076924	1.896734	-0.357552
C	0.687752	0.224308	0.006725
C	1.830152	-0.504155	0.241057
C	6.593089	-0.149819	-0.790395
C	7.399152	0.732672	-1.446020
S	6.698210	2.316524	-1.541956
C	4.524051	-1.592268	0.756301
C	4.834661	-1.858099	2.089701
C	5.022777	-3.173657	2.510706
C	4.900654	-4.222715	1.600994

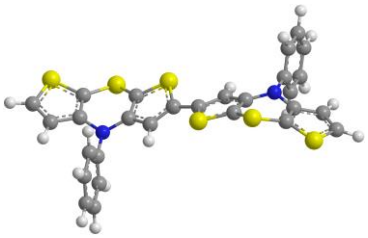
C	4.590173	-3.956265	0.267687
C	4.401912	-2.642510	-0.157086
H	-8.366704	-0.551469	-1.887426
H	-6.847860	1.188677	-0.638748
H	-1.815202	1.556291	0.487238
H	-4.161811	2.427595	-1.192023
H	-4.494534	4.769811	-0.442057
H	-5.046618	5.245298	1.929394
H	-5.263780	3.377383	3.547577
H	-4.925982	1.032671	2.785597
H	1.815203	-1.556290	0.487236
H	6.847859	-1.188678	-0.638764
H	8.366699	0.551465	-1.887450
H	4.925983	-1.032666	2.785587
H	5.263781	-3.377377	3.547572
H	5.046620	-5.245295	1.929392
H	4.494537	-4.769812	-0.442061
H	4.161813	-2.427597	-1.192031

SCF Done: E(RB3LYP) = -3575.59932258 A.U. after 1 cycles

E(HOMO) = -4.840 eV

E(LUMO) = -1.768 eV

11.5 Computed xyz-coordinates of dithienothiazine dimer (wave trans conformer)



C	-5.294986	-1.815245	-0.420076
C	-5.357130	-0.514909	0.019315
N	-4.337182	0.425116	-0.248420
C	-3.030187	-0.068947	-0.446165
C	-2.786041	-1.335109	-0.924736
S	-4.040023	-2.444148	-1.509665

S	-6.636226	-2.763422	0.155132
C	-7.313107	-1.375005	0.944943
C	-6.530222	-0.267965	0.803569
C	-1.828191	0.627749	-0.125131
C	-0.688097	-0.104910	-0.357075
S	-1.085084	-1.702575	-0.966082
C	-4.520757	1.799516	0.136831
C	-4.864943	2.737037	-0.836676
C	-5.044822	4.073370	-0.482375
C	-4.881693	4.472720	0.843029
C	-4.537577	3.534757	1.816169
C	-4.356090	2.198396	1.465853
C	2.808650	1.584224	0.095730
C	3.002968	0.227740	0.215849
N	4.277617	-0.335852	0.434663
C	5.398668	0.387975	-0.029307
C	5.391314	1.755430	-0.162598
S	4.064082	2.805822	0.377216
S	1.153954	1.978645	-0.269244
C	0.691837	0.288035	-0.169807
C	1.788496	-0.505618	0.070618
C	6.635586	-0.188487	-0.464957
C	7.521259	0.743660	-0.917817
S	6.870023	2.350539	-0.861130
C	4.397623	-1.752759	0.656552
C	4.608539	-2.221378	1.953054
C	4.731151	-3.590407	2.185933
C	4.641392	-4.490528	1.125451
C	4.429990	-4.021229	-0.170851
C	4.308969	-2.653539	-0.407900
H	-8.250588	-1.466368	1.470921
H	-6.775601	0.692294	1.233256
H	-1.809296	1.628992	0.280861

H -4.989103 2.411658 -1.862666

H -5.312121 4.799710 -1.241056

H -5.021706 5.511816 1.117791

H -4.409531 3.842546 2.847488

H -4.087538 1.464364 2.216885

H 1.724964 -1.579541 0.172946

H 6.849916 -1.246892 -0.434074

H 8.522030 0.588088 -1.289440

H 4.674781 -1.509986 2.767601

H 4.895070 -3.951902 3.194454

H 4.735421 -5.554826 1.307778

H 4.360180 -4.718572 -0.997638

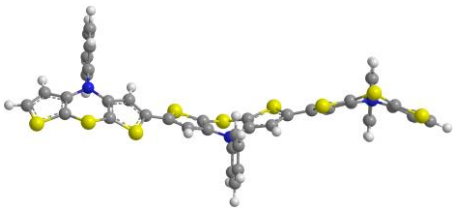
H 4.146871 -2.281452 -1.412986

SCF Done: E(RB3LYP) = -3575.59923686 A.U. after 1 cycles

E(HOMO) = -4.847 eV

E(LUMO) = -1.768 eV

11.6 Computed xyz-coordinates of dithienothiazine trimer (all-trans wave/wave conformer)



C -7.103173 -1.367657 0.096076

C -7.090102 -0.023501 0.388293

N -8.238213 0.663052 0.835968

C -9.496519 0.147610 0.451535

C -9.696521 -1.182625 0.172292

S -8.473835 -2.449671 0.409224

S -5.575045 -1.917043 -0.527516

C -4.871974 -0.323655 -0.307304

C -5.810346 0.564061 0.163978

C -10.682984 0.924422 0.249561

C -11.737820 0.174360 -0.178241

S -11.316453 -1.496073 -0.381570

C	-8.134025	2.047756	1.214916
C	-8.145210	2.383359	2.568471
C	-8.052014	3.719920	2.953654
C	-7.945166	4.719777	1.988391
C	-7.933584	4.383363	0.634913
C	-8.029813	3.048918	0.245794
C	-3.483207	-0.086158	-0.636395
C	-2.443228	-0.984822	-0.668178
C	-1.202966	-0.408655	-1.071140
C	-1.315687	0.934954	-1.340315
S	-2.935139	1.520304	-1.084643
N	0.029215	-1.093512	-1.130946
C	1.204969	-0.348649	-0.903167
C	1.278855	1.002895	-1.147006
S	0.006802	1.952258	-1.940906
C	2.427843	-0.870921	-0.388095
C	3.409689	0.078989	-0.233914
S	2.817686	1.669208	-0.683467
C	0.048113	-2.525299	-0.987827
C	0.053592	-3.118029	0.277358
C	0.069067	-4.506766	0.391809
C	0.074319	-5.303037	-0.753106
C	0.065056	-4.709602	-2.014466
C	0.053273	-3.320920	-2.133325
C	4.764895	-0.087539	0.245266
S	5.168664	-1.398817	1.340033
C	6.824120	-0.866995	1.423502
C	7.053262	0.236149	0.634649
C	5.873340	0.676367	-0.033995
S	8.045149	-1.624487	2.462576
C	9.407834	-1.188536	1.408769
C	9.449367	-0.060717	0.625047
N	8.337859	0.798374	0.476344

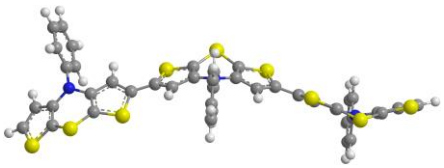
S	10.883429	-2.105995	1.311087
C	11.579270	-0.923499	0.249759
C	10.710825	0.087309	-0.037641
C	8.482172	2.029914	-0.254013
C	8.577449	3.229524	0.450974
C	8.710168	4.433127	-0.239678
C	8.749499	4.438858	-1.633019
C	8.655027	3.238938	-2.337559
C	8.520231	2.034006	-1.650800
H	-5.586450	1.600067	0.374487
H	-10.741349	1.989190	0.422540
H	-12.743828	0.499262	-0.393232
H	-8.226551	1.595173	3.307434
H	-8.061057	3.978138	4.006223
H	-7.871223	5.758445	2.289238
H	-7.851991	5.158591	-0.118145
H	-8.025504	2.780345	-0.804332
H	-2.556028	-2.024082	-0.394340
H	2.584553	-1.917873	-0.171085
H	0.044812	-2.492668	1.162606
H	0.074430	-4.965106	1.373913
H	0.085077	-6.382998	-0.661819
H	0.069003	-5.325791	-2.906045
H	0.048422	-2.845595	-3.106939
H	5.851090	1.516610	-0.713124
H	12.591206	-1.053226	-0.100912
H	10.954658	0.912521	-0.690709
H	8.546845	3.209827	1.533821
H	8.783680	5.363789	0.310887
H	8.853296	5.375171	-2.169073
H	8.684064	3.239934	-3.421015
H	8.443307	1.097965	-2.191926

SCF Done: E(RB3LYP) = -5362.80054646 A.U. after 6 cycles

E(HOMO) = -4.797 eV

E(LUMO) = -1.844 eV

11.7 Computed xyz-coordinates of dithienothiazine trimer (all-trans wave/crescent conformer)



C	-6.254610	-10.428900	1.510680
C	-5.312290	-11.161600	0.830345
N	-4.506530	-10.601600	-0.185641
C	-4.234620	-9.219500	-0.112573
C	-5.092140	-8.333830	0.497714
S	-6.704810	-8.759280	1.102660
S	-7.003500	-11.350700	2.782870
C	-6.076420	-12.751600	2.349460
C	-5.218630	-12.504900	1.319030
C	-3.064840	-8.577860	-0.615675
C	-3.034970	-7.224040	-0.377129
S	-4.449520	-6.717600	0.530031
C	-3.647260	-11.456800	-0.960489
C	-2.404660	-11.861800	-0.466446
C	-1.589870	-12.691300	-1.234620
C	-2.013990	-13.118600	-2.492640
C	-3.254670	-12.714900	-2.983220
C	-4.071700	-11.883700	-2.218640
C	0.130158	-5.159480	-1.375520
C	-0.922257	-4.275360	-1.327230
N	-0.761005	-2.897330	-1.581930
C	0.504364	-2.328070	-1.324860
C	1.667070	-3.060210	-1.379450
S	1.764550	-4.743740	-1.927840
S	-0.345282	-6.769260	-0.918782
C	-2.016870	-6.263530	-0.744709

C	-2.146960	-4.913740	-0.971917
C	0.732564	-0.981141	-0.916203
C	2.054160	-0.700062	-0.663139
S	3.054640	-2.121520	-0.907204
C	-1.917120	-2.043970	-1.661900
C	-2.367980	-1.630280	-2.915230
C	-3.482280	-0.798702	-3.013180
C	-4.147120	-0.382550	-1.860820
C	-3.696150	-0.797114	-0.607969
C	-2.580850	-1.626370	-0.505506
C	3.135510	2.972580	0.128722
C	4.082130	2.148210	0.691387
N	5.206910	2.650890	1.377980
C	5.677640	3.930800	1.010270
C	4.854860	4.893760	0.477858
S	3.090850	4.733820	0.338078
S	1.920900	2.078530	-0.738069
C	2.650630	0.555398	-0.259592
C	3.795150	0.768767	0.471493
C	7.040320	4.366400	1.081980
C	7.215480	5.630190	0.601752
S	5.736250	6.321510	0.015635
C	6.087830	1.741170	2.061200
C	5.995820	1.620770	3.447680
C	6.839590	0.743405	4.126990
C	7.773870	-0.013701	3.422080
C	7.866280	0.107950	2.035810
C	7.025480	0.984816	1.353290
H	-6.221550	-13.673600	2.890470
H	-4.546280	-13.247100	0.913841
H	-2.288990	-9.094670	-1.162270
H	-2.082600	-11.527700	0.513140
H	-0.625846	-13.003600	-0.850028

H -1.378740 -13.764000 -3.088240

H -3.587310 -13.044700 -3.960590

H -5.037900 -11.561000 -2.587720

H -3.095340 -4.398450 -0.919108

H -0.056591 -0.253089 -0.793914

H -1.842150 -1.963010 -3.802180

H -3.830290 -0.478368 -3.988330

H -5.014190 0.263189 -1.938100

H -4.210220 -0.474281 0.289900

H -2.223140 -1.949600 0.465288

H 4.396370 -0.036241 0.869473

H 7.844380 3.763590 1.478500

H 8.127890 6.203440 0.549558

H 5.263570 2.214420 3.981840

H 6.765410 0.651460 5.204330

H 8.428650 -0.696829 3.950670

H 8.592540 -0.478737 1.485270

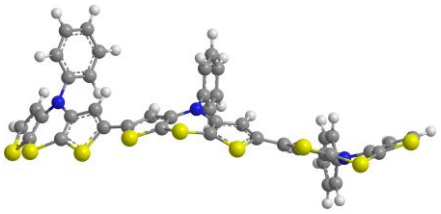
H 7.092470 1.085600 0.276132

SCF Done: E(RB3LYP) = -5362.80062687 A.U. after 1 cycles

E(HOMO) = -4.810 eV

E(LUMO) = -1.823 eV

11.8 Computed xyz-coordinates of dithienothiazine trimer (all-cis wave/crescent conformer)



C -8.905430 -1.223710 -0.987552

C -8.209620 -0.298502 -0.247536

N -6.954370 -0.581983 0.335339

C -6.152200 -1.560490 -0.288177

C -6.687380 -2.582090 -1.038340

S -8.423100 -2.923680 -1.173020

S -10.360300 -0.553379 -1.668040

C	-10.050700	0.969691	-0.897676
C	-8.880830	0.965910	-0.197730
C	-4.727790	-1.611280	-0.245134
C	-4.192940	-2.648630	-0.971157
S	-5.456580	-3.573560	-1.764190
C	-6.339390	0.391912	1.198110
C	-5.653410	1.487020	0.666481
C	-5.062880	2.416310	1.520450
C	-5.157200	2.255280	2.902640
C	-5.843100	1.163050	3.431290
C	-6.434100	0.230397	2.580110
C	-0.594285	-4.103790	-1.487770
C	-0.467609	-2.742270	-1.338070
N	0.785020	-2.092770	-1.355190
C	1.917380	-2.843820	-0.972285
C	1.976780	-4.211410	-1.103490
S	0.738574	-5.200290	-1.900270
S	-2.245310	-4.627930	-1.333700
C	-2.791810	-2.970220	-1.149110
C	-1.727720	-2.100230	-1.155650
C	3.085060	-2.309310	-0.352213
C	4.019060	-3.262820	-0.025723
S	3.451320	-4.867630	-0.454264
C	0.841564	-0.655987	-1.290710
C	1.130580	0.064751	-2.448980
C	1.196350	1.456550	-2.402950
C	0.970898	2.127520	-1.202160
C	0.681078	1.405840	-0.044316
C	0.618036	0.014488	-0.085437
C	7.465120	-3.229090	1.835490
C	7.375020	-2.058710	1.117760
N	8.387220	-1.076730	1.147990
C	9.186920	-1.000390	2.310040

C	9.420320	-2.087850	3.116630
S	8.905850	-3.744750	2.733170
S	6.030400	-4.200370	1.684050
C	5.327140	-3.050380	0.560354
C	6.155290	-1.967710	0.384383
C	9.795000	0.190862	2.822840
C	10.459600	-0.019057	3.994480
S	10.341300	-1.664450	4.531270
C	8.293850	0.064887	0.276973
C	9.066980	0.097280	-0.883226
C	8.989640	1.194440	-1.739730
C	8.140540	2.257890	-1.438120
C	7.367570	2.224960	-0.277724
C	7.442930	1.130470	0.581474
H	-10.755100	1.778260	-1.015350
H	-8.506970	1.824650	0.340696
H	-4.121010	-0.926438	0.328984
H	-5.585060	1.606560	-0.408659
H	-4.530710	3.264910	1.106380
H	-4.697370	2.979490	3.565160
H	-5.918090	1.034790	4.504860
H	-6.968630	-0.624600	2.976520
H	-1.847970	-1.030460	-1.067130
H	3.221880	-1.259880	-0.136174
H	1.301010	-0.470416	-3.375500
H	1.420980	2.014300	-3.304650
H	1.020060	3.209770	-1.167980
H	0.506340	1.924540	0.891195
H	0.397681	-0.553376	0.811126
H	5.912450	-1.148780	-0.276946
H	9.740850	1.152590	2.333670
H	11.012500	0.694767	4.584890
H	9.721500	-0.737135	-1.105040

H 9.591440 1.216830 -2.640830

H 8.080570 3.110230 -2.105040

H 6.706230 3.050300 -0.040597

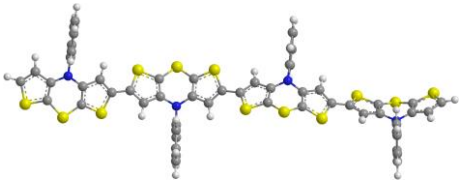
H 6.846070 1.098250 1.485730

SCF Done: E(RB3LYP) = -5362.79856047 A.U. after 1 cycles

E(HOMO) = -4.813 eV

E(LUMO) = -1.797 eV

11.9 Computed xyz-coordinates of dithienothiazine tetramer



C -11.167473 -1.575041 -0.210921

C -11.198730 -0.313703 0.337511

N -12.363167 0.226324 0.921853

C -13.608691 -0.253361 0.458977

C -13.764745 -1.510357 -0.073041

S -12.492066 -2.750054 -0.100067

S -9.630966 -1.932149 -0.944501

C -8.983964 -0.385318 -0.425275

C -9.946147 0.356921 0.217868

C -14.826642 0.500004 0.426584

C -15.860897 -0.193402 -0.128234

S -15.381903 -1.773654 -0.660078

C -12.300803 1.503343 1.582259

C -12.278346 1.546097 2.976070

C -12.222573 2.774462 3.632888

C -12.187367 3.958679 2.898458

C -12.209509 3.915194 1.504639

C -12.267495 2.689451 0.844500

C -7.610665 -0.031460 -0.712784

C -6.528917 -0.860539 -0.893247

C -5.319891 -0.164871 -1.189177

C	-5.500270	1.197715	-1.230882
S	-7.144696	1.651816	-0.886761
N	-4.054380	-0.767474	-1.357509
C	-2.918569	-0.011634	-0.998088
C	-2.914269	1.363588	-1.010794
S	-4.232752	2.366225	-1.645897
C	-1.671730	-0.550131	-0.564379
C	-0.741817	0.408730	-0.237499
S	-1.414866	2.019785	-0.420915
C	-3.960016	-2.202660	-1.420758
C	-3.961902	-2.970815	-0.253735
C	-3.869772	-4.358644	-0.337424
C	-3.778265	-4.979559	-1.582887
C	-3.777617	-4.211345	-2.745972
C	-3.867841	-2.822483	-2.666562
C	0.617855	0.232460	0.223890
S	1.113824	-1.269114	0.986548
C	2.721816	-0.651520	1.237802
C	2.870323	0.622266	0.741687
C	1.666406	1.119942	0.163060
S	3.988570	-1.548469	2.095154
C	5.320866	-0.761291	1.226796
C	5.282105	0.525729	0.743739
N	4.105823	1.303853	0.761488
S	6.874060	-1.506147	0.982583
C	7.515995	-0.023294	0.296372
C	6.541185	0.943506	0.221301
C	4.156736	2.684365	0.357484
C	8.899260	0.050824	-0.121114
C	9.973399	-0.677038	0.333816
C	11.198317	-0.358154	-0.322426
C	11.038502	0.618124	-1.277992
S	9.393189	1.178909	-1.372183

N	12.459139	-0.909657	-0.010845
C	13.596791	-0.099183	-0.220894
C	13.624959	0.899021	-1.164536
S	12.331443	1.192536	-2.347008
C	14.815061	-0.164460	0.529849
C	15.721646	0.778766	0.146544
S	15.113810	1.799131	-1.117927
C	12.539782	-2.028381	0.890538
C	12.682461	-3.312681	0.365710
C	12.761198	-4.409324	1.222654
C	12.697867	-4.223664	2.602679
C	12.555556	-2.939195	3.127115
C	12.476125	-1.840481	2.273704
C	4.134491	3.678308	1.335660
C	4.175575	5.020848	0.962910
C	4.240290	5.370085	-0.384988
C	4.263623	4.375546	-1.362395
C	4.220844	3.032314	-0.994193
H	-9.755114	1.340570	0.622775
H	-14.920835	1.507356	0.805289
H	-16.882010	0.126909	-0.264562
H	-12.304794	0.617464	3.533660
H	-12.205353	2.804897	4.716132
H	-12.142607	4.913176	3.410066
H	-12.182836	4.834279	0.930787
H	-12.287467	2.647778	-0.238425
H	-6.590236	-1.935035	-0.796990
H	-1.462561	-1.609676	-0.525767
H	-4.035211	-2.481014	0.710418
H	-3.871053	-4.953272	0.568708
H	-3.707678	-6.059284	-1.645976
H	-3.705935	-4.691020	-3.715184
H	-3.866933	-2.212526	-3.561998

H 1.585869 2.094548 -0.296655

H 6.725500 1.935355 -0.166001

H 9.894948 -1.405872 1.127761

H 15.002208 -0.885607 1.312206

H 16.715210 0.944712 0.532748

H 12.730566 -3.441324 -0.709027

H 12.871815 -5.406144 0.811839

H 12.759137 -5.076902 3.268300

H 12.506181 -2.791563 4.199728

H 12.365522 -0.839418 2.674443

H 4.084948 3.391607 2.379312

H 4.157938 5.791380 1.724845

H 4.272621 6.414257 -0.673853

H 4.313306 4.644046 -2.411252

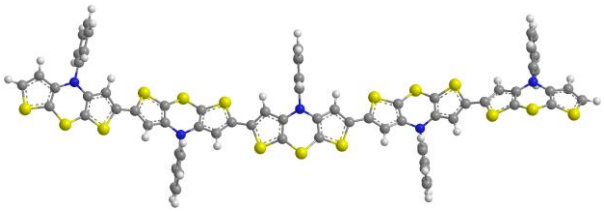
H 4.235936 2.254188 -1.748622

SCF Done: E(RB3LYP) = -7150.00180560 A.U. after 5 cycles

E(HOMO) = -4.776 eV

E(LUMO) = -1.883 eV

11.10 Computed xyz-coordinates of dithienothiazine pentamer



C -6.977511 0.075806 -1.918137

C -7.184978 -1.138037 -1.306066

N -8.467017 -1.716501 -1.196169

C -9.578093 -0.847037 -1.168722

C -9.558906 0.388145 -1.772262

S -8.230143 0.985115 -2.783913

S -5.318813 0.591387 -1.805906

C -4.884270 -0.876807 -0.947537

C -5.985306 -1.677361 -0.755450

C -10.800418 -1.091377 -0.476788

C	-11.695644	-0.050782	-0.556956
S	-11.024639	1.281946	-1.482424
C	-8.602823	-3.063563	-0.708525
C	-8.783320	-4.100168	-1.624157
C	-8.916620	-5.411663	-1.171567
C	-8.869690	-5.687890	0.193979
C	-8.689106	-4.651087	1.108958
C	-8.555310	-3.338394	0.660584
C	-13.027969	0.038893	-0.000464
C	-3.512759	-1.113994	-0.550879
C	-2.526272	-0.196764	-0.276386
C	-1.284180	-0.789661	0.095842
C	-1.347882	-2.163378	0.111584
S	-2.903461	-2.752702	-0.397248
S	-13.945928	-1.417166	0.344430
C	-15.266215	-0.477276	0.977348
C	-15.040299	0.874794	0.863194
C	-13.757459	1.162096	0.311191
N	-0.100170	-0.082115	0.394440
C	1.126756	-0.736430	0.154055
C	1.249070	-2.106119	0.172464
S	-0.037525	-3.223587	0.665084
S	-16.683676	-1.194137	1.767141
C	-17.765244	0.147840	1.335808
C	-17.360722	1.452841	1.189809
N	-16.001694	1.836575	1.238712
C	2.358114	-0.089556	-0.158275
C	3.395377	-0.962453	-0.388318
S	2.850443	-2.626496	-0.264702
S	-19.482658	-0.030825	1.119662
C	-19.658393	1.679142	0.887853
C	-18.462647	2.332100	0.935248
C	-0.133927	1.356421	0.447281

C	-15.661273	3.233880	1.178551
C	-0.120289	2.114107	-0.726418
C	-0.154836	3.505094	-0.653627
C	-0.202854	4.139430	0.587583
C	-0.216736	3.381464	1.757266
C	-0.182292	1.989442	1.688809
C	-15.655929	3.916143	-0.040780
C	-15.323538	5.268735	-0.077276
C	-14.996978	5.940700	1.100502
C	-15.002870	5.258510	2.315978
C	-15.334566	3.904967	2.356532
C	4.772585	-0.665030	-0.716878
S	5.197934	0.864829	-1.465435
C	6.873791	0.401453	-1.542313
C	7.092071	-0.843595	-1.001029
C	5.888649	-1.446285	-0.530742
S	8.130716	1.403674	-2.290323
C	9.435020	0.766923	-1.269313
C	9.470687	-0.509938	-0.759793
N	8.383126	-1.400185	-0.879487
S	10.871967	1.667749	-0.881149
C	11.579003	0.266893	-0.093636
C	10.701314	-0.791601	-0.096994
C	8.524973	-2.765448	-0.446615
C	12.910634	0.339663	0.467088
C	13.939260	1.185911	0.125862
C	15.115778	0.999622	0.909160
C	14.966910	0.002349	1.844266
S	13.393632	-0.739105	1.765504
N	16.332298	1.690894	0.729364
C	17.525816	1.009198	1.053910
C	17.566935	0.008035	1.994154
S	16.200536	-0.437146	3.039882

C	18.800275	1.217605	0.433935
C	19.760829	0.373611	0.906745
S	19.142620	-0.723940	2.099291
C	16.372389	2.830443	-0.147959
C	16.247268	4.108933	0.395567
C	16.275879	5.225323	-0.438606
C	16.431936	5.065807	-1.814573
C	16.556598	3.787365	-2.357736
C	16.524814	2.668609	-1.527465
C	8.690608	-3.766367	-1.403603
C	8.821713	-5.095164	-1.003451
C	8.789335	-5.423425	0.350883
C	8.624215	-4.421846	1.307182
C	8.490207	-3.092531	0.911322
H	-5.943712	-2.614416	-0.218826
H	-11.001678	-1.998246	0.075322
H	-8.817281	-3.870650	-2.682496
H	-9.056642	-6.215321	-1.885113
H	-8.973326	-6.708105	0.544951
H	-8.652204	-4.862615	2.171282
H	-8.414571	-2.527469	1.365895
H	-2.691284	0.870740	-0.308146
H	-13.377524	2.165184	0.179248
H	2.476519	0.984363	-0.181718
H	-20.640075	2.096033	0.725546
H	-18.362517	3.399282	0.800721
H	-0.083167	1.613799	-1.687235
H	-0.144173	4.091753	-1.564878
H	-0.229455	5.221593	0.642199
H	-0.254378	3.871534	2.723182
H	-0.192748	1.387530	2.589630
H	-15.911293	3.387516	-0.951965
H	-15.319655	5.796206	-1.024099

H -14.738274 6.992823 1.070195

H -14.749283 5.777731 3.232909

H -15.343112 3.361801 3.293976

H 5.854682 -2.416521 -0.056052

H 10.939174 -1.753717 0.333799

H 13.864703 1.909207 -0.673604

H 18.987125 1.966009 -0.322339

H 20.800837 0.322169 0.624597

H 16.128921 4.218017 1.467043

H 16.178226 6.217296 -0.013015

H 16.455474 5.934487 -2.462363

H 16.675480 3.659649 -3.427453

H 16.616738 1.672076 -1.943817

H 8.714789 -3.496144 -2.452557

H 8.949859 -5.871286 -1.748973

H 8.892097 -6.456809 0.661230

H 8.597538 -4.674245 2.360862

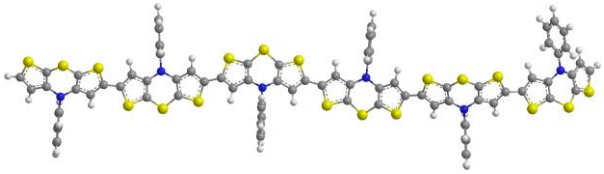
H 8.358166 -2.309028 1.648553

SCF Done: E(RB3LYP) = -8937.20306495 A.U. after 1 cycles

E(HOMO) = -4.771 eV

E(LUMO) = -1.891 eV

11.11 Computed xyz-coordinates of dithienothiazine hexamer



C 2.873749 -1.256029 -0.917885

C 3.111832 0.080183 -0.697596

N 4.408474 0.635391 -0.724357

C 5.492358 -0.213617 -0.419317

C 5.438107 -1.575243 -0.606227

S 4.107821 -2.429516 -1.412776

S 1.192337 -1.662318 -0.724196

C	0.792352	0.009691	-0.370028
C	1.919961	0.796203	-0.383203
C	6.743315	0.206269	0.121315
C	7.618560	-0.828810	0.349639
S	6.885501	-2.370092	-0.059557
C	4.566846	2.062314	-0.626034
C	4.701945	2.811813	-1.794495
C	4.850954	4.195699	-1.718834
C	4.867563	4.829758	-0.477524
C	4.732487	4.079426	0.690286
C	4.579524	2.696253	0.618929
C	8.967602	-0.776847	0.871350
C	-0.578732	0.402406	-0.126721
C	-1.628024	-0.361880	0.326482
C	-2.847828	0.364851	0.457065
C	-2.703978	1.688244	0.111527
S	-1.096987	2.048337	-0.448141
S	9.451416	0.507689	1.964977
C	11.049504	-0.167810	2.106739
C	11.204472	-1.296346	1.336306
C	10.011234	-1.639860	0.635575
N	-4.084287	-0.181456	0.863194
C	-5.257866	0.438549	0.383380
C	-5.298747	1.767184	0.030590
S	-3.972029	2.915794	0.288026
S	12.302406	0.493215	3.174045
C	13.651197	-0.073384	2.171199
C	13.615977	-1.207070	1.394073
N	12.440071	-1.968816	1.223347
C	-6.510458	-0.211502	0.180062
C	-7.481543	0.614476	-0.335212
S	-6.843697	2.224078	-0.624718
S	15.201593	0.716128	2.109215

C	15.829767	-0.525469	1.038486
C	14.862929	-1.459113	0.750078
C	-4.138586	-1.552794	1.298944
C	12.503097	-3.225958	0.525138
C	-4.154352	-2.596638	0.370466
C	-4.206410	-3.916692	0.813146
C	-4.241165	-4.195492	2.179307
C	-4.224351	-3.152499	3.103828
C	-4.173423	-1.830217	2.665079
C	12.537734	-3.268373	-0.871062
C	12.597408	-4.496946	-1.525896
C	12.622795	-5.681288	-0.789934
C	12.588471	-5.636854	0.602827
C	12.528795	-4.409914	1.261735
C	-8.857856	0.306015	-0.657320
S	-9.344109	-1.343867	-1.008559
C	-10.981452	-0.834758	-1.308972
C	-11.144669	0.517814	-1.123584
C	-9.929392	1.162496	-0.749983
S	-12.262770	-1.934452	-1.850693
C	-13.572762	-0.985700	-1.119819
C	-13.549132	0.380157	-0.960496
N	-12.400401	1.151768	-1.232832
S	-15.087019	-1.677925	-0.614665
C	-15.737486	-0.085652	-0.264240
C	-14.791206	0.888296	-0.478671
C	-12.472726	2.587998	-1.180788
C	-17.097472	0.061765	0.207871
C	-18.180221	-0.753434	-0.023017
C	-19.373266	-0.314198	0.622881
C	-19.179592	0.840069	1.345377
S	-17.543032	1.420488	1.225716
N	-20.638996	-0.926487	0.503049

C	-21.777862	-0.096728	0.605447
C	-21.772443	1.075261	1.322555
S	-20.422733	1.615672	2.343993
C	-23.034022	-0.323469	-0.044801
C	-23.934708	0.673562	0.185727
S	-23.277105	1.937481	1.175363
C	-20.746215	-2.202709	-0.153258
C	-20.817554	-3.360058	0.621687
C	-20.917703	-4.605581	0.003610
C	-20.947808	-4.695215	-1.387049
C	-20.876699	-3.537543	-2.161578
C	-20.775188	-2.290839	-1.547493
C	-12.508230	3.308785	-2.374321
C	-12.572267	4.700874	-2.343651
C	-12.602806	5.372319	-1.122440
C	-12.567432	4.650855	0.070497
C	-12.500139	3.259195	0.044263
C	22.744006	1.202874	-3.100813
S	22.671776	-0.526381	-2.982753
C	21.591179	-0.414793	-1.622828
C	21.277872	0.888126	-1.319763
C	21.952754	1.817178	-2.176127
S	21.023854	-1.819597	-0.694305
C	19.495908	-1.056609	-0.216136
C	19.332521	0.294741	-0.018863
N	20.349913	1.227948	-0.310357
S	18.042369	-1.949705	0.129480
C	17.202583	-0.476196	0.582995
C	18.020790	0.618825	0.436990
C	20.171633	2.608541	0.053972
C	19.396354	3.463438	-0.733770
C	19.238811	4.797053	-0.361707
C	19.853435	5.278456	0.793985

C	20.626369	4.424232	1.578769
C	20.786180	3.089433	1.209931
H	1.902134	1.853114	-0.158400
H	6.998434	1.240969	0.300327
H	4.689717	2.304690	-2.751887
H	4.955720	4.775910	-2.628202
H	4.984894	5.905687	-0.419495
H	4.743506	4.569874	1.656719
H	4.469750	2.107188	1.522130
H	-1.525448	-1.405408	0.588156
H	9.934833	-2.482857	-0.036017
H	-6.692724	-1.245685	0.435234
H	15.030486	-2.290907	0.081011
H	-4.125794	-2.372369	-0.689608
H	-4.218999	-4.725559	0.091867
H	-4.281072	-5.223106	2.521631
H	-4.251110	-3.365931	4.166046
H	-4.160282	-1.009100	3.371808
H	12.517605	-2.343880	-1.436571
H	12.623961	-4.528166	-2.608926
H	12.669387	-6.635851	-1.301209
H	12.608340	-6.555486	1.177560
H	12.501900	-4.359938	2.343698
H	-9.856829	2.220142	-0.540286
H	-14.987042	1.940374	-0.328484
H	-18.131137	-1.630112	-0.652950
H	-23.251277	-1.192533	-0.648506
H	-24.950498	0.749820	-0.169517
H	-20.794297	-3.274843	1.701566
H	-20.972842	-5.503253	0.608426
H	-21.026165	-5.664029	-1.866722
H	-20.898825	-3.603944	-3.243171
H	-20.717538	-1.387082	-2.143145

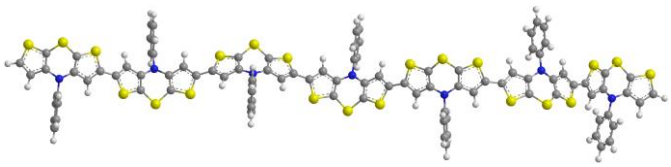
H	-12.485870	2.773390	-3.316020
H	-12.599860	5.258565	-3.272534
H	-12.653712	6.454738	-1.099607
H	-12.589743	5.170036	1.021603
H	-12.467915	2.692366	0.967570
H	23.367426	1.659161	-3.853813
H	21.853461	2.890019	-2.097419
H	17.689587	1.629237	0.629702
H	18.921965	3.083107	-1.631150
H	18.636774	5.458432	-0.973988
H	19.729630	6.316146	1.081502
H	21.105393	4.794820	2.477585
H	21.384253	2.414042	1.810023

SCF Done: E(RB3LYP) = -10724.4042312 A.U. after 5 cycles

E(HOMO) = -4.762 eV

E(LUMO) = -1.900 eV

11.12 Computed xyz-coordinates of dithienothiazine heptamer



C	-0.942906	0.878186	1.144383
C	-0.694029	-0.286175	0.456448
N	0.614703	-0.752688	0.207935
C	1.645174	0.207803	0.127554
C	1.576627	1.414664	0.783559
S	0.304587	1.855791	1.939430
S	-2.640368	1.258958	1.194566
C	-3.030029	-0.200217	0.300697
C	-1.890177	-0.897901	-0.021137
C	2.841528	0.077300	-0.637677
C	3.659371	1.180239	-0.570189
S	2.935174	2.437351	0.417907
C	0.800542	-2.050691	-0.385448

C	1.076771	-3.140225	0.440215
C	1.258040	-4.405284	-0.116478
C	1.165376	-4.581682	-1.496105
C	0.888486	-3.491763	-2.320928
C	0.703800	-2.225988	-1.768190
C	4.938327	1.403195	-1.209964
C	-4.407451	-0.533854	0.006450
C	-5.479028	0.309261	-0.168383
C	-6.697801	-0.371412	-0.458973
C	-6.531739	-1.735650	-0.511952
S	-4.901003	-2.211782	-0.139056
S	5.330120	0.602401	-2.721330
C	6.868970	1.412510	-2.792385
C	7.075281	2.228846	-1.704873
C	5.968809	2.218324	-0.805686
N	-7.951385	0.247039	-0.650394
C	-9.103397	-0.503054	-0.333438
C	-9.123184	-1.877621	-0.372545
S	-7.797999	-2.883814	-0.988044
S	7.984296	1.257175	-4.162758
C	9.433809	1.611140	-3.203541
C	9.454088	2.411715	-2.085772
N	8.279647	2.935867	-1.505525
C	-10.352864	0.042517	0.082900
C	-11.301343	-0.910843	0.369116
S	-10.643936	-2.526144	0.169548
S	11.022232	1.043713	-3.632591
C	11.737831	1.928251	-2.295839
C	10.772528	2.586414	-1.571567
C	-8.032414	1.683817	-0.691887
C	8.384733	3.866813	-0.412760
C	-8.016746	2.434343	0.486352
C	-8.097197	3.824020	0.423648

C	-8.192523	4.464025	-0.811833
C	-8.208256	3.713165	-1.986089
C	-8.128299	2.322625	-1.927765
C	8.613459	3.416472	0.889969
C	8.712895	4.334760	1.933282
C	8.585137	5.699858	1.678096
C	8.357553	6.147149	0.377614
C	8.256798	5.231720	-0.668834
C	-12.668388	-0.723831	0.804643
S	-13.142900	0.750085	1.632216
C	-14.772913	0.166417	1.810661
C	-14.943387	-1.074388	1.243129
C	-13.738234	-1.577088	0.670762
S	-16.041930	1.052348	2.675847
C	-17.364586	0.365579	1.712701
C	-17.348659	-0.894486	1.162114
N	-16.200384	-1.713203	1.189645
S	-18.875712	1.182236	1.436387
C	-19.536259	-0.236753	0.641321
C	-18.594808	-1.235292	0.558555
C	-16.283252	-3.080142	0.747720
C	-20.898543	-0.232419	0.153072
C	-21.973104	0.491365	0.613210
C	-23.170626	0.269044	-0.128252
C	-22.988972	-0.629436	-1.153656
S	-21.358328	-1.235530	-1.211876
N	-24.429487	0.834520	0.166246
C	-25.577689	0.083346	-0.169991
C	-25.584852	-0.831420	-1.195224
S	-24.239388	-1.070090	-2.331161
C	-26.832359	0.127712	0.519957
C	-27.744529	-0.749260	0.012716
S	-27.100160	-1.681179	-1.300842

C	-24.522390	1.867397	1.163893
C	-24.576045	3.200513	0.757663
C	-24.662151	4.214749	1.710200
C	-24.695337	3.898286	3.067304
C	-24.641711	2.565072	3.473053
C	-24.554206	1.548562	2.524016
C	-16.333519	-4.097837	1.700307
C	-16.407748	-5.428492	1.292284
C	-16.433105	-5.742514	-0.065635
C	-16.383281	-4.724525	-1.017470
C	-16.307337	-3.392867	-0.613824
C	24.554723	-3.287689	1.968543
C	24.275897	-2.331709	2.915114
N	22.995817	-1.749950	3.052881
C	22.176801	-1.699700	1.905396
C	22.295423	-2.603626	0.875336
S	23.336768	-4.039356	0.915758
S	26.237445	-3.731471	1.965998
C	26.550103	-2.658124	3.292423
C	25.434538	-1.976504	3.678809
C	21.165077	-0.726647	1.654430
C	20.536199	-0.886739	0.442302
S	21.224853	-2.235422	-0.445601
C	22.748704	-0.839500	4.139837
C	22.103587	-1.308055	5.284030
C	21.857664	-0.441125	6.347759
C	22.254251	0.892756	6.268188
C	22.899194	1.360764	5.123505
C	23.148527	0.496881	4.059054
C	19.466616	-0.100880	-0.133834
S	19.242826	1.575899	0.334222
C	17.903302	1.740578	-0.765132
C	17.631901	0.567853	-1.429968

C	18.528396	-0.479065	-1.064990
S	17.052867	3.272506	-1.041681
C	15.524092	2.501045	-1.504003
C	15.425279	1.272807	-2.114263
N	16.543122	0.436158	-2.318054
S	13.970930	3.260297	-1.303106
C	13.170025	1.909697	-2.088017
C	14.078136	0.941049	-2.443880
C	16.391276	-0.773932	-3.082396
C	15.862850	-1.927693	-2.497802
C	15.723374	-3.087783	-3.257020
C	16.108583	-3.097238	-4.597380
C	16.634489	-1.944830	-5.179048
C	16.777071	-0.782672	-4.422614
H	-1.903374	-1.809374	-0.601436
H	3.100668	-0.813120	-1.192455
H	1.147990	-2.987655	1.510524
H	1.472680	-5.250349	0.527266
H	1.307879	-5.565520	-1.927978
H	0.814495	-3.625831	-3.393862
H	0.485146	-1.375048	-2.402995
H	-5.393612	1.385627	-0.124201
H	5.943468	2.781228	0.116314
H	-10.550392	1.103602	0.137436
H	10.994222	3.165696	-0.686706
H	-7.942344	1.929634	1.442691
H	-8.084955	4.405196	1.338381
H	-8.254474	5.545109	-0.858497
H	-8.282858	4.207669	-2.947591
H	-8.139753	1.726008	-2.832077
H	8.712246	2.354025	1.080738
H	8.890144	3.983867	2.943283
H	8.663071	6.412533	2.490986

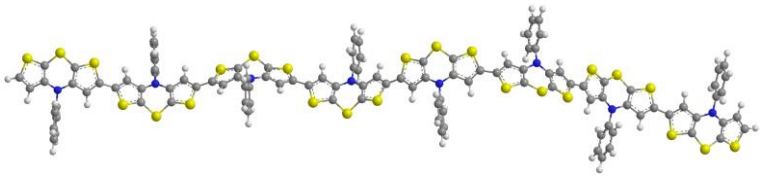
H	8.258211	7.207379	0.176020
H	8.079881	5.564923	-1.684473
H	-13.672203	-2.527701	0.161047
H	-18.796546	-2.196937	0.108635
H	-21.915135	1.148740	1.468927
H	-27.040160	0.787733	1.349469
H	-28.761903	-0.912748	0.332241
H	-24.549946	3.431762	-0.300563
H	-24.703393	5.249764	1.391266
H	-24.762210	4.687653	3.807052
H	-24.666025	2.315510	4.527505
H	-24.509840	0.510431	2.832732
H	-16.313939	-3.838409	2.752072
H	-16.446408	-6.217332	2.034469
H	-16.491311	-6.777518	-0.382097
H	-16.401999	-4.965638	-2.073958
H	-16.266222	-2.596745	-1.348234
H	27.546056	-2.594945	3.702267
H	25.427809	-1.251550	4.479721
H	20.891965	0.044453	2.360587
H	21.799562	-2.346943	5.330898
H	21.355971	-0.808016	7.235645
H	22.061653	1.566346	7.095228
H	23.209431	2.397246	5.058771
H	23.651067	0.853354	3.167270
H	18.468543	-1.481560	-1.463676
H	13.791429	0.010175	-2.911847
H	15.564511	-1.913020	-1.455824
H	15.313840	-3.982101	-2.801878
H	15.998910	-4.000592	-5.186164
H	16.934984	-1.948900	-6.220339
H	17.185075	0.120269	-4.860997

SCF Done: E(RB3LYP) = -12511.6054618 A.U. after 6 cycles

E(HOMO) = -4.767 eV

E(LUMO) = -1.888 eV

11.13 Computed xyz-coordinates of dithienothiazine octamer



C	-4.811830	0.162976	1.361760
C	-4.567900	-0.000262	0.018322
N	-3.262270	-0.010802	-0.517477
C	-2.266870	0.708995	0.176228
C	-2.334650	0.938291	1.530580
S	-3.551280	0.224932	2.607320
S	-6.514610	0.247423	1.712710
C	-6.910990	0.024130	0.017321
C	-5.770470	-0.079409	-0.743365
C	-1.110890	1.299840	-0.413383
C	-0.323211	1.980830	0.484418
S	-1.029100	1.942280	2.091250
C	-3.070390	-0.335039	-1.906600
C	-2.707350	-1.635660	-2.255360
C	-2.518380	-1.968230	-3.595800
C	-2.690050	-1.002660	-4.586410
C	-3.053390	0.297598	-4.236760
C	-3.245380	0.633652	-2.898100
C	0.913614	2.693100	0.245992
C	-8.291650	-0.034310	-0.411935
C	-9.401210	0.519627	0.181594
C	-10.611700	0.273074	-0.530216
C	-10.401600	-0.462212	-1.673440
S	-8.734750	-0.924020	-1.858490
S	1.266310	3.356150	-1.340290
C	2.769180	4.020440	-0.767001

C	2.994470	3.725870	0.557310
C	1.930900	2.967610	1.129180
N	-11.895500	0.698641	-0.128762
C	-13.000800	-0.066765	-0.556125
C	-12.975000	-0.826580	-1.702020
S	-11.649800	-0.823238	-2.881440
S	3.832140	5.026960	-1.768410
C	5.307910	4.590100	-0.886903
C	5.348750	4.254710	0.445991
N	4.181970	4.095990	1.223230
C	-14.244700	-0.172265	0.132944
C	-15.144000	-1.010820	-0.482064
S	-14.442200	-1.735100	-1.918720
S	6.892990	4.618190	-1.605030
C	7.634320	4.201380	-0.069350
C	6.680160	4.032950	0.905734
C	-12.032600	1.552490	1.022030
C	4.298000	3.886220	2.642290
C	-11.939600	1.029790	2.314370
C	-12.077400	1.873660	3.414530
C	-12.310100	3.235900	3.226540
C	-12.404300	3.754910	1.936300
C	-12.265100	2.914370	0.832865
C	4.587500	2.619960	3.157130
C	4.696460	2.440350	4.534720
C	4.518260	3.521530	5.397420
C	4.230400	4.784190	4.881770
C	4.119420	4.967890	3.504480
C	-16.494400	-1.344020	-0.082635
S	-16.970700	-1.265450	1.604900
C	-18.574300	-1.818400	1.214350
C	-18.736300	-2.023610	-0.135675
C	-17.545200	-1.751090	-0.870182

S	-19.822100	-2.137620	2.433060
C	-21.173200	-1.789880	1.335990
C	-21.147100	-2.004100	-0.022230
N	-19.974400	-2.393940	-0.702455
S	-22.725300	-1.224090	1.880350
C	-23.383200	-1.362650	0.258804
C	-22.414800	-1.765130	-0.630089
C	-20.037600	-2.730930	-2.100280
C	-24.771400	-1.041070	0.004994
C	-25.844100	-1.137520	0.859384
C	-27.073700	-0.701744	0.283716
C	-26.917900	-0.273282	-1.014060
S	-25.271200	-0.420615	-1.558690
N	-28.333000	-0.750124	0.918963
C	-29.471600	-0.919596	0.099868
C	-29.503200	-0.512271	-1.212050
S	-28.215400	0.423021	-2.002210
C	-30.690100	-1.562740	0.492285
C	-31.599700	-1.632930	-0.520713
S	-30.995200	-0.947663	-1.994970
C	-28.403000	-1.102360	2.312780
C	-28.518900	-0.089595	3.264460
C	-28.583400	-0.412739	4.619160
C	-28.533300	-1.745890	5.022770
C	-28.417000	-2.758270	4.070530
C	-28.350700	-2.439270	2.715820
C	-19.987000	-4.073000	-2.476400
C	-20.041700	-4.418560	-3.825660
C	-20.149400	-3.425380	-4.797780
C	-20.200000	-2.083680	-4.420890
C	-20.142400	-1.733660	-3.073240
C	20.656100	-1.964450	-1.403120
C	20.384200	-2.093900	-0.061498

N	19.097500	-1.873240	0.474939
C	18.247200	-0.982317	-0.212984
C	18.357500	-0.756342	-1.565100
S	19.430800	-1.662860	-2.648980
S	22.346200	-2.191770	-1.753850
C	22.692000	-2.501770	-0.061052
C	21.550600	-2.400290	0.698764
C	17.210700	-0.203894	0.380856
C	16.554700	0.610152	-0.512121
S	17.247100	0.462928	-2.118520
C	18.852000	-2.164520	1.862960
C	18.254600	-3.377290	2.205700
C	18.013800	-3.679000	3.545140
C	18.368200	-2.770300	4.540940
C	18.965000	-1.557570	4.197280
C	19.208800	-1.252640	2.859640
C	15.455800	1.520500	-0.271923
C	24.037000	-2.816900	0.368755
C	25.231200	-2.491580	-0.230039
C	26.373600	-2.950900	0.488853
C	26.029400	-3.616760	1.642230
S	24.305200	-3.754440	1.828530
S	15.215300	2.228920	1.315620
C	13.844500	3.135710	0.741885
C	13.576400	2.885330	-0.583494
C	14.500300	1.962690	-1.156010
N	27.714200	-2.781480	0.084192
C	28.654000	-3.741800	0.520613
C	28.488700	-4.464080	1.677720
S	27.190500	-4.182830	2.857910
S	12.958500	4.302400	1.741970
C	11.431500	4.109060	0.860500
C	11.338700	3.786440	-0.472878

N	12.466900	3.447470	-1.249770
C	29.841800	-4.120640	-0.184604
C	30.534400	-5.112930	0.443224
S	29.750100	-5.642470	1.897100
S	9.870010	4.382100	1.579320
C	9.072750	4.088470	0.043108
C	9.988950	3.775390	-0.932634
C	28.002400	-1.983840	-1.078750
C	12.319700	3.259630	-2.669160
C	28.419000	-0.663540	-0.910355
C	28.697300	0.125028	-2.025780
C	28.561400	-0.404866	-3.307780
C	28.144900	-1.725360	-3.475440
C	27.863600	-2.516000	-2.363140
C	11.820500	2.060450	-3.183910
C	11.684900	1.900690	-4.561540
C	12.045400	2.935300	-5.424390
C	12.542300	4.131250	-4.908820
C	12.680300	4.294790	-3.531370
H	-5.788870	-0.187217	-1.818400
H	-0.856490	1.197590	-1.458660
H	-2.575420	-2.374950	-1.474370
H	-2.236120	-2.979580	-3.864350
H	-2.541680	-1.262030	-5.628270
H	-3.188900	1.050300	-5.004700
H	-3.529270	1.641750	-2.618790
H	-9.350340	1.114390	1.082400
H	1.927720	2.622540	2.153180
H	-14.475100	0.379692	1.033070
H	6.920220	3.742140	1.918400
H	-11.761100	-0.030357	2.452890
H	-12.004600	1.466920	4.416490
H	-12.417900	3.890350	4.083740

H	-12.585200	4.812980	1.786870
H	-12.334900	3.303750	-0.175786
H	4.726170	1.784420	2.480680
H	4.920760	1.457540	4.932720
H	4.603540	3.379600	6.468560
H	4.091320	5.626330	5.549630
H	3.895420	5.943240	3.089270
H	-17.475900	-1.834460	-1.945330
H	-22.609700	-1.918170	-1.681900
H	-25.760500	-1.526580	1.864010
H	-30.875900	-1.946580	1.484760
H	-32.593600	-2.051780	-0.496873
H	-28.557400	0.942188	2.936010
H	-28.673100	0.376468	5.356560
H	-28.583900	-1.996120	6.076170
H	-28.376500	-3.795820	4.381330
H	-28.258300	-3.220860	1.970490
H	-19.906000	-4.834030	-1.709460
H	-20.002100	-5.462100	-4.115660
H	-20.193300	-3.695480	-5.846550
H	-20.282000	-1.309030	-5.174440
H	-20.177700	-0.692688	-2.773190
H	21.547300	-2.520950	1.772580
H	16.940200	-0.269067	1.425100
H	17.983700	-4.073600	1.421040
H	17.549700	-4.622210	3.808910
H	18.180500	-3.005900	5.582100
H	19.242500	-0.849224	4.969220
H	19.675000	-0.313210	2.585760
H	25.294000	-1.912170	-1.140160
H	14.447400	1.624500	-2.180880
H	30.161800	-3.666870	-1.111220
H	31.460900	-5.574960	0.139737

H 9.707030 3.525960 -1.945510

H 28.521000 -0.265323 0.092139

H 29.020300 1.150900 -1.892110

H 28.778700 0.208892 -4.174320

H 28.037400 -2.140030 -4.471050

H 27.537200 -3.542330 -2.485700

H 11.541500 1.261260 -2.506860

H 11.297800 0.969793 -4.959340

H 11.939100 2.809160 -6.495630

H 12.823000 4.937130 -5.576900

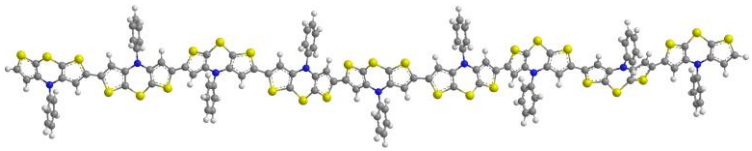
H 13.065200 5.218600 -3.116250

SCF Done: E(RB3LYP) = -14298.8067877 A.U. after 7 cycles

E(HOMO) = -4.761 eV

E(LUMO) = -1.891 eV

11.14 Computed xyz-coordinates of dithienothiazine nonamer



C -8.500730 1.068150 1.346900

C -8.231810 1.028400 -0.001003

N -6.931390 1.203840 -0.520073

C -6.022820 1.971840 0.237803

C -6.123870 2.095140 1.603970

S -7.264530 1.184080 2.613010

S -10.203600 0.926969 1.679350

C -10.561400 0.777287 -0.032520

C -9.412510 0.862857 -0.782702

C -4.927450 2.716400 -0.290502

C -4.218160 3.403880 0.665692

S -4.928980 3.178960 2.254590

C -6.701730 1.006510 -1.927140

C -6.224460 -0.226963 -2.369660

C -6.002930 -0.438720 -3.729510

C	-6.255390	0.580883	-4.645860
C	-6.732300	1.814090	-4.202420
C	-6.958170	2.028880	-2.844220
C	-3.053450	4.246490	0.497988
C	-11.922100	0.580872	-0.483693
C	-13.095500	0.945528	0.133240
C	-14.261400	0.600287	-0.611152
C	-13.955300	-0.016027	-1.801760
S	-12.242600	-0.250276	-1.996430
S	-2.773060	5.084850	-1.018300
C	-1.330270	5.822990	-0.383455
C	-1.069650	5.424610	0.906701
C	-2.058360	4.525990	1.404470
N	-15.590900	0.820408	-0.194324
C	-16.579200	-0.065169	-0.673422
C	-16.452900	-0.732381	-1.869390
S	-15.148700	-0.452244	-3.039610
S	-0.358477	7.003980	-1.281470
C	1.157220	6.589930	-0.458434
C	1.236560	6.135340	0.836884
N	0.090674	5.827800	1.601090
C	-17.788400	-0.398213	0.005110
C	-18.560300	-1.315510	-0.667409
S	-17.773200	-1.829320	-2.149820
S	2.728140	6.781410	-1.183820
C	3.513710	6.270930	0.300688
C	2.584950	5.955670	1.263750
C	-15.842300	1.591250	0.994991
C	0.233444	5.503090	2.996120
C	-15.734200	1.009540	2.260630
C	-15.983100	1.774770	3.398280
C	-16.336500	3.118170	3.274160
C	-16.441700	3.697030	2.010540

C	-16.195600	2.934600	0.869855
C	0.644834	4.229180	3.396290
C	0.779536	3.938480	4.752470
C	0.503380	4.915810	5.708230
C	0.091842	6.185720	5.307030
C	-0.043504	6.480810	3.951440
C	-19.841000	-1.874860	-0.290093
S	-20.275200	-2.044470	1.401830
C	-21.795100	-2.777150	0.974558
C	-21.964800	-2.859790	-0.387612
C	-20.845000	-2.343630	-1.103500
S	-22.948200	-3.399840	2.169040
C	-24.366000	-3.144400	1.132760
C	-24.349300	-3.208140	-0.240966
N	-23.152900	-3.343130	-0.976735
S	-25.968500	-2.886110	1.757500
C	-26.647400	-2.953460	0.140343
C	-25.656900	-3.105060	-0.800869
C	-23.209500	-3.510300	-2.405390
C	-28.076000	-2.830870	-0.055818
C	-29.091200	-3.180390	0.802806
C	-30.392400	-2.893590	0.295209
C	-30.349300	-2.321710	-0.955002
S	-28.718800	-2.149880	-1.540250
N	-31.607000	-3.207390	0.941489
C	-32.726600	-3.486540	0.126376
C	-32.866200	-2.964040	-1.136650
S	-31.774500	-1.753720	-1.844360
C	-33.806000	-4.364230	0.467976
C	-34.720700	-4.490210	-0.534978
S	-34.285800	-3.571070	-1.940290
C	-31.580600	-3.685590	2.298670
C	-31.852300	-2.795230	3.337220

C	-31.827500	-3.239780	4.658300
C	-31.532200	-4.572120	4.942120
C	-31.260600	-5.462080	3.903210
C	-31.283800	-5.021400	2.581500
C	-22.964700	-4.770090	-2.951210
C	-23.006200	-4.948110	-4.333180
C	-23.294800	-3.870140	-5.168440
C	-23.540500	-2.610920	-4.621570
C	-23.496000	-2.427780	-3.240960
C	16.474200	0.297279	-1.505620
C	16.157200	0.034034	-0.193598
N	14.868900	0.259108	0.336189
C	14.072000	1.248040	-0.277571
C	14.230100	1.612880	-1.594150
S	15.305500	0.793679	-2.743940
S	18.158000	0.012359	-1.842700
C	18.438400	-0.503162	-0.188710
C	17.283300	-0.421558	0.552318
C	13.040400	1.991620	0.367337
C	12.433600	2.914100	-0.451508
S	13.169400	2.915790	-2.044740
C	14.581200	-0.143791	1.687980
C	13.909100	-1.345280	1.909970
C	13.622400	-1.749880	3.212880
C	14.006000	-0.955204	4.291950
C	14.678300	0.246135	4.068740
C	14.967400	0.653808	2.768100
C	11.347700	3.820560	-0.144776
C	19.748800	-0.950338	0.231740
C	20.980400	-0.619322	-0.281958
C	22.067500	-1.246330	0.395227
C	21.643500	-2.043540	1.432620
S	19.909200	-2.096950	1.551140

S	11.108500	4.398380	1.495400
C	9.748720	5.362430	0.993880
C	9.481810	5.222530	-0.347761
C	10.400600	4.343450	-0.992934
N	23.429600	-1.108790	0.054245
C	24.293600	-2.176850	0.375937
C	24.041700	-3.044790	1.412450
S	22.722200	-2.855910	2.583280
S	8.848520	6.435800	2.081100
C	7.319470	6.274950	1.197150
C	7.229400	6.067410	-0.159141
N	8.367930	5.835610	-0.960952
C	25.491900	-2.505820	-0.323368
C	26.131200	-3.616860	0.173637
S	25.225000	-4.316440	1.504430
S	5.754010	6.414020	1.944950
C	4.957500	6.225010	0.391873
C	5.877650	6.041950	-0.612883
C	23.811900	-0.176895	-0.974207
C	8.236800	5.800680	-2.393770
C	24.343600	1.058730	-0.606586
C	24.721100	1.972290	-1.589600
C	24.567000	1.652120	-2.937430
C	24.035300	0.415944	-3.303960
C	23.657100	-0.500207	-2.324570
C	7.738630	4.666830	-3.040880
C	7.621060	4.656630	-4.429410
C	8.000840	5.774360	-5.171850
C	8.498910	6.904050	-4.524640
C	8.617350	6.918630	-3.135910
C	27.363500	-4.229340	-0.273703
S	27.890000	-4.057500	-1.939400
C	29.289500	-5.047200	-1.636410

C	29.357600	-5.459710	-0.326083
C	28.254700	-4.989720	0.445835
S	30.443000	-5.522780	-2.896620
C	31.813400	-5.673300	-1.775420
C	31.697100	-6.043150	-0.457341
N	30.444700	-6.206600	0.175081
S	33.473400	-5.440400	-2.243690
C	34.012300	-5.904280	-0.661313
C	32.973800	-6.179140	0.177944
C	30.386800	-6.728010	1.514990
C	30.033000	-8.063260	1.708390
C	29.968600	-8.585440	2.999250
C	30.257800	-7.775440	4.096120
C	30.611600	-6.440390	3.902380
C	30.676300	-5.914450	2.613550
H	-9.411950	0.827838	-1.862750
H	-4.654890	2.715730	-1.336180
H	-6.030560	-1.009370	-1.645680
H	-5.632250	-1.398220	-4.070970
H	-6.081560	0.415557	-5.702840
H	-6.930910	2.608390	-4.912560
H	-7.332200	2.983580	-2.492680
H	-13.125600	1.473360	1.075790
H	-2.022880	4.086420	2.390910
H	-18.090300	0.050862	0.940484
H	2.856480	5.586340	2.242220
H	-15.457300	-0.034649	2.349320
H	-15.900000	1.322080	4.379510
H	-16.529200	3.711730	4.160330
H	-16.716300	4.740710	1.910950
H	-16.275000	3.370440	-0.118923
H	0.857835	3.474250	2.648180
H	1.099560	2.950050	5.061100

H	0.608588	4.687570	6.762540
H	-0.123750	6.947400	6.047280
H	-0.361346	7.463810	3.625020
H	-20.794000	-2.302290	-2.182070
H	-25.859300	-3.175030	-1.859980
H	-28.914700	-3.648470	1.760590
H	-33.893300	-4.869180	1.418980
H	-35.628400	-5.073280	-0.540296
H	-32.080800	-1.762620	3.101780
H	-32.039000	-2.545650	5.463360
H	-31.513300	-4.916670	5.969610
H	-31.029900	-6.498580	4.120420
H	-31.072700	-5.707210	1.769110
H	-22.744100	-5.599100	-2.289460
H	-22.815200	-5.927940	-4.755160
H	-23.328000	-4.010060	-6.242710
H	-23.763700	-1.770490	-5.268500
H	-23.680700	-1.450840	-2.809250
H	17.243200	-0.662307	1.604910
H	12.734900	1.824210	1.390250
H	13.615900	-1.951770	1.061390
H	13.099600	-2.683820	3.383220
H	13.782100	-1.270680	5.304440
H	14.978200	0.865957	4.905700
H	15.489900	1.585920	2.586520
H	21.109400	0.076407	-1.098770
H	10.346900	4.088550	-2.041630
H	25.882600	-1.921730	-1.144350
H	5.597150	5.871270	-1.642340
H	24.456800	1.293690	0.445014
H	25.134000	2.932070	-1.301730
H	24.860500	2.363350	-3.700800
H	23.915200	0.163794	-4.351160

H 23.244200 -1.463310 -2.601800

H 7.446690 3.800910 -2.457910

H 7.233970 3.776520 -4.929610

H 7.908890 5.764190 -6.251750

H 8.795110 7.774250 -5.098810

H 9.001980 7.789760 -2.619130

H 28.136000 -5.191540 1.500760

H 35.069400 -5.939830 -0.448456

H 33.104500 -6.473860 1.209000

H 29.811200 -8.681190 0.846495

H 29.693100 -9.623270 3.146490

H 30.207600 -8.182500 5.099410

H 30.836500 -5.807770 4.753230

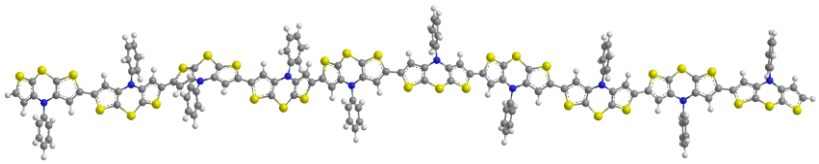
H 30.949300 -4.877460 2.455370

SCF Done: E(RB3LYP) = -16086.0080771 A.U. after 6 cycles

E(HOMO) = -4.767 eV

E(LUMO) = -1.886 eV

11.15 Computed xyz-coordinates of dithienothiazine decamer



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C 12.302100 0.997838 0.069962

N 11.012100 1.199770 0.605137

C 10.123400 2.019320 -0.121613

C 10.219000 2.182280 -1.484000

S 11.321900 1.266740 -2.530290

S 14.256500 0.880405 -1.629650

C 14.621900 0.664434 0.073687

C 13.482200 0.767493 0.835861

C 9.055890 2.780770 0.438323

C 8.361990 3.520110 -0.490228

S 9.054560 3.323340 -2.090960

C	10.787000	0.970306	2.008120
C	10.260200	-0.254048	2.418720
C	10.041300	-0.496641	3.773830
C	10.346400	0.482939	4.717430
C	10.872600	1.707140	4.305890
C	11.095300	1.952790	2.952420
C	7.224710	4.391480	-0.287603
C	15.978300	0.409274	0.506963
C	17.157500	0.714241	-0.131182
C	18.318500	0.324712	0.598669
C	18.003300	-0.263857	1.801070
S	16.284900	-0.417969	2.024560
S	6.954750	5.155850	1.269050
C	5.543820	5.974490	0.661587
C	5.284910	5.655290	-0.650759
C	6.248920	4.751800	-1.186690
N	19.650000	0.485989	0.160955
C	20.611400	-0.423819	0.650281
C	20.474800	-1.065690	1.858750
S	19.189800	-0.729149	3.035080
S	4.602340	7.137310	1.613790
C	3.083570	6.822520	0.753369
C	3.004090	6.442260	-0.565670
N	4.147450	6.135540	-1.334060
C	21.803400	-0.806835	-0.032196
C	22.553100	-1.734710	0.650801
S	21.763800	-2.196520	2.148930
S	1.511820	7.028850	1.472260
C	0.726949	6.627660	-0.045702
C	1.655380	6.333980	-1.015660
C	19.912000	1.191690	-1.066510
C	4.008200	5.888130	-2.745170
C	19.706100	0.574134	-2.302740

C	19.969600	1.273410	-3.478720
C	20.439500	2.585280	-3.421780
C	20.644800	3.199140	-2.187310
C	20.380900	2.503620	-1.008270
C	3.569080	4.647440	-3.214350
C	3.439950	4.430880	-4.584840
C	3.747880	5.449640	-5.486060
C	4.185340	6.686840	-5.016020
C	4.316250	6.907440	-3.645870
C	23.814500	-2.337160	0.275212
S	24.235000	-2.543420	-1.416090
C	25.736500	-3.311340	-0.985250
C	25.911000	-3.378330	0.377170
C	24.809400	-2.821530	1.090720
S	26.866700	-3.983470	-2.174960
C	28.296200	-3.746540	-1.150600
C	28.284900	-3.788780	0.223964
N	27.089200	-3.884390	0.967028
S	29.901100	-3.533140	-1.786510
C	30.586100	-3.590060	-0.171404
C	29.597000	-3.705660	0.776408
C	27.149500	-4.035660	2.397330
C	32.017600	-3.492750	0.017507
C	33.023000	-3.869620	-0.841132
C	34.331100	-3.600570	-0.341662
C	34.303100	-3.014870	0.902587
S	32.678400	-2.807640	1.492030
N	35.537400	-3.941270	-0.989877
C	36.656900	-4.227540	-0.177075
C	36.810600	-3.693700	1.079570
S	35.740600	-2.459990	1.780170
C	37.722200	-5.123840	-0.514850
C	38.640500	-5.251720	0.484462

S	38.226200	-4.311500	1.881990
C	35.496500	-4.436540	-2.340550
C	35.778400	-3.564670	-3.391960
C	35.739700	-4.025990	-4.706970
C	35.420000	-5.356610	-4.971800
C	35.138300	-6.228080	-3.920010
C	35.175500	-5.770640	-2.604340
C	26.886900	-5.284860	2.958970
C	26.933100	-5.447710	4.342650
C	27.243900	-4.365120	5.163860
C	27.507300	-3.116500	4.601230
C	27.458700	-2.948590	3.218800
C	-12.613600	1.276860	1.248490
C	-12.337600	1.134370	-0.091115
N	-11.040300	1.303830	-0.620227
C	-10.155500	2.152930	0.076809
C	-10.265300	2.383100	1.428300
S	-11.388200	1.529350	2.505240
S	-14.312700	1.109580	1.588470
C	-14.658000	0.807127	-0.105478
C	-13.509100	0.867033	-0.858136
C	-9.076970	2.879640	-0.507585
C	-8.387680	3.658360	0.391650
S	-9.098960	3.544070	1.992160
C	-10.802600	1.015920	-2.010430
C	-10.253800	-0.216560	-2.363650
C	-10.021200	-0.514225	-3.705470
C	-10.335300	0.418082	-4.692930
C	-10.883500	1.650550	-4.338670
C	-11.119000	1.951550	-2.998690
C	-7.241100	4.510160	0.159544
C	-16.009600	0.530579	-0.541598
C	-17.196800	0.893936	0.048949

C	-18.347900	0.457614	-0.670268
C	-18.017100	-0.227393	-1.815860
S	-16.296600	-0.412629	-1.994090
S	-6.956290	5.206450	-1.426110
C	-5.539870	6.035320	-0.845986
C	-5.289780	5.767810	0.479539
C	-6.265900	4.897570	1.047900
N	-19.685500	0.659532	-0.268232
C	-20.640200	-0.291862	-0.686250
C	-20.485500	-1.036760	-1.832020
S	-19.190900	-0.791835	-3.019790
S	-4.579780	7.146030	-1.840590
C	-3.067930	6.843610	-0.963881
C	-2.997710	6.517440	0.370085
N	-4.148520	6.262390	1.146560
C	-21.839400	-0.619468	0.011459
C	-22.573400	-1.612970	-0.592519
S	-21.762500	-2.200630	-2.034280
S	-1.491590	6.990880	-1.686980
C	-0.716731	6.639270	-0.151611
C	-1.651900	6.403940	0.827787
C	-19.956500	1.477690	0.885117
C	-4.018080	6.072430	2.567370
C	-20.332700	2.807770	0.700449
C	-20.594000	3.615340	1.806320
C	-20.482100	3.094410	3.094310
C	-20.106200	1.763930	3.277790
C	-19.841100	0.954203	2.175320
C	-3.597810	4.846650	3.090100
C	-3.478850	4.685400	4.469120
C	-3.778040	5.744640	5.325520
C	-4.196460	6.966890	4.802070
C	-4.317240	7.132180	3.423230

C	-23.830400	-2.191870	-0.170299
S	-24.301700	-2.151530	1.520150
C	-25.765400	-3.024940	1.169520
C	-25.892300	-3.305820	-0.170546
C	-24.784900	-2.826100	-0.929912
S	-26.913800	-3.542100	2.417550
C	-28.313800	-3.522760	1.327690
C	-28.255100	-3.780860	-0.021936
N	-27.032800	-3.939670	-0.707831
S	-29.945900	-3.277000	1.877680
C	-30.574400	-3.618670	0.274441
C	-29.550200	-3.842270	-0.615388
C	-27.035400	-4.330820	-2.092770
C	-32.000900	-3.618050	0.033586
C	-33.021400	-3.842640	0.927312
C	-34.320300	-3.740520	0.348501
C	-34.270900	-3.437020	-0.992049
S	-32.635200	-3.295430	-1.571210
N	-35.535500	-3.983280	1.023030
C	-36.612900	-4.492490	0.264714
C	-36.741300	-4.254250	-1.082420
S	-35.697400	-3.151800	-2.005790
C	-37.653400	-5.342250	0.762104
C	-38.528100	-5.728870	-0.209464
S	-38.099700	-5.099190	-1.768090
C	-35.528800	-4.147690	2.452460
C	-35.194700	-5.375010	3.030870
C	-35.192400	-5.510320	4.417780
C	-35.520700	-4.423170	5.227310
C	-35.852100	-3.199070	4.648740
C	-35.857200	-3.060200	3.261690
C	-26.706600	-5.644230	-2.427250
C	-26.698600	-6.039430	-3.764000

C	-27.021400	-5.124650	-4.765080
C	-27.350100	-3.811490	-4.429570
C	-27.355800	-3.411400	-3.094780
H	13.487800	0.698332	1.914240
H	8.791680	2.756070	1.485890
H	10.026200	-1.005380	1.673950
H	9.632120	-1.448970	4.090430
H	10.175100	0.293536	5.770780
H	11.111800	2.470450	5.037150
H	11.507400	2.900680	2.625890
H	17.196300	1.229540	-1.080220
H	6.209870	4.367380	-2.195810
H	22.110100	-0.383900	-0.978122
H	1.382970	6.028080	-2.015540
H	19.343000	-0.446528	-2.338440
H	19.809500	0.793499	-4.437220
H	20.644900	3.127290	-4.337660
H	21.009300	4.218690	-2.140260
H	20.535000	2.967700	-0.041434
H	3.330750	3.860410	-2.508150
H	3.099180	3.467930	-4.947150
H	3.646910	5.279040	-6.551650
H	4.425230	7.480580	-5.713880
H	4.654980	7.863910	-3.265950
H	24.765100	-2.763050	2.168790
H	29.802600	-3.762770	1.835690
H	32.834200	-4.344280	-1.793330
H	37.797200	-5.640150	-1.460780
H	39.539900	-5.847440	0.491324
H	36.025600	-2.533120	-3.171110
H	35.959200	-3.346210	-5.522070
H	35.390200	-5.714220	-5.994560
H	34.888700	-7.263190	-4.122520

H	34.956600	-6.442060	-1.782050
H	26.648700	-6.117630	2.308090
H	26.728300	-6.419320	4.776960
H	27.280600	-4.493240	6.239500
H	27.748000	-2.272550	5.237210
H	27.658000	-1.980030	2.774840
H	-13.502900	0.741693	-1.931390
H	-8.801820	2.802190	-1.549730
H	-10.014100	-0.931173	-1.585360
H	-9.594860	-1.472790	-3.977540
H	-10.153900	0.185561	-5.735910
H	-11.129400	2.377360	-5.104110
H	-11.547500	2.906350	-2.716420
H	-17.248200	1.481950	0.954207
H	-6.235260	4.554320	2.072030
H	-22.161400	-0.116246	0.911955
H	-1.386840	6.135150	1.840250
H	-20.417300	3.198580	-0.306540
H	-20.886000	4.648800	1.660450
H	-20.687000	3.722850	3.953280
H	-20.017600	1.356170	4.278060
H	-19.545900	-0.079934	2.310450
H	-3.366660	4.027820	2.418470
H	-3.153010	3.733900	4.873010
H	-3.685090	5.617160	6.397840
H	-4.429460	7.791930	5.465110
H	-4.641500	8.076260	3.001980
H	-24.708200	-2.931840	-2.002650
H	-29.717700	-4.076270	-1.657050
H	-32.849100	-4.092240	1.964540
H	-37.743400	-5.642360	1.795930
H	-39.402000	-6.353610	-0.109832
H	-34.938500	-6.215170	2.395700

H -34.933200 -6.463130 4.864680

H -35.517500 -4.530310 6.305880

H -36.107500 -2.352220 5.275050

H -36.114200 -2.115360 2.797800

H -26.460600 -6.344680 -1.638100

H -26.442600 -7.060620 -4.021330

H -27.016700 -5.433320 -5.804050

H -27.600100 -3.097620 -5.205830

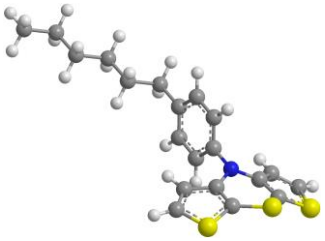
H -27.606800 -2.391540 -2.826830

SCF Done: E(RB3LYP) = -17873.2093630 A.U. after 6 cycles

E(HOMO) = -4.759 eV

E(LUMO) = -1.899 eV

11.16 Computed xyz-coordinates and excitation energies of dithienothiazine monomer **1a**



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N -1.79305100 -0.10301900 0.23968800

C -2.79530900 -1.07379400 0.02207000

C -4.13468700 -0.79912800 0.16721300

S -4.78150500 0.73114300 0.79669400

S -3.57289000 3.39357000 -0.23644500

C -1.87040800 3.48758400 -0.55438200

C -1.24757800 2.28556100 -0.38503400

C -2.56564100 -2.42076100 -0.41001900

C -3.72168400 -3.12299600 -0.58863900

S -5.12862800 -2.16186900 -0.26461300

C -0.40824100 -0.49015400 0.17611900

C 0.24116900 -0.65151500 -1.04963000

C 1.58281100 -1.02422000 -1.08411200

C	2.30477500	-1.24390500	0.09616500
C	1.63673100	-1.08461200	1.31596600
C	0.29460400	-0.71130700	1.35971500
C	3.77312400	-1.60054000	0.05409400
C	4.68996900	-0.36125900	0.05443200
C	6.18053600	-0.71408500	0.00812600
C	7.09438000	0.51656500	0.00721900
C	8.58819600	0.17485000	-0.04011200
C	9.49040000	1.41272500	-0.04242600
H	-1.43451300	4.42877300	-0.85218200
H	-0.18991100	2.13620800	-0.54745100
H	-1.58371800	-2.84032400	-0.57530000
H	-0.30448800	-0.48763200	-1.97218300
H	2.07495200	-1.14906700	-2.04333200
H	2.17079800	-1.25625500	2.24500600
H	-0.21500300	-0.59190200	2.30893900
H	4.02099000	-2.22854300	0.91624100
H	3.97906000	-2.19618800	-0.84142100
H	4.43591400	0.27138300	-0.80443900
H	4.48187600	0.23685900	0.94958500
H	6.42930700	-1.34972100	0.86764800
H	6.38270100	-1.31622500	-0.88700400
H	6.84332500	1.15246100	-0.85172400
H	6.89087000	1.11852400	0.90237000
H	8.84046300	-0.45899600	0.81873500
H	8.79209900	-0.42703500	-0.93409800
H	10.54813500	1.13647800	-0.07584000
H	9.28481500	2.04867400	-0.90946000
H	9.33236500	2.01726900	0.85642500
H	-3.83708300	-4.15060700	-0.89723900

SCF Done: E(RB3LYP) = -1788.39791194 A.U. after 1 cycles

E(HOMO) = -5.012 eV

E(LUMO) = -1.077 eV

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1096 eV 398.71 nm f=0.0047 <S**2>=0.000

98 -> 99 0.69271

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2024.23286014

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6147 eV 343.00 nm f=0.0001 <S**2>=0.000

98 ->100 0.69576

Excited State 3: Singlet-A 3.7823 eV 327.80 nm f=0.0021 <S**2>=0.000

98 -> 99 -0.11556

98 ->100 0.10174

98 ->102 0.65899

98 ->103 -0.16126

Excited State 4: Singlet-A 3.7971 eV 326.52 nm f=0.0806 <S**2>=0.000

98 ->101 0.68893

Excited State 5: Singlet-A 4.0824 eV 303.70 nm f=0.0003 <S**2>=0.000

98 ->102 0.17868

98 ->103 0.67437

Excited State 6: Singlet-A 4.2391 eV 292.48 nm f=0.0021 <S**2>=0.000

98 ->104 0.70181

Excited State 7: Singlet-A 4.7108 eV 263.19 nm f=0.0067 <S**2>=0.000

97 -> 99 0.26403

98 ->105 0.63369

Excited State 8: Singlet-A 4.7890 eV 258.90 nm f=0.0006 <S**2>=0.000

98 ->106 0.69461

Excited State 9: Singlet-A 4.8640 eV 254.90 nm f=0.1890 <S**2>=0.000

97 -> 99 0.63437

98 ->105 -0.25998

98 ->109 0.10133

Excited State 10: Singlet-A 5.1742 eV 239.62 nm f=0.0303 <S**2>=0.000

93 ->100 0.17967

94 ->100 0.25268

95 -> 99 0.50463

95 ->102 -0.20182

96 -> 99 0.28368

Excited State 11: Singlet-A 5.1984 eV 238.50 nm f=0.0178 <S**2>=0.000

94 ->100 -0.11274

95 -> 99 -0.23121

96 -> 99 0.62290

Excited State 12: Singlet-A 5.2387 eV 236.67 nm f=0.0037 <S**2>=0.000

97 ->100 0.69246

Excited State 13: Singlet-A 5.3443 eV 231.99 nm f=0.0451 <S**2>=0.000

94 -> 99 0.12887

97 ->101 0.66639

Excited State 14: Singlet-A 5.3953 eV 229.80 nm f=0.0015 <S**2>=0.000

97 ->102 0.65320

98 ->109 0.19982

Excited State 15: Singlet-A 5.4723 eV 226.57 nm f=0.1012 <S**2>=0.000

97 ->102 -0.17937

97 ->103 0.22415

98 ->109 0.61837

Excited State 16: Singlet-A 5.4928 eV 225.72 nm f=0.0048 <S**2>=0.000

96 ->100 0.68988

Excited State 17: Singlet-A 5.5038 eV 225.27 nm f=0.0265 <S**2>=0.000

94 -> 99 0.51175

94 ->100 0.12360

95 -> 99 -0.29789

95 ->100 -0.11413

95 ->102 -0.26917

96 ->100 0.12219

Excited State 18: Singlet-A 5.5543 eV 223.22 nm f=0.1203 <S**2>=0.000

93 -> 99 -0.23086

93 ->100 -0.13517

94 -> 99 0.36607

94 ->100 -0.20567

95 -> 99 0.27207

95 ->102 0.33600

98 ->107 -0.10182

Excited State 19: Singlet-A 5.6044 eV 221.23 nm f=0.1197 <S**2>=0.000

96 ->101 0.62476

97 ->103 -0.25931

98 ->109 0.11073

Excited State 20: Singlet-A 5.6375 eV 219.93 nm f=0.0178 <S**2>=0.000

94 -> 99 0.10540

98 ->107 0.60844

98 ->108 -0.25660

98 ->111 0.10095

Excited State 21: Singlet-A 5.6529 eV 219.33 nm f=0.1653 <S**2>=0.000

94 ->104 0.11628

96 ->101 0.25796

96 ->104 -0.12000

97 ->102 0.15034

97 ->103 0.55684

98 ->109 -0.16745

Excited State 22: Singlet-A 5.6655 eV 218.84 nm f=0.0025 <S**2>=0.000

94 ->103 0.11116

96 ->102 0.30094

96 ->103 -0.15587

97 ->104 0.54608

Excited State 23: Singlet-A 5.6812 eV 218.23 nm f=0.0087 <S**2>=0.000

96 ->102 0.60201

97 ->104 -0.30671

Excited State 24: Singlet-A 5.7560 eV 215.40 nm f=0.0358 <S**2>=0.000

93 -> 99 0.56585

94 ->100 -0.15045

95 ->100 -0.26238

95 ->102 0.19125

97 ->104 -0.13342

Excited State 25: Singlet-A 5.7870 eV 214.25 nm f=0.0021 <S**2>=0.000

95 ->101 0.70343

Excited State 26: Singlet-A 5.8915 eV 210.45 nm f=0.2809 <S**2>=0.000

93 ->102 -0.10916

94 -> 99 -0.13251

94 ->102 -0.13433

95 ->100 -0.35360

96 ->103 0.35807

98 ->107 0.11496

98 ->110 -0.24232

98 ->112 -0.27485

Excited State 27: Singlet-A 5.9395 eV 208.75 nm f=0.0913 <S**2>=0.000

93 -> 99 0.21459

94 ->102 0.30206

95 ->100 0.34649

96 ->103 0.44238

Excited State 28: Singlet-A 5.9719 eV 207.61 nm f=0.0022 <S**2>=0.000

94 ->102 0.12680

95 ->100 0.12664

96 ->103 -0.31176

98 ->107 0.22147

98 ->108 0.38953

98 ->110 -0.29655

98 ->111 -0.12595

98 ->112 -0.17517

Excited State 29: Singlet-A 5.9788 eV 207.37 nm f=0.0387 <S**2>=0.000

94 ->101 0.66407

96 ->104 0.13392

97 ->105 0.11709

Excited State 30: Singlet-A 5.9999 eV 206.64 nm f=0.0101 <S**2>=0.000

94 ->101 -0.14672

96 ->104 0.64907

97 ->103 0.10290

97 ->105 0.10611

Excited State 31: Singlet-A 6.0154 eV 206.11 nm f=0.0072 <S**2>=0.000

94 ->102 -0.17845

96 ->103 0.12277

98 ->107 0.17941

98 ->108 0.42141

98 ->110 0.20453

98 ->112 0.39064

Excited State 32: Singlet-A 6.0286 eV 205.66 nm f=0.0251 <S**2>=0.000

93 ->100 0.47399

94 ->100 -0.46535

95 ->102 -0.13755

97 ->104 -0.10244

Excited State 33: Singlet-A 6.1772 eV 200.71 nm f=0.0017 <S**2>=0.000

93 ->101 0.45128

93 ->104 -0.16611

94 ->104 0.23117

96 ->104 0.10616

97 ->103 -0.12046

97 ->105 -0.39798

Excited State 34: Singlet-A 6.1914 eV 200.25 nm f=0.1334 <S**2>=0.000

93 ->102 -0.42350

94 ->102 0.44275

95 ->100 -0.16637

98 ->110 0.13763

98 ->114 -0.11359

Excited State 35: Singlet-A 6.2303 eV 199.00 nm f=0.0089 <S**2>=0.000

93 ->101 0.50734

93 ->104 0.14748

94 ->104 -0.20132

96 ->106 -0.14180

97 ->105 0.31016

98 ->118 -0.12067

Excited State 36: Singlet-A 6.2536 eV 198.26 nm f=0.0021 <S**2>=0.000

98 ->108 0.16284

98 ->110 0.50057

98 ->112 -0.41749

98 ->116 -0.11604

Excited State 37: Singlet-A 6.2612 eV 198.02 nm f=0.0013 <S**2>=0.000

98 ->108 0.20646

98 ->111 0.64329

Excited State 38: Singlet-A 6.3839 eV 194.21 nm f=0.0596 <S**2>=0.000

93 ->101 0.12656

96 ->106 0.36779

98 ->114 -0.27935

98 ->115 0.33539

98 ->118 0.34191

Excited State 39: Singlet-A 6.4091 eV 193.45 nm f=0.0022 <S**2>=0.000

93 ->103 -0.13367

94 ->103 0.23412

95 ->103 0.10345

96 ->105 -0.11108

97 ->106 0.59966

Excited State 40: Singlet-A 6.4489 eV 192.26 nm f=0.0149 <S**2>=0.000

94 ->103 0.15535

97 ->106 -0.20524

98 ->113 0.39936

98 ->115 -0.30155

98 ->117 -0.12282

98 ->118 0.31749

Excited State 41: Singlet-A 6.4583 eV 191.98 nm f=0.0080 <S**2>=0.000

93 ->103 -0.19230

94 ->103 0.36110

95 ->103 0.23414

97 ->104 -0.11727

97 ->106 -0.28160

98 ->113 -0.17260

98 ->114 -0.26665

98 ->117 0.12069

98 ->118 -0.18332

Excited State 42: Singlet-A 6.4922 eV 190.97 nm f=0.1496 <S**2>=0.000

93 ->102 -0.16178

94 ->103 0.20019

95 ->103 0.22359

96 ->105 0.46121

98 ->114 0.27108

98 ->115 0.15472

98 ->116 -0.13840

Excited State 43: Singlet-A 6.5298 eV 189.87 nm f=0.0051 <S**2>=0.000

93 ->103 0.12997

94 ->103 -0.27574

95 ->103 0.58701

96 ->105 -0.17434

Excited State 44: Singlet-A 6.5459 eV 189.41 nm f=0.0104 <S**2>=0.000

92 -> 99 0.65010

92 ->102 0.13572

Excited State 45: Singlet-A 6.5581 eV 189.06 nm f=0.0901 <S**2>=0.000

93 ->102 0.14081

94 ->103 -0.11082

96 ->105 0.26773

98 ->113 0.43251

98 ->114 -0.27651

98 ->115 0.13509

98 ->117 0.11709

98 ->118 -0.19337

Excited State 46: Singlet-A 6.5766 eV 188.52 nm f=0.3355 <S**2>=0.000

93 ->102 0.26369

94 ->103 -0.10907

96 ->105 0.33916

96 ->109 -0.10540

98 ->113 -0.28604

98 ->114 -0.11408

98 ->115 -0.33128

98 ->116 0.15024

98 ->118 0.10190

Excited State 47: Singlet-A 6.6112 eV 187.54 nm f=0.0478 <S**2>=0.000

96 ->106 0.55051

98 ->113 0.10623

98 ->114 0.14207

98 ->115 -0.14402

98 ->118 -0.35112

Excited State 48: Singlet-A 6.6317 eV 186.96 nm f=0.0084 <S**2>=0.000

95 ->104 0.66377

97 ->105 0.18179

Excited State 49: Singlet-A 6.6783 eV 185.65 nm f=0.0281 <S**2>=0.000

93 ->100 -0.11904

93 ->104 -0.17967

94 ->104 0.48337

95 ->102 -0.11558

95 ->104 -0.18471

97 ->105 0.36367

Excited State 50: Singlet-A 6.6837 eV 185.50 nm f=0.2766 <S**2>=0.000

93 ->100 0.37048

93 ->103 -0.16709

94 ->100 0.24760

94 ->104 0.14730

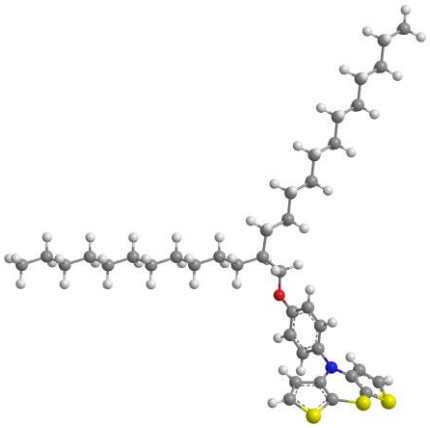
95 -> 99 -0.10532

95 ->102 0.36328

95 ->103 0.11458

97 ->105 0.11373

11.17 Computed xyz-coordinates and excitation energies of dithienothiazine monomer **1c**



C	8.515545	-1.431205	-1.099820
C	7.249409	-0.953752	-0.860249
N	6.309529	-1.653291	-0.071553
C	6.814350	-2.517918	0.924598
C	8.046780	-3.118265	0.827155
S	9.084050	-3.043124	-0.613829
S	9.478620	-0.299356	-2.006612
C	8.139195	0.798875	-2.110121
C	7.039675	0.334264	-1.451773
C	6.158013	-2.835783	2.158029

C	6.901988	-3.651186	2.958002
S	8.439758	-4.036807	2.252689
C	4.969410	-1.145697	0.042960
C	4.663129	-0.096877	0.919194
C	3.366423	0.383467	1.012382
C	2.346084	-0.175112	0.227140
C	2.646724	-1.224264	-0.648537
C	3.955739	-1.700049	-0.731763
O	1.111088	0.367253	0.388846
C	0.020260	-0.121919	-0.408239
C	-1.223434	0.704945	-0.084056
C	-1.035509	2.169664	-0.528860
C	-2.467850	0.052609	-0.722590
C	-2.023378	3.159940	0.100279
C	-1.805517	4.606303	-0.359957
C	-2.789656	5.601155	0.265918
C	-2.575362	7.049509	-0.188045
C	-3.570043	8.038844	0.430035
C	-3.357856	9.488875	-0.019538
C	-4.358751	10.474442	0.594571
C	-4.148116	11.925346	0.147760
C	-5.151090	12.909793	0.760246
C	-4.933482	14.356807	0.308341
C	-3.000258	-1.191867	0.002005
C	-4.237894	-1.792658	-0.674348
C	-4.816032	-3.005724	0.063763
C	-6.048976	-3.606502	-0.620524
C	-6.646412	-4.804479	0.126862
C	-7.874484	-5.407319	-0.564394
C	-8.483756	-6.595810	0.188537
C	-9.707633	-7.201059	-0.508139
C	-10.323411	-8.384337	0.247279
C	-11.544282	-8.992503	-0.452250

C	-12.154518	-10.171953	0.310809
H	8.251502	1.726168	-2.649978
H	6.108756	0.879113	-1.390249
H	5.175759	-2.474692	2.425928
H	6.646042	-4.049476	3.927402
H	5.446653	0.341776	1.526437
H	3.118081	1.194548	1.686226
H	1.880418	-1.675320	-1.263240
H	4.192358	-2.512495	-1.408702
H	0.272002	-0.027125	-1.471989
H	-0.139054	-1.181212	-0.183597
H	-1.342613	0.689107	1.007198
H	-0.018565	2.484538	-0.274691
H	-1.111094	2.219192	-1.623665
H	-3.271848	0.793774	-0.762123
H	-2.242191	-0.198019	-1.768008
H	-3.054222	2.867245	-0.131081
H	-1.929785	3.111248	1.192756
H	-0.778948	4.911835	-0.119831
H	-1.890039	4.654439	-1.453337
H	-3.815284	5.294878	0.022070
H	-2.708539	5.549885	1.359437
H	-1.552856	7.359777	0.063484
H	-2.648690	7.100056	-1.282180
H	-4.591928	7.728244	0.176145
H	-3.498961	7.986087	1.524215
H	-2.337807	9.801790	0.238668
H	-3.424736	9.541436	-1.113990
H	-5.378492	10.161394	0.335110
H	-4.293030	10.420646	1.689052
H	-3.129319	12.240622	0.408734
H	-4.212633	11.980398	-0.946871
H	-6.169046	12.595436	0.499463

H -5.086578 12.855678 1.853823

H -5.664061 15.031892 0.762829

H -3.935599 14.711176 0.585907

H -5.026335 14.449255 -0.778494

H -2.221602 -1.960969 0.065460

H -3.248251 -0.922296 1.036357

H -3.983129 -2.081693 -1.702154

H -5.012799 -1.019742 -0.758697

H -4.041220 -3.777864 0.155916

H -5.078199 -2.712964 1.088664

H -5.782216 -3.912871 -1.640308

H -6.816839 -2.829242 -0.727248

H -5.878180 -5.580421 0.240294

H -6.919736 -4.495402 1.144091

H -7.598156 -5.725016 -1.578159

H -8.638318 -4.628426 -0.687115

H -7.719414 -7.373377 0.316253

H -8.765215 -6.276348 1.200328

H -9.424367 -7.525254 -1.517937

H -10.469629 -6.422019 -0.641025

H -9.561559 -9.163094 0.383707

H -10.610872 -8.059925 1.255977

H -11.256580 -9.318858 -1.459070

H -12.305098 -8.214520 -0.590206

H -13.021408 -10.582748 -0.214310

H -11.426978 -10.980433 0.434983

H -12.483935 -9.867802 1.309466

SCF Done: E(RB3LYP) = -2846.73803084 A.U. after 6 cycles

E (HOMO) = -4.974 eV

E (LUMO) = -1.047 eV

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1207 eV 397.29 nm f=0.0044 <S**2>=0.000

178 -> 179 0.69058

178 -> 181 0.10323

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2846.62334562

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.7196 eV 333.33 nm f=0.0009 <S**2>=0.000

178 -> 179 -0.11956

178 -> 180 -0.14758

178 -> 181 0.66699

178 -> 183 -0.11984

Excited State 3: Singlet-A 3.8041 eV 325.92 nm f=0.0847 <S**2>=0.000

178 -> 180 0.67939

178 -> 181 0.14808

Excited State 4: Singlet-A 3.8897 eV 318.75 nm f=0.0004 <S**2>=0.000

178 -> 182 0.69502

Excited State 5: Singlet-A 4.0907 eV 303.09 nm f=0.0002 <S**2>=0.000

178 -> 181 0.13376

178 -> 183 0.67849

Excited State 6: Singlet-A 4.2431 eV 292.20 nm f=0.0021 <S**2>=0.000

178 -> 184 0.70180

Excited State 7: Singlet-A 4.7228 eV 262.52 nm f=0.0082 <S**2>=0.000

176 -> 179 0.26737

178 -> 185 0.62648

Excited State 8: Singlet-A 4.7737 eV 259.72 nm f=0.0250 <S**2>=0.000

173 -> 182 0.11305

177 -> 179 0.67143

177 -> 181 -0.11398

Excited State 9: Singlet-A 4.8030 eV 258.14 nm f=0.0008 <S**2>=0.000

178 -> 186 0.69437

Excited State 10: Singlet-A 4.8725 eV 254.46 nm f=0.1850 <S**2>=0.000

176 -> 179 0.63090

178 -> 185 -0.26799

Excited State 11: Singlet-A 5.1807 eV 239.32 nm f=0.0402 <S**2>=0.000

173 -> 182 -0.15996

174 -> 182 0.12925

175 -> 179 -0.17816

177 -> 179 0.16413

177 -> 180 -0.11305

177 -> 181 0.58553

177 -> 182 0.15480

Excited State 12: Singlet-A 5.1955 eV 238.64 nm f=0.0294 <S**2>=0.000

175 -> 179 0.66274

177 -> 181 0.15626

Excited State 13: Singlet-A 5.2835 eV 234.66 nm f=0.0016 <S**2>=0.000

177 -> 180 0.69159

177 -> 181 0.13048

Excited State 14: Singlet-A 5.3319 eV 232.53 nm f=0.0140 <S**2>=0.000

176 -> 180 -0.30161

176 -> 181 0.60989

Excited State 15: Singlet-A 5.3500 eV 231.75 nm f=0.0516 <S**2>=0.000

174 -> 179 -0.12556

176 -> 180 0.59572

176 -> 181 0.30327

Excited State 16: Singlet-A 5.4652 eV 226.86 nm f=0.0314 <S**2>=0.000

176 -> 182 0.41324

176 -> 183 0.21643

178 -> 192 0.49004

Excited State 17: Singlet-A 5.5242 eV 224.44 nm f=0.0552 <S**2>=0.000

175 -> 180 -0.12686

176 -> 182 0.51466

178 -> 192 -0.43177

Excited State 18: Singlet-A 5.5498 eV 223.40 nm f=0.0654 <S**2>=0.000

174 -> 179 0.61733

175 -> 181 0.15258

175 -> 183 -0.12390

177 -> 182 0.12439

Excited State 19: Singlet-A 5.5957 eV 221.57 nm f=0.0377 <S**2>=0.000

174 -> 179 -0.15176

175 -> 180 -0.31065

175 -> 181 0.57742

Excited State 20: Singlet-A 5.6092 eV 221.04 nm f=0.1757 <S**2>=0.000

175 -> 180 0.56901

175 -> 181 0.31199

176 -> 182 0.14856

176 -> 183 -0.14026

Excited State 21: Singlet-A 5.6360 eV 219.99 nm f=0.4138 <S**2>=0.000

173 -> 179 -0.28718

174 -> 181 -0.13901

176 -> 184 0.15596

177 -> 181 -0.15593

177 -> 182 0.55271

Excited State 22: Singlet-A 5.6653 eV 218.85 nm f=0.0988 <S**2>=0.000

174 -> 184 0.13260

175 -> 180 0.14796

175 -> 184 0.11837

176 -> 181 0.13879

176 -> 182 -0.10032

176 -> 183 0.59125

178 -> 192 -0.17239

Excited State 23: Singlet-A 5.6736 eV 218.53 nm f=0.0348 <S**2>=0.000

174 -> 179 0.10208

174 -> 183 0.14074

175 -> 181 0.12187

176 -> 184 0.59788

177 -> 182 -0.13665

Excited State 24: Singlet-A 5.6843 eV 218.12 nm f=0.0032 <S**2>=0.000

176 -> 184 -0.10392

178 -> 187 0.51803

178 -> 189 -0.22530

178 -> 190 0.15164

178 -> 191 0.26292

178 -> 193 -0.10316

178 -> 194 -0.16218

178 -> 196 0.12633

Excited State 25: Singlet-A 5.7653 eV 215.05 nm f=0.0122 <S**2>=0.000

175 -> 182 0.68477

Excited State 26: Singlet-A 5.8566 eV 211.70 nm f=0.1742 <S**2>=0.000

173 -> 179 0.38724

174 -> 179 -0.16455

175 -> 183 -0.24317

177 -> 182 0.10884

178 -> 187 0.21691

178 -> 191 -0.12943

178 -> 194 0.15474

178 -> 195 -0.10540

178 -> 197 0.17208

178 -> 199 -0.16805

178 -> 200 -0.18180

Excited State 27: Singlet-A 5.8976 eV 210.23 nm f=0.0156 <S**2>=0.000

173 -> 179 0.40635

174 -> 181 -0.17407

177 -> 182 0.12363

178 -> 187 -0.32408

178 -> 189 -0.10972

178 -> 191 0.22882

178 -> 193 -0.11454

178 -> 194 -0.17745

178 -> 195 0.11258

178 -> 196 0.11093

Excited State 28: Singlet-A 5.9362 eV 208.86 nm f=0.0010 <S**2>=0.000

173 -> 179 0.18436

174 -> 181 -0.13196

175 -> 183 0.55587

178 -> 187 0.17648

178 -> 189 0.12396

178 -> 191 -0.14952

Excited State 29: Singlet-A 5.9640 eV 207.89 nm f=0.0095 <S**2>=0.000

175 -> 183 -0.17136

178 -> 187 0.16281

178 -> 188 0.52029

178 -> 189 0.17307

178 -> 190 -0.25042

178 -> 197 -0.12111

178 -> 199 0.11825

178 -> 200 0.15198

Excited State 30: Singlet-A 5.9913 eV 206.94 nm f=0.0080 <S**2>=0.000

175 -> 184 0.55451

176 -> 183 -0.10188

176 -> 185 -0.10816

178 -> 188 -0.21847

178 -> 197 -0.10332

178 -> 199 0.11332

178 -> 200 0.16156

Excited State 31: Singlet-A 5.9922 eV 206.91 nm f=0.0227 <S**2>=0.000

174 -> 181 0.11303

175 -> 183 0.14612

175 -> 184 0.34766

177 -> 183 -0.13456

178 -> 188 0.33649

178 -> 189 -0.15915

178 -> 191 0.12152

178 -> 197 0.16628

178 -> 199 -0.18296

178 -> 200 -0.25684

Excited State 32: Singlet-A 6.0166 eV 206.07 nm f=0.0279 <S**2>=0.000

174 -> 180 0.51028

177 -> 183 -0.42579

Excited State 33: Singlet-A 6.0205 eV 205.94 nm f=0.0222 <S**2>=0.000

174 -> 180 0.40552

177 -> 183 0.52050

Excited State 34: Singlet-A 6.0606 eV 204.58 nm f=0.0092 <S**2>=0.000

174 -> 181 0.12791

178 -> 189 0.57389

178 -> 191 0.17729

178 -> 193 -0.13142

178 -> 194 -0.15347

178 -> 200 -0.20818

Excited State 35: Singlet-A 6.0938 eV 203.46 nm f=0.0047 <S**2>=0.000

174 -> 181 -0.13186

178 -> 188 0.22243

178 -> 189 0.11131

178 -> 190 0.58486

178 -> 194 0.20111

178 -> 200 0.10733

Excited State 36: Singlet-A 6.1195 eV 202.60 nm f=0.0445 <S**2>=0.000

173 -> 181 0.24392

174 -> 180 -0.11543

174 -> 181 0.40787

177 -> 184 0.41002

Excited State 37: Singlet-A 6.1219 eV 202.52 nm f=0.0340 <S**2>=0.000

173 -> 181 -0.17409

174 -> 181 -0.33092

176 -> 184 -0.10009

177 -> 184 0.52706

Excited State 38: Singlet-A 6.1515 eV 201.55 nm f=0.0007 <S**2>=0.000

178 -> 190 -0.12483

178 -> 191 0.44143

178 -> 194 0.47962

178 -> 196 -0.10128

178 -> 200 0.15237

Excited State 39: Singlet-A 6.2095 eV 199.67 nm f=0.0029 <S**2>=0.000

173 -> 180 -0.19601

173 -> 184 -0.15073

174 -> 180 0.10911

174 -> 184 -0.32571

175 -> 184 0.12976

176 -> 183 0.12245

176 -> 185 0.47579

177 -> 184 0.15249

Excited State 40: Singlet-A 6.2293 eV 199.03 nm f=0.0001 <S**2>=0.000

178 -> 191 0.23194

178 -> 193 0.59251

178 -> 194 -0.19976

178 -> 195 -0.15639

178 -> 200 0.10622

Excited State 41: Singlet-A 6.2534 eV 198.27 nm f=0.0003 <S**2>=0.000

178 -> 191 -0.12430

178 -> 193 0.28537

178 -> 194 0.19660

178 -> 195 0.48203

178 -> 196 0.31423

178 -> 200 -0.10546

Excited State 42: Singlet-A 6.2707 eV 197.72 nm f=0.0017 <S**2>=0.000

173 -> 180 0.64085

175 -> 186 0.13669

176 -> 185 0.11652

Excited State 43: Singlet-A 6.2712 eV 197.70 nm f=0.0143 <S**2>=0.000

173 -> 182 0.23212

174 -> 182 0.63446

Excited State 44: Singlet-A 6.3270 eV 195.96 nm f=0.0004 <S**2>=0.000

178 -> 190 -0.11400

178 -> 194 0.11553

178 -> 195 -0.40582

178 -> 196 0.50200

178 -> 203 0.17312

Excited State 45: Singlet-A 6.3892 eV 194.05 nm f=0.0616 <S**2>=0.000

173 -> 180 -0.14053

175 -> 186 0.36882

178 -> 208 0.39655

178 -> 210 0.19482

178 -> 211 -0.30631

Excited State 46: Singlet-A 6.4215 eV 193.08 nm f=0.0012 <S**2>=0.000

174 -> 183 0.21426

175 -> 185 0.11896

176 -> 186 0.62481

178 -> 207 -0.10666

Excited State 47: Singlet-A 6.4531 eV 192.13 nm f=0.0123 <S**2>=0.000

174 -> 183 -0.10511

176 -> 186 0.11404

178 -> 195 0.11273

178 -> 196 0.11846

178 -> 197 0.53886

178 -> 200 0.25130

178 -> 205 0.11059

178 -> 207 0.14704

Excited State 48: Singlet-A 6.4703 eV 191.62 nm f=0.0750 <S**2>=0.000

173 -> 181 0.13996

173 -> 183 -0.12242

174 -> 183 -0.32225

175 -> 185 -0.20033

176 -> 186 0.23026

178 -> 197 -0.20638

178 -> 198 -0.20733

178 -> 199 -0.10832

178 -> 207 0.32406

Excited State 49: Singlet-A 6.4808 eV 191.31 nm f=0.0024 <S**2>=0.000

174 -> 183 -0.10028

178 -> 197 -0.12750

178 -> 198 0.64654

178 -> 199 -0.12021

Excited State 50: Singlet-A 6.4886 eV 191.08 nm f=0.0023 <S**2>=0.000

178 -> 198 -0.13966

178 -> 199 -0.24483

178 -> 200 0.13501

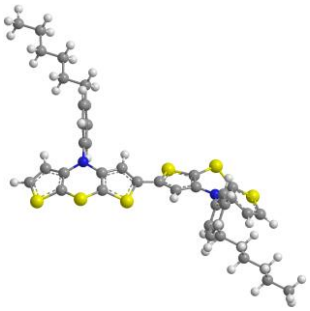
178 -> 207 -0.13066

178 -> 208 0.40589

178 -> 210 -0.18160

178 -> 211 0.37512

11.18 Computed xyz-coordinates and excitation energies of dithienothiazine dimer **4** (crescent trans conformer)



C	3.385420	4.467990	-1.104600
C	4.195820	3.397270	-0.813448
N	3.719700	2.237940	-0.161931
C	2.354480	1.919950	-0.315235
C	1.399020	2.875430	-0.573448
S	1.700340	4.623860	-0.563288
S	4.225860	5.695680	-2.007900
C	5.696110	4.777520	-1.938930
C	5.531270	3.586800	-1.296140
C	1.800400	0.607656	-0.251207
C	0.443362	0.571429	-0.470457
S	-0.176844	2.177590	-0.812905
C	4.652140	1.208480	0.214659
C	5.115980	0.280059	-0.719773
C	6.024040	-0.701926	-0.333085
C	6.489360	-0.779407	0.985466
C	6.010290	0.155690	1.910030
C	5.101060	1.141070	1.532610
C	-1.399060	-2.875420	-0.573605
C	-2.354510	-1.919960	-0.315294
N	-3.719720	-2.237960	-0.161966
C	-4.195870	-3.397240	-0.813548
C	-3.385480	-4.467940	-1.104800
S	-1.700380	-4.623850	-0.563558
S	0.176796	-2.177560	-0.813073

C	-0.443395	-0.571427	-0.470483
C	-1.800430	-0.607669	-0.251193
C	-5.531340	-3.586730	-1.296210
C	-5.696200	-4.777410	-1.939070
S	-4.225950	-5.695570	-2.008150
C	-4.652140	-1.208510	0.214720
C	-5.100970	-1.141130	1.532710
C	-6.010160	-0.155766	1.910220
C	-6.489300	0.779357	0.985720
C	-6.024080	0.701911	-0.332868
C	-5.116060	-0.280062	-0.719652
C	-7.513840	1.815620	1.388010
C	7.513920	-1.815680	1.387650
C	8.962730	-1.319760	1.212910
C	10.011800	-2.360910	1.618470
C	11.452400	-1.866550	1.446870
C	12.510400	-2.900860	1.849110
C	13.945600	-2.396010	1.674230
C	-8.962660	1.319710	1.213330
C	-10.011700	2.360860	1.618970
C	-11.452300	1.866510	1.447450
C	-12.510300	2.900820	1.849760
C	-13.945500	2.395980	1.674950
H	6.593810	5.176260	-2.385010
H	6.326480	2.868080	-1.161520
H	2.381980	-0.273340	-0.020032
H	4.765180	0.328528	-1.744470
H	6.375120	-1.420210	-1.066760
H	6.349820	0.111460	2.939660
H	4.733160	1.860660	2.254600
H	-2.382000	0.273311	-0.019936
H	-6.326550	-2.868020	-1.161500
H	-6.593920	-5.176120	-2.385140

H -4.733010 -1.860740 2.254650

H -6.349620 -0.111563 2.939880

H -6.375220 1.420220 -1.066490

H -4.765330 -0.328500 -1.744370

H -7.356250 2.098480 2.434050

H -7.371030 2.721680 0.789974

H 7.356400 -2.098580 2.433690

H 7.371080 -2.721720 0.789588

H 9.101920 -0.408429 1.806510

H 9.117830 -1.031730 0.166364

H 9.849770 -2.650040 2.664700

H 9.867370 -3.271660 1.023260

H 11.595300 -0.955208 2.041910

H 11.612700 -1.575720 0.400623

H 12.350400 -3.191670 2.894400

H 12.368600 -3.811260 1.254160

H 14.675000 -3.156310 1.967040

H 14.145000 -2.127340 0.631976

H 14.128300 -1.506620 2.285630

H -9.101820 0.408364 1.806910

H -9.117820 1.031710 0.166785

H -9.849610 2.649960 2.665210

H -9.867300 3.271620 1.023780

H -11.595200 0.955157 2.042480

H -11.612700 1.575690 0.401209

H -12.350200 3.191610 2.895040

H -12.368500 3.811230 1.254810

H -14.128200 1.506580 2.286360

H -14.674900 3.156280 1.967810

H -14.144900 2.127320 0.632710

SCF Done: E(RB3LYP) = -4047.49790764 A.U. after 1 cycles

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5463 eV 486.92 nm f=0.2834 <S**2>=0.000

195 -> 196 0.69434

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -4047.40415378

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.7749 eV 446.81 nm f=0.0004 <S**2>=0.000

194 -> 196 0.68664

195 -> 197 0.13807

Excited State 3: Singlet-A 3.2268 eV 384.23 nm f=0.0000 <S**2>=0.000

194 -> 196 -0.15309

194 -> 198 -0.21281

195 -> 197 0.63871

Excited State 4: Singlet-A 3.3361 eV 371.64 nm f=0.0743 <S**2>=0.000

194 -> 197 -0.33703

195 -> 198 0.58965

195 -> 204 0.10512

Excited State 5: Singlet-A 3.5547 eV 348.79 nm f=0.0000 <S**2>=0.000

194 -> 200 -0.27701

195 -> 199 0.63966

Excited State 6: Singlet-A 3.5797 eV 346.36 nm f=0.0005 <S**2>=0.000

194 -> 199 -0.31664

195 -> 200 0.62140

Excited State 7: Singlet-A 3.7045 eV 334.68 nm f=0.0095 <S**2>=0.000

194 -> 197 0.36858

194 -> 201 -0.16060

194 -> 203 -0.16051

195 -> 198 0.33366

195 -> 202 0.40277

195 -> 204 -0.14132

Excited State 8: Singlet-A 3.7221 eV 333.10 nm f=0.0000 <S**2>=0.000

194 -> 202 -0.26182

195 -> 197 0.13813

195 -> 201 0.57590

195 -> 203 0.23095

Excited State 9: Singlet-A 3.7587 eV 329.86 nm f=0.0384 <S**2>=0.000

194 -> 197 0.45392

194 -> 201 0.21538

195 -> 198 0.16927

195 -> 202 -0.44590

Excited State 10: Singlet-A 3.8065 eV 325.71 nm f=0.0002 <S**2>=0.000

194 -> 200 0.11702

194 -> 204 0.19615

195 -> 201 -0.28096

195 -> 203 0.57306

195 -> 205 -0.11572

Excited State 11: Singlet-A 3.8652 eV 320.77 nm f=0.0001 <S**2>=0.000

194 -> 198 0.65913

195 -> 197 0.20151

Excited State 12: Singlet-A 3.9445 eV 314.32 nm f=0.1259 <S**2>=0.000

193 -> 196 -0.28924

194 -> 197 0.14711

194 -> 199 0.14596

194 -> 203 0.29544

195 -> 202 0.13012

195 -> 204 0.47510

Excited State 13: Singlet-A 4.0019 eV 309.82 nm f=0.4853 <S**2>=0.000

193 -> 196 0.60956

194 -> 203 0.12597

195 -> 202 0.13386

195 -> 204 0.23642

195 -> 206 -0.10782

Excited State 14: Singlet-A 4.0348 eV 307.29 nm f=0.0186 <S**2>=0.000

194 -> 199 0.57706

195 -> 200 0.29986

195 -> 204 -0.11835

195 -> 206 0.15153

Excited State 15: Singlet-A 4.0482 eV 306.27 nm f=0.0000 <S**2>=0.000

194 -> 200 0.58237

194 -> 206 0.11214

195 -> 199 0.24917

195 -> 203 -0.10292

195 -> 205 -0.22544

Excited State 16: Singlet-A 4.1101 eV 301.66 nm f=0.0631 <S**2>=0.000

193 -> 196 0.14335

194 -> 199 -0.17639

194 -> 201 -0.14809

194 -> 205 -0.24463

195 -> 206 0.56799

Excited State 17: Singlet-A 4.1266 eV 300.45 nm f=0.0001 <S**2>=0.000

194 -> 200 0.23841

194 -> 202 0.10004

194 -> 204 0.10683

194 -> 206 -0.27011

195 -> 199 0.13532

195 -> 205 0.53857

195 -> 207 -0.14051

Excited State 18: Singlet-A 4.2132 eV 294.27 nm f=0.0094 <S**2>=0.000

194 -> 201 0.61831

195 -> 202 0.27150

195 -> 206 0.17417

Excited State 19: Singlet-A 4.2224 eV 293.64 nm f=0.0001 <S**2>=0.000

192 -> 196 -0.10699

194 -> 202 0.60325

195 -> 201 0.24986

195 -> 205 -0.10846

195 -> 207 -0.17880

Excited State 20: Singlet-A 4.2397 eV 292.44 nm f=0.0002 <S**2>=0.000

192 -> 196 0.38177

194 -> 202 0.19653

194 -> 204 -0.18816

195 -> 203 0.15228

195 -> 207 0.46532

Excited State 21: Singlet-A 4.3256 eV 286.63 nm f=0.0027 <S**2>=0.000

191 -> 196 0.47998

194 -> 203 0.38090

194 -> 207 0.18328

195 -> 204 -0.25173

Excited State 22: Singlet-A 4.3411 eV 285.60 nm f=0.0001 <S**2>=0.000

192 -> 196 0.54229

194 -> 204 0.19178

194 -> 206 0.10561

195 -> 203 -0.14759

195 -> 205 -0.13978

195 -> 207 -0.25601

195 -> 208 -0.18771

Excited State 23: Singlet-A 4.3928 eV 282.24 nm f=0.0518 <S**2>=0.000

191 -> 196 0.47650

194 -> 203 -0.42189

194 -> 205 0.14968

195 -> 204 0.22861

Excited State 24: Singlet-A 4.4726 eV 277.21 nm f=0.0005 <S**2>=0.000

192 -> 196 0.16820

194 -> 204 -0.21404

194 -> 206 -0.31222

194 -> 209 0.13108

195 -> 205 -0.13619

195 -> 207 -0.23139

195 -> 208 0.45458

Excited State 25: Singlet-A 4.6072 eV 269.11 nm f=0.0004 <S**2>=0.000

194 -> 204 0.51114

194 -> 211 0.10360

195 -> 203 -0.15087

195 -> 207 0.17132

195 -> 208 0.37363

195 -> 210 -0.10526

Excited State 26: Singlet-A 4.6165 eV 268.57 nm f=0.0156 <S**2>=0.000

194 -> 203 0.11726

194 -> 205 0.15821

194 -> 207 -0.11528

194 -> 208 0.28274

194 -> 210 0.17485

195 -> 209 0.55161

Excited State 27: Singlet-A 4.6567 eV 266.25 nm f=0.1121 <S**2>=0.000

191 -> 196 -0.14396

194 -> 205 0.55108

194 -> 207 0.31813

195 -> 206 0.18519

Excited State 28: Singlet-A 4.7076 eV 263.37 nm f=0.0002 <S**2>=0.000

190 -> 196 0.69459

Excited State 29: Singlet-A 4.7166 eV 262.87 nm f=0.0068 <S**2>=0.000

189 -> 196 0.68419

Excited State 30: Singlet-A 4.7231 eV 262.51 nm f=0.0055 <S**2>=0.000

189 -> 196 -0.15210

194 -> 205 -0.16635

194 -> 207 0.43831

194 -> 208 0.30302

195 -> 204 0.19067

195 -> 206 -0.13762

195 -> 211 0.25253

Excited State 31: Singlet-A 4.7242 eV 262.44 nm f=0.0000 <S**2>=0.000

194 -> 206 0.41974

194 -> 209 0.29105

195 -> 205 0.23812

195 -> 207 -0.13763

195 -> 208 0.12892

195 -> 210 0.32829

Excited State 32: Singlet-A 4.7921 eV 258.73 nm f=0.0000 <S**2>=0.000

186 -> 196 -0.15616

194 -> 204 0.19481

194 -> 206 -0.32012

194 -> 209 0.15743

195 -> 205 -0.11987

195 -> 207 0.18039

195 -> 208 -0.16343

195 -> 210 0.44279

Excited State 33: Singlet-A 4.8165 eV 257.42 nm f=0.0018 <S**2>=0.000

186 -> 196 -0.12794

188 -> 196 -0.15277

193 -> 197 0.63880

195 -> 210 -0.11760

Excited State 34: Singlet-A 4.8989 eV 253.08 nm f=0.0246 <S**2>=0.000

187 -> 196 -0.15430

192 -> 197 -0.11223

193 -> 198 0.38766

194 -> 205 0.14361

194 -> 207 -0.23470

194 -> 208 0.23445

194 -> 210 -0.20171

195 -> 206 0.15752

195 -> 209 -0.18383

195 -> 211 0.23742

Excited State 35: Singlet-A 4.9027 eV 252.89 nm f=0.0169 <S**2>=0.000

188 -> 196 0.67096

193 -> 197 0.13088

Excited State 36: Singlet-A 4.9178 eV 252.11 nm f=0.0492 <S**2>=0.000

187 -> 196 0.53144

193 -> 198 -0.26602

194 -> 207 -0.20663

194 -> 208 0.15514

194 -> 210 -0.11097

195 -> 209 -0.12977

195 -> 211 0.14411

Excited State 37: Singlet-A 4.9593 eV 250.00 nm f=0.0723 <S**2>=0.000

187 -> 196 0.40782

192 -> 197 -0.14415

193 -> 198 0.45099

194 -> 208 -0.17816

194 -> 210 0.12385

195 -> 211 -0.12958

Excited State 38: Singlet-A 5.0355 eV 246.22 nm f=0.0000 <S**2>=0.000

186 -> 196 0.63679

193 -> 197 0.15874

195 -> 210 0.12211

Excited State 39: Singlet-A 5.0838 eV 243.88 nm f=0.0009 <S**2>=0.000

185 -> 196 0.16159

193 -> 199 0.65190

Excited State 40: Singlet-A 5.1137 eV 242.45 nm f=0.3337 <S**2>=0.000

184 -> 196 -0.13672

191 -> 198 -0.27255

192 -> 197 0.56211

193 -> 198 0.17629

193 -> 200 -0.11727

Excited State 41: Singlet-A 5.1207 eV 242.12 nm f=0.0033 <S**2>=0.000

184 -> 196 -0.14661

192 -> 199 -0.13236

193 -> 200 0.65540

Excited State 42: Singlet-A 5.1287 eV 241.75 nm f=0.0260 <S**2>=0.000

185 -> 196 0.51291

191 -> 197 -0.33123

192 -> 198 0.24991

193 -> 199 -0.13301

Excited State 43: Singlet-A 5.1466 eV 240.90 nm f=0.0188 <S**2>=0.000

185 -> 196 0.41175

191 -> 197 0.38452

192 -> 198 -0.33458

193 -> 199 -0.10758

193 -> 201 -0.12737

Excited State 44: Singlet-A 5.1746 eV 239.60 nm f=0.0494 <S**2>=0.000

184 -> 196 0.62074

192 -> 197 0.11188

193 -> 198 0.10519

193 -> 200 0.13041

195 -> 214 0.14269

Excited State 45: Singlet-A 5.2485 eV 236.23 nm f=0.0029 <S**2>=0.000

193 -> 202 -0.19145

194 -> 208 -0.38980

194 -> 210 -0.21663

195 -> 209 0.22523

195 -> 211 0.42361

Excited State 46: Singlet-A 5.2591 eV 235.75 nm f=0.0021 <S**2>=0.000

187 -> 199 0.16749

188 -> 200 0.15657

189 -> 197 -0.23513

189 -> 201 -0.14398

190 -> 198 0.18974

190 -> 202 0.15295

193 -> 201 0.44840

194 -> 209 -0.18987

Excited State 47: Singlet-A 5.2650 eV 235.49 nm f=0.0010 <S**2>=0.000

184 -> 200 -0.10795

185 -> 199 0.13087

187 -> 200 0.23055

188 -> 199 0.21584

189 -> 198 -0.26663

189 -> 202 -0.20061

190 -> 197 0.34209

190 -> 201 0.20083

193 -> 202 0.18570

Excited State 48: Singlet-A 5.2743 eV 235.07 nm f=0.0004 <S**2>=0.000

185 -> 196 -0.13297

187 -> 199 0.17105

188 -> 200 0.15884

189 -> 197 -0.25724

189 -> 201 -0.14613

190 -> 198 0.21105

190 -> 202 0.14592

193 -> 201 -0.28929

194 -> 209 0.30359

195 -> 210 -0.17991

Excited State 49: Singlet-A 5.2750 eV 235.04 nm f=0.0002 <S**2>=0.000

193 -> 201 0.37850

194 -> 209 0.42481

195 -> 208 -0.13636

195 -> 210 -0.25916

Excited State 50: Singlet-A 5.2902 eV 234.36 nm f=0.0278 <S**2>=0.000

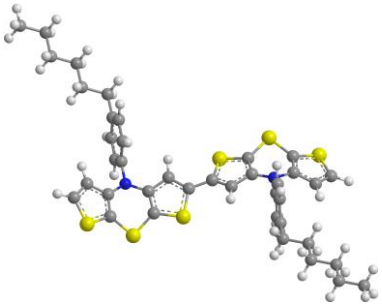
190 -> 197 -0.12409

192 -> 201 -0.11094

193 -> 202 0.60107

194 -> 210 -0.12393

11.19 Computed xyz-coordinates and excitation energies of dithienothiazine dimer **4** (wave trans conformer)



C	-3.145100	-4.501360	-1.076350
C	-3.970440	-3.495760	-0.634111
N	-3.706130	-2.130910	-0.884778
C	-2.359230	-1.751760	-1.067790
C	-1.406400	-2.621310	-1.545440
S	-1.751380	-4.252320	-2.150200
S	-3.667360	-6.066330	-0.521906
C	-5.042830	-5.358180	0.263240
C	-5.068080	-4.001210	0.135378
C	-1.808210	-0.480486	-0.729962
C	-0.453507	-0.392188	-0.946363
S	0.181192	-1.907700	-1.563740
C	-4.670200	-1.139310	-0.486611
C	-5.503950	-0.570813	-1.448130
C	-6.439590	0.392735	-1.078330
C	-6.563900	0.807268	0.252479
C	-5.717310	0.228179	1.206050

C	-4.778730	-0.734765	0.845762
C	1.361700	3.037130	-0.463073
C	2.311480	2.056360	-0.295777
N	3.664810	2.351060	-0.029469
C	4.165010	3.588730	-0.489894
C	3.361280	4.688830	-0.669015
S	1.651070	4.766840	-0.193236
S	-0.193966	2.377770	-0.878686
C	0.423442	0.740296	-0.738450
C	1.767150	0.746975	-0.448579
C	5.520720	3.845050	-0.875366
C	5.706920	5.113800	-1.338010
S	4.234390	6.030990	-1.351200
C	4.577390	1.276050	0.257286
C	4.910860	0.997668	1.581930
C	5.779740	-0.050056	1.876900
C	6.333540	-0.838610	0.861796
C	5.989820	-0.545263	-0.463528
C	5.121000	0.499276	-0.768024
C	7.299360	-1.955520	1.185420
C	8.767910	-1.490470	1.241780
C	9.740660	-2.626540	1.574760
C	11.205400	-2.179190	1.638110
C	12.178400	-3.315250	1.973370
C	13.639800	-2.861680	2.037000
C	-7.607840	1.823100	0.656811
C	-8.948840	1.179250	1.060530
C	-10.009300	2.207080	1.469410
C	-11.346300	1.575180	1.872630
C	-12.410600	2.599770	2.282300
C	-13.743800	1.960480	2.681110
H	-5.747970	-5.993100	0.776590
H	-5.838620	-3.377650	0.564753

H	-2.391170	0.332690	-0.321894
H	-5.411560	-0.884978	-2.481180
H	-7.079460	0.831430	-1.836930
H	-5.789430	0.538468	2.243390
H	-4.127140	-1.170860	1.594550
H	2.344100	-0.156971	-0.314661
H	6.314350	3.115670	-0.803278
H	6.621860	5.571810	-1.680040
H	4.481210	1.600190	2.373640
H	6.025510	-0.261963	2.912340
H	6.400690	-1.146820	-1.267730
H	4.858030	0.709553	-1.798570
H	7.029650	-2.400620	2.148940
H	7.204940	-2.747150	0.434797
H	8.863180	-0.693634	1.988890
H	9.039660	-1.043440	0.278028
H	9.457220	-3.073710	2.536240
H	9.637260	-3.421910	0.825594
H	11.309000	-1.383110	2.386750
H	11.490200	-1.732690	0.676505
H	12.075300	-4.110260	1.224940
H	11.893200	-3.761910	2.933650
H	14.306300	-3.694200	2.279030
H	13.965300	-2.442580	1.079550
H	13.780600	-2.090050	2.800560
H	-7.780320	2.517910	-0.171703
H	-7.231280	2.418430	1.495230
H	-9.323130	0.577888	0.223559
H	-8.775570	0.481190	1.888200
H	-10.174900	2.905640	0.639235
H	-9.626690	2.808820	2.303760
H	-11.728600	0.972985	1.038240
H	-11.180800	0.876027	2.702610

H -12.574900 3.299040 1.453490

H -12.029600 3.200580 3.117010

H -13.617700 1.281010 3.530050

H -14.479800 2.716950 2.967460

H -14.166700 1.381310 1.854070

SCF Done: E(RB3LYP) = -4047.49782907 A.U. after 1 cycles

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5741 eV 481.66 nm f=0.2667 <S**2>=0.000

195 -> 196 0.69374

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -4047.40311538

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.8060 eV 441.86 nm f=0.0006 <S**2>=0.000

194 -> 196 0.68352

195 -> 197 0.14881

Excited State 3: Singlet-A 3.2424 eV 382.39 nm f=0.0013 <S**2>=0.000

194 -> 196 -0.16516

194 -> 198 -0.21339

195 -> 197 0.63618

Excited State 4: Singlet-A 3.3481 eV 370.31 nm f=0.0757 <S**2>=0.000

194 -> 197 -0.33989

195 -> 198 0.58872

Excited State 5: Singlet-A 3.5694 eV 347.35 nm f=0.0033 <S**2>=0.000

194 -> 200 0.26951

195 -> 199 0.61910

195 -> 200 0.15272

Excited State 6: Singlet-A 3.5918 eV 345.19 nm f=0.0002 <S**2>=0.000

194 -> 199 0.30602

195 -> 199 -0.14879

195 -> 200 0.60099

Excited State 7: Singlet-A 3.7138 eV 333.85 nm f=0.0100 <S**2>=0.000

194 -> 197 0.40820

194 -> 201 0.10206

194 -> 203 -0.12187

195 -> 198 0.34245

195 -> 201 0.24147

195 -> 202 0.22333

195 -> 203 -0.18558

Excited State 8: Singlet-A 3.7339 eV 332.05 nm f=0.0037 <S**2>=0.000

194 -> 197 -0.13606

194 -> 201 0.21311

194 -> 202 0.14165

195 -> 197 -0.13836

195 -> 201 0.51087

195 -> 202 -0.28960

195 -> 204 0.11265

Excited State 9: Singlet-A 3.7554 eV 330.15 nm f=0.0226 <S**2>=0.000

194 -> 197 -0.36893

194 -> 202 -0.22197

195 -> 198 -0.12160

195 -> 201 0.21189

195 -> 202 0.46779

Excited State 10: Singlet-A 3.8565 eV 321.49 nm f=0.0043 <S**2>=0.000

194 -> 197 0.17252

194 -> 200 0.13644

194 -> 205 -0.14958

195 -> 201 0.17004

195 -> 203 0.57294

195 -> 204 0.16350

Excited State 11: Singlet-A 3.8757 eV 319.90 nm f=0.0023 <S**2>=0.000

194 -> 198 0.65156

195 -> 197 0.20545

Excited State 12: Singlet-A 3.9710 eV 312.22 nm f=0.0675 <S**2>=0.000

193 -> 196 -0.25034

194 -> 199 0.16756

194 -> 203 -0.22021

194 -> 204 -0.20037

195 -> 202 0.15530

195 -> 204 0.34291

195 -> 205 0.34680

Excited State 13: Singlet-A 4.0008 eV 309.90 nm f=0.3401 <S**2>=0.000

193 -> 196 0.50599

194 -> 204 -0.13566

194 -> 206 0.10500

195 -> 202 0.10315

195 -> 204 0.36588

195 -> 205 -0.13233

Excited State 14: Singlet-A 4.0399 eV 306.90 nm f=0.1528 <S**2>=0.000

193 -> 196 0.32487

194 -> 199 0.44414

195 -> 200 -0.23488

195 -> 204 -0.18994

195 -> 205 0.20725

Excited State 15: Singlet-A 4.0639 eV 305.09 nm f=0.0538 <S**2>=0.000

193 -> 196 0.17871

194 -> 199 -0.18303

194 -> 200 0.48534

194 -> 207 0.10020

195 -> 199 -0.21335

195 -> 200 0.11229

195 -> 204 -0.14017

195 -> 205 0.26368

Excited State 16: Singlet-A 4.0902 eV 303.13 nm f=0.0343 <S**2>=0.000

193 -> 196 -0.14301

194 -> 199 0.35734

194 -> 200 0.34835

194 -> 203 0.11427

195 -> 199 -0.17275

195 -> 200 -0.16593

195 -> 203 -0.11917

195 -> 205 -0.31753

195 -> 206 0.11615

Excited State 17: Singlet-A 4.1155 eV 301.26 nm f=0.0076 <S**2>=0.000

194 -> 200 -0.14317

194 -> 204 0.22851

194 -> 206 0.21220

195 -> 206 0.55189

Excited State 18: Singlet-A 4.2201 eV 293.79 nm f=0.0022 <S**2>=0.000

194 -> 201 0.19430

194 -> 202 0.59086

195 -> 202 0.26027

Excited State 19: Singlet-A 4.2306 eV 293.06 nm f=0.0098 <S**2>=0.000

194 -> 201 0.59895

194 -> 202 -0.19747

195 -> 201 -0.24572

Excited State 20: Singlet-A 4.2763 eV 289.93 nm f=0.0038 <S**2>=0.000

191 -> 196 0.11959

192 -> 196 0.28662

194 -> 204 -0.13736

194 -> 205 0.19162

194 -> 207 -0.11567

195 -> 203 0.13561

195 -> 204 -0.11330

195 -> 206 0.10305

195 -> 207 0.50631

Excited State 21: Singlet-A 4.3315 eV 286.24 nm f=0.0079 <S**2>=0.000

192 -> 196 0.59492

194 -> 205 -0.17098

195 -> 203 -0.11195

195 -> 207 -0.15554

195 -> 208 0.16568

Excited State 22: Singlet-A 4.3418 eV 285.56 nm f=0.0017 <S**2>=0.000

191 -> 196 0.50855

194 -> 203 0.35487

194 -> 206 0.10934

194 -> 207 0.12794

195 -> 205 0.19726

Excited State 23: Singlet-A 4.4072 eV 281.32 nm f=0.0221 <S**2>=0.000

191 -> 196 -0.39300

194 -> 203 0.44133

194 -> 205 0.13214

194 -> 206 0.10708

195 -> 205 0.21369

195 -> 207 0.15421

Excited State 24: Singlet-A 4.5046 eV 275.24 nm f=0.0034 <S**2>=0.000

192 -> 196 -0.17402

194 -> 204 -0.12168

194 -> 205 -0.29645

194 -> 206 0.23899

194 -> 208 0.11171

195 -> 204 -0.15808

195 -> 207 0.12541

195 -> 208 0.44989

Excited State 25: Singlet-A 4.5509 eV 272.44 nm f=0.0905 <S**2>=0.000

191 -> 196 0.20157

194 -> 204 0.44289

194 -> 207 -0.26324

195 -> 204 0.14095

195 -> 206 -0.17997

195 -> 207 0.13672

195 -> 208 0.11099

195 -> 209 -0.23800

Excited State 26: Singlet-A 4.6365 eV 267.41 nm f=0.0140 <S**2>=0.000

194 -> 205 0.51292

194 -> 208 0.12390

195 -> 203 0.10582

195 -> 207 -0.17343

195 -> 208 0.35487

Excited State 27: Singlet-A 4.7022 eV 263.67 nm f=0.0035 <S**2>=0.000

194 -> 204 -0.12865

194 -> 206 -0.24428

194 -> 207 -0.19374

194 -> 208 0.30852

195 -> 206 0.17665

195 -> 209 -0.17851

195 -> 210 0.32853

195 -> 211 -0.17771

Excited State 28: Singlet-A 4.7270 eV 262.29 nm f=0.0060 <S**2>=0.000

194 -> 204 0.30012

194 -> 206 -0.16862

194 -> 207 0.17589

194 -> 208 0.16815

194 -> 209 -0.14495

195 -> 204 0.13131

195 -> 207 0.18695

195 -> 209 0.40680

195 -> 210 0.16337

Excited State 29: Singlet-A 4.7341 eV 261.89 nm f=0.0089 <S**2>=0.000

190 -> 196 0.68826

Excited State 30: Singlet-A 4.7385 eV 261.65 nm f=0.0003 <S**2>=0.000

189 -> 196 0.68758

Excited State 31: Singlet-A 4.7725 eV 259.79 nm f=0.0038 <S**2>=0.000

194 -> 203 -0.10186

194 -> 206 0.38562

194 -> 210 0.13498

194 -> 211 0.10616

195 -> 206 -0.16635

195 -> 208 -0.19437

195 -> 210 0.42368

195 -> 211 0.10522

Excited State 32: Singlet-A 4.8034 eV 258.12 nm f=0.0054 <S**2>=0.000

186 -> 196 0.16300

188 -> 196 0.10327

193 -> 197 0.64141

Excited State 33: Singlet-A 4.8507 eV 255.60 nm f=0.0240 <S**2>=0.000

194 -> 207 0.48170

194 -> 209 0.26993

195 -> 204 0.13674

195 -> 205 -0.11315

195 -> 207 0.17622

195 -> 209 -0.27449

Excited State 34: Singlet-A 4.8943 eV 253.32 nm f=0.0142 <S**2>=0.000

187 -> 196 0.11602

188 -> 196 0.33418

194 -> 206 0.23683

194 -> 207 0.10642

194 -> 208 0.27776

194 -> 210 -0.22946

195 -> 206 -0.14690

195 -> 210 -0.15671

195 -> 211 -0.29040

Excited State 35: Singlet-A 4.9158 eV 252.21 nm f=0.0053 <S**2>=0.000

187 -> 196 0.31289

188 -> 196 -0.13693

192 -> 197 0.12441

193 -> 198 0.57282

Excited State 36: Singlet-A 4.9407 eV 250.94 nm f=0.0201 <S**2>=0.000

188 -> 196 0.56829

193 -> 197 -0.10321

193 -> 198 0.13794

194 -> 208 -0.20151

194 -> 210 0.13238

195 -> 211 0.17100

Excited State 37: Singlet-A 4.9670 eV 249.61 nm f=0.1216 <S**2>=0.000

187 -> 196 0.59189

192 -> 197 -0.13574

193 -> 198 -0.25927

Excited State 38: Singlet-A 5.0432 eV 245.84 nm f=0.0048 <S**2>=0.000

186 -> 196 0.59562

193 -> 197 -0.15928

193 -> 199 0.21344

193 -> 203 -0.13256

Excited State 39: Singlet-A 5.0832 eV 243.91 nm f=0.0174 <S**2>=0.000

186 -> 196 -0.19187

193 -> 199 0.59950

193 -> 200 0.22450

Excited State 40: Singlet-A 5.0919 eV 243.49 nm f=0.2833 <S**2>=0.000

184 -> 196 0.11053

191 -> 197 -0.18065

191 -> 198 -0.18450

192 -> 197 0.53840

192 -> 198 0.22195

193 -> 198 -0.16534

Excited State 41: Singlet-A 5.1208 eV 242.12 nm f=0.0031 <S**2>=0.000

186 -> 196 0.11086

192 -> 199 -0.11912

193 -> 199 -0.18997

193 -> 200 0.62698

Excited State 42: Singlet-A 5.1344 eV 241.48 nm f=0.0805 <S**2>=0.000

185 -> 196 -0.17638

191 -> 197 0.45640

191 -> 198 -0.22836

192 -> 197 0.15674

192 -> 198 -0.27535

193 -> 200 0.11717

194 -> 209 0.10317

Excited State 43: Singlet-A 5.1596 eV 240.30 nm f=0.0034 <S**2>=0.000

185 -> 196 0.63416

192 -> 198 -0.10562

193 -> 201 -0.11407

Excited State 44: Singlet-A 5.1806 eV 239.32 nm f=0.0110 <S**2>=0.000

184 -> 196 0.57022

194 -> 209 -0.21251

195 -> 209 -0.12658

195 -> 214 0.11787

Excited State 45: Singlet-A 5.2361 eV 236.79 nm f=0.0861 <S**2>=0.000

184 -> 196 0.21044

193 -> 201 0.40493

194 -> 208 0.13803

194 -> 209 0.34175

195 -> 209 0.22746

195 -> 211 0.12680

Excited State 46: Singlet-A 5.2630 eV 235.58 nm f=0.0406 <S**2>=0.000

184 -> 196 -0.12405

187 -> 199 -0.10014

189 -> 197 0.13385

190 -> 198 0.10729

191 -> 198 -0.10052

193 -> 201 0.47693

194 -> 209 -0.23342

195 -> 209 -0.14109

Excited State 47: Singlet-A 5.2691 eV 235.30 nm f=0.0142 <S**2>=0.000

184 -> 196 0.13355

187 -> 199 -0.12922

187 -> 200 0.17683

188 -> 199 -0.15928

188 -> 200 0.12433

189 -> 197 0.14807

189 -> 198 0.14525

189 -> 202 0.13509

190 -> 197 0.32289

190 -> 198 0.17327

190 -> 202 0.22242

193 -> 201 -0.14342

194 -> 208 0.11856

195 -> 211 0.11050

Excited State 48: Singlet-A 5.2730 eV 235.13 nm f=0.0075 <S**2>=0.000

187 -> 199 -0.14220

187 -> 200 -0.15784

188 -> 199 0.15398

188 -> 200 0.12943

189 -> 197 0.23837

189 -> 198 -0.23131

189 -> 201 -0.23058

190 -> 197 -0.17701

190 -> 198 0.12102

190 -> 201 0.13997

193 -> 201 -0.11260

193 -> 202 -0.16463

194 -> 208 0.15247

195 -> 211 0.14591

Excited State 49: Singlet-A 5.2781 eV 234.90 nm f=0.0027 <S**2>=0.000

184 -> 196 0.12733

189 -> 197 0.15304

190 -> 198 0.10271

193 -> 202 0.42812

194 -> 208 -0.23894

194 -> 209 0.10106

194 -> 210 -0.15152

195 -> 209 0.10644

195 -> 210 0.13016

195 -> 211 -0.20679

Excited State 50: Singlet-A 5.2923 eV 234.27 nm f=0.0140 <S**2>=0.000

184 -> 196 -0.11917

192 -> 199 -0.10911

192 -> 202 0.10017

193 -> 202 0.45653

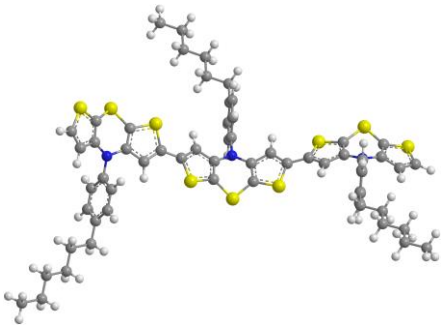
194 -> 208 0.24384

194 -> 210 0.16439

195 -> 210 -0.16341

195 -> 211 0.27450

11.20 Computed xyz-coordinates and excitation energies of dithienothiazine trimer **5** (all-trans conformer 1)



C	-8.596771	0.799570	3.197016
C	-8.692522	-0.297012	2.374657
N	-7.922407	-0.434569	1.198597
C	-6.677290	0.226232	1.155838
C	-6.420669	1.361950	1.888732
S	-7.640678	2.249453	2.822227
S	-9.579087	0.632526	4.624102
C	-10.165510	-0.904294	4.072770
C	-9.604852	-1.275517	2.886945
C	-5.545423	-0.191524	0.395727
C	-4.442704	0.612727	0.563111
S	-4.772822	1.893062	1.717695
C	-8.168163	-1.549198	0.322388
C	-7.634699	-2.810838	0.594148
C	-7.892639	-3.874869	-0.265923
C	-8.684739	-3.707460	-1.408435
C	-9.209081	-2.435913	-1.667079
C	-8.955259	-1.365097	-0.813290
C	-1.072648	-0.339914	-1.174437
C	-1.018419	1.009063	-0.911823
N	0.107767	1.796362	-1.229200
C	1.360691	1.150039	-1.288751
C	1.490868	-0.184745	-1.592298
S	0.152439	-1.233393	-2.096466
S	-2.539930	-1.064025	-0.582876

C	-3.136493	0.498158	-0.048662
C	-2.203053	1.482106	-0.274746
C	2.613233	1.758471	-0.982679
C	3.678833	0.892763	-1.055408
S	3.143359	-0.722668	-1.486695
C	0.057601	3.222721	-1.044088
C	-0.101611	4.050183	-2.154702
C	-0.138810	5.432858	-1.993693
C	-0.021176	6.017647	-0.727430
C	0.137907	5.172634	0.377703
C	0.179191	3.789076	0.226444
C	7.304961	2.275040	-0.581875
C	7.356433	0.925170	-0.321652
N	8.555532	0.265390	0.018653
C	9.764042	0.830573	-0.445807
C	9.900723	2.172385	-0.708257
S	8.661776	3.394108	-0.349214
S	5.716146	2.787623	-1.071308
C	5.082118	1.167595	-0.835042
C	6.081839	0.301013	-0.460567
C	10.957143	0.098897	-0.751488
C	11.953045	0.892608	-1.237754
S	11.464689	2.551917	-1.371004
C	8.520588	-1.128447	0.375520
C	8.596406	-1.492715	1.718933
C	8.565102	-2.837796	2.079086
C	8.457449	-3.843786	1.112017
C	8.377955	-3.461121	-0.232641
C	8.409528	-2.119206	-0.602298
C	-8.997316	-4.877234	-2.313328
C	-10.277785	-5.629257	-1.899793
C	-10.590684	-6.826201	-2.804139
C	-11.865648	-7.575388	-2.400866

C	-12.177643	-8.781364	-3.294568
C	-13.454537	-9.521868	-2.886355
C	8.469407	-5.303715	1.504253
C	9.892301	-5.892071	1.574748
C	9.914317	-7.375114	1.960600
C	11.328634	-7.960853	2.034831
C	11.360513	-9.447000	2.410261
C	12.778263	-10.021534	2.481748
C	-0.097130	7.517386	-0.554539
C	-1.538519	8.033077	-0.373613
C	-1.610981	9.553336	-0.195769
C	-3.039808	10.080881	-0.023189
C	-3.113502	11.601393	0.157922
C	-4.543726	12.122322	0.326812
H	-10.888553	-1.441702	4.666284
H	-9.830869	-2.206096	2.386837
H	-5.558306	-1.038780	-0.274968
H	-7.019282	-2.955346	1.474935
H	-7.469922	-4.850084	-0.047433
H	-9.820158	-2.279144	-2.549932
H	-9.361774	-0.382367	-1.021673
H	-2.369323	2.519500	-0.022032
H	2.716635	2.796176	-0.699638
H	-0.189719	3.604680	-3.138658
H	-0.256110	6.066809	-2.866424
H	0.238735	5.602364	1.368924
H	0.311123	3.147579	1.090400
H	5.907697	-0.746319	-0.258638
H	11.062054	-0.966598	-0.607658
H	12.950192	0.606083	-1.533534
H	8.675904	-0.718906	2.473466
H	8.620701	-3.109054	3.128240
H	8.287175	-4.222326	-1.000592

H	8.345343	-1.837521	-1.647242
H	-9.108062	-4.523086	-3.343543
H	-8.154995	-5.576872	-2.308172
H	-11.122204	-4.929912	-1.909869
H	-10.172966	-5.970534	-0.863027
H	-10.685813	-6.481461	-3.841749
H	-9.741689	-7.521543	-2.789323
H	-12.715706	-6.881232	-2.422457
H	-11.773589	-7.912594	-1.360266
H	-12.267182	-8.445518	-4.334787
H	-11.329279	-9.476012	-3.270428
H	-14.326562	-8.862136	-2.936546
H	-13.646668	-10.377090	-3.540230
H	-13.382291	-9.896894	-1.860498
H	7.983870	-5.424290	2.478392
H	7.879723	-5.879774	0.783541
H	10.482069	-5.315916	2.297544
H	10.382243	-5.759373	0.602756
H	9.322798	-7.946530	1.233863
H	9.416691	-7.505183	2.930173
H	11.828201	-7.823365	1.066985
H	11.918159	-7.392142	2.765598
H	10.861470	-9.585481	3.377054
H	10.772621	-10.015579	1.679541
H	12.766702	-11.082155	2.747885
H	13.291679	-9.925219	1.519740
H	13.379390	-9.497005	3.231244
H	0.349147	8.007118	-1.426493
H	0.499741	7.814181	0.314135
H	-1.989528	7.538939	0.495121
H	-2.137084	7.735237	-1.242686
H	-1.010072	9.844182	0.675399
H	-1.147823	10.040927	-1.063180

H -3.504760 9.591768 0.842593

H -3.640271 9.792100 -0.895573

H -2.647063 12.089847 -0.706228

H -2.514995 11.889438 1.030704

H -5.024975 11.677213 1.203462

H -4.560844 13.208369 0.453863

H -5.157826 11.879806 -0.546274

SCF Done: E(RB3LYP) = -6070.64849976 A.U. after 14 cycles

E(HOMO) = -4.775 eV

E(LUMO) = -1.824 eV

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4253 eV 511.22 nm f=0.4411 <S**2>=0.000

290 -> 293 0.11106

291 -> 294 -0.12464

292 -> 293 0.68016

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -6070.55937247

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6278 eV 471.83 nm f=0.0591 <S**2>=0.000

290 -> 294 -0.10105

291 -> 293 -0.36680

292 -> 294 0.57778

Excited State 3: Singlet-A 2.7260 eV 454.82 nm f=0.0143 <S**2>=0.000

290 -> 293 0.21473

290 -> 294 0.22373

291 -> 293 0.47490

291 -> 294 0.22425

292 -> 294 0.34490

Excited State 4: Singlet-A 2.7301 eV 454.15 nm f=0.0432 <S**2>=0.000

290 -> 293 0.39724

290 -> 294 -0.13384

291 -> 293 -0.22949

291 -> 294 0.47124

292 -> 294 -0.17246

Excited State 5: Singlet-A 3.0141 eV 411.35 nm f=0.0353 <S**2>=0.000

290 -> 293 0.51958

291 -> 294 -0.44125

292 -> 293 -0.17194

Excited State 6: Singlet-A 3.1121 eV 398.39 nm f=0.0181 <S**2>=0.000

290 -> 294 0.63240

291 -> 293 -0.28603

Excited State 7: Singlet-A 3.2735 eV 378.75 nm f=0.0139 <S**2>=0.000

290 -> 295 -0.13595

291 -> 294 -0.10766

291 -> 296 -0.37508

292 -> 295 0.54214

Excited State 8: Singlet-A 3.2966 eV 376.10 nm f=0.0415 <S**2>=0.000

290 -> 294 -0.12754

290 -> 296 -0.16179

291 -> 295 -0.42285

292 -> 296 0.49311

Excited State 9: Singlet-A 3.5020 eV 354.04 nm f=0.0387 <S**2>=0.000

290 -> 295 0.13685

290 -> 297 0.17909

291 -> 296 0.15063

292 -> 295 0.10816

292 -> 297 0.59903

292 -> 299 -0.10904

Excited State 10: Singlet-A 3.5693 eV 347.36 nm f=0.0015 <S**2>=0.000

290 -> 298 -0.17452

291 -> 297 -0.14947

291 -> 298 -0.30313

291 -> 299 -0.24565

292 -> 298 0.50592

292 -> 299 0.12537

Excited State 11: Singlet-A 3.5785 eV 346.47 nm f=0.0061 <S**2>=0.000

290 -> 299 -0.15576

291 -> 297 0.12298

291 -> 298 -0.28149

291 -> 299 0.30155

292 -> 297 0.10328

292 -> 298 -0.11379

292 -> 299 0.46996

Excited State 12: Singlet-A 3.5976 eV 344.63 nm f=0.0540 <S**2>=0.000

290 -> 295 0.18063

290 -> 300 0.14243

290 -> 303 -0.10174

291 -> 296 0.23162

292 -> 295 0.19515

292 -> 297 -0.13511

292 -> 300 0.47640

292 -> 303 -0.20510

Excited State 13: Singlet-A 3.6715 eV 337.69 nm f=0.0008 <S**2>=0.000

290 -> 296 0.19404

291 -> 295 0.39282

292 -> 296 0.46750

292 -> 300 0.10873

292 -> 302 0.11968

Excited State 14: Singlet-A 3.6918 eV 335.84 nm f=0.0030 <S**2>=0.000

290 -> 295 -0.11318

290 -> 300 0.11025

290 -> 303 0.14959

291 -> 296 -0.14929

292 -> 295 -0.14814

292 -> 297 0.16078

292 -> 299 -0.12965

292 -> 300 0.42941

292 -> 301 -0.18779

292 -> 303 0.24573

292 -> 304 0.11541

292 -> 305 0.13605

Excited State 15: Singlet-A 3.7183 eV 333.44 nm f=0.0001 <S**2>=0.000

290 -> 305 0.10221

291 -> 296 0.14978

291 -> 301 -0.13855

291 -> 302 -0.14739

291 -> 304 0.11966

292 -> 295 0.27345

292 -> 301 0.15159

292 -> 303 0.47151

Excited State 16: Singlet-A 3.7404 eV 331.48 nm f=0.0057 <S**2>=0.000

290 -> 301 -0.13560

291 -> 295 -0.21595

291 -> 296 -0.15497

291 -> 301 -0.33807

291 -> 302 0.11252

292 -> 301 0.39485

292 -> 302 0.20045

292 -> 304 -0.10088

Excited State 17: Singlet-A 3.7467 eV 330.92 nm f=0.0130 <S**2>=0.000

290 -> 295 0.11157

290 -> 302 -0.13081

291 -> 296 0.24435

291 -> 302 0.34994

292 -> 295 0.13209

292 -> 301 -0.15726

292 -> 302 0.41485

Excited State 18: Singlet-A 3.8386 eV 323.00 nm f=0.0130 <S**2>=0.000

290 -> 306 0.11440

291 -> 296 0.12952

291 -> 300 -0.12338

291 -> 304 -0.26810

292 -> 301 0.19398

292 -> 303 -0.16029

292 -> 304 0.44241

292 -> 305 0.22046

Excited State 19: Singlet-A 3.8635 eV 320.91 nm f=0.0610 <S**2>=0.000

290 -> 303 0.10562

291 -> 296 0.14394

291 -> 297 0.29001

291 -> 299 -0.15334

291 -> 300 0.12206

291 -> 303 -0.18512

291 -> 305 0.22929

292 -> 302 -0.13510

292 -> 304 -0.20175

292 -> 305 0.32166

Excited State 20: Singlet-A 3.9066 eV 317.37 nm f=0.3964 <S**2>=0.000

288 -> 293 -0.15109

289 -> 293 0.43380

289 -> 294 0.30618

290 -> 295 -0.19442

291 -> 296 0.15318

291 -> 297 -0.14116

291 -> 299 0.10119

292 -> 306 -0.16498

Excited State 21: Singlet-A 3.9299 eV 315.49 nm f=0.1450 <S**2>=0.000

288 -> 293 0.10493

289 -> 293 0.41805

289 -> 294 -0.17997

290 -> 295 0.19926

290 -> 296 -0.11678

291 -> 297 0.35945

Excited State 22: Singlet-A 3.9335 eV 315.20 nm f=0.0745 <S**2>=0.000

289 -> 293 -0.24852

289 -> 294 0.17116

290 -> 298 0.18775

291 -> 297 0.34998

291 -> 299 0.13963

292 -> 298 0.29024

292 -> 305 -0.14561

292 -> 306 -0.18502

Excited State 23: Singlet-A 3.9577 eV 313.27 nm f=0.0389 <S**2>=0.000

289 -> 293 -0.10839

289 -> 294 0.10304

290 -> 297 0.11546

290 -> 299 0.24032

291 -> 298 0.30853

291 -> 299 -0.24965

292 -> 297 0.13385

292 -> 299 0.42282

Excited State 24: Singlet-A 3.9655 eV 312.66 nm f=0.1559 <S**2>=0.000

288 -> 293 0.11537

289 -> 294 -0.16503

290 -> 295 0.21604

290 -> 296 0.15626

290 -> 298 0.13509

291 -> 297 -0.20100

291 -> 298 0.22875

291 -> 299 0.22149

291 -> 304 -0.12820

291 -> 305 0.10874

292 -> 298 0.21249

292 -> 299 0.10081

292 -> 305 0.21568

292 -> 306 -0.17298

Excited State 25: Singlet-A 3.9725 eV 312.11 nm f=0.2455 <S**2>=0.000

288 -> 293 -0.13022

289 -> 294 0.37570

290 -> 295 0.41963

291 -> 296 -0.20331

291 -> 298 -0.11155

292 -> 298 -0.15273

292 -> 306 -0.14110

Excited State 26: Singlet-A 3.9971 eV 310.19 nm f=0.0228 <S**2>=0.000

290 -> 295 0.12410

290 -> 296 -0.37663

291 -> 295 0.15834

291 -> 297 -0.14423

291 -> 299 0.11030

291 -> 300 0.46623

292 -> 304 0.10525

Excited State 27: Singlet-A 4.0139 eV 308.89 nm f=0.1500 <S**2>=0.000

288 -> 293 -0.14440

289 -> 294 0.19613

290 -> 296 0.22055

290 -> 304 0.14766

291 -> 295 -0.10987

291 -> 298 0.14308

291 -> 304 0.12303

292 -> 298 0.18428

292 -> 304 0.13490

292 -> 306 0.40079

Excited State 28: Singlet-A 4.0338 eV 307.37 nm f=0.0022 <S**2>=0.000

290 -> 296 0.39994

291 -> 295 -0.15888

291 -> 299 -0.12323

291 -> 300 0.43733

291 -> 305 -0.10829

292 -> 306 -0.14450

Excited State 29: Singlet-A 4.0652 eV 304.99 nm f=0.0059 <S**2>=0.000

288 -> 293 0.12951

289 -> 294 0.12433

290 -> 295 -0.11953

290 -> 297 0.31042

290 -> 299 -0.11989

291 -> 299 0.10548

291 -> 305 -0.13249

291 -> 308 -0.13523

292 -> 297 -0.14149

292 -> 305 0.15421

292 -> 307 0.33362

292 -> 308 0.11052

292 -> 309 -0.12466

Excited State 30: Singlet-A 4.0860 eV 303.43 nm f=0.0029 <S**2>=0.000

288 -> 293 0.15457

290 -> 297 -0.20444

290 -> 300 0.12845

290 -> 309 -0.11177

291 -> 300 0.12053

291 -> 303 0.13088

291 -> 307 0.21155

291 -> 308 0.17071

292 -> 301 0.11742

292 -> 307 0.29358

292 -> 308 -0.26940

Excited State 31: Singlet-A 4.0900 eV 303.14 nm f=0.0056 <S**2>=0.000

290 -> 297 0.34535

290 -> 299 -0.10332

290 -> 303 0.10468

291 -> 305 0.11881

291 -> 308 0.18301

291 -> 309 -0.16478

292 -> 297 -0.13594

292 -> 305 -0.12379

292 -> 307 -0.13436

292 -> 308 -0.32467

Excited State 32: Singlet-A 4.1170 eV 301.15 nm f=0.0075 <S**2>=0.000

288 -> 293 -0.14248

290 -> 297 0.24222

290 -> 302 0.22162

291 -> 302 -0.34449

291 -> 307 0.10066

292 -> 302 0.36506

292 -> 309 0.17183

Excited State 33: Singlet-A 4.1255 eV 300.53 nm f=0.0029 <S**2>=0.000

290 -> 301 0.24107

291 -> 301 0.46168

292 -> 301 0.40570

292 -> 308 0.10775

Excited State 34: Singlet-A 4.1328 eV 300.00 nm f=0.0441 <S**2>=0.000

288 -> 293 0.41550

289 -> 294 0.18224

290 -> 297 -0.14891

290 -> 302 0.12806

291 -> 302 -0.26521

291 -> 303 -0.10065

291 -> 307 -0.11613

291 -> 309 -0.12541

292 -> 302 0.21100

292 -> 309 -0.19489

Excited State 35: Singlet-A 4.1550 eV 298.40 nm f=0.0884 <S**2>=0.000

288 -> 293 0.37113

289 -> 294 0.16096

291 -> 302 0.10825

291 -> 303 0.13749

291 -> 305 0.10201

291 -> 306 -0.13854

292 -> 303 -0.10548

292 -> 307 -0.14600

292 -> 308 0.11662

292 -> 309 0.31001

Excited State 36: Singlet-A 4.1821 eV 296.47 nm f=0.0031 <S**2>=0.000

290 -> 299 -0.12326

290 -> 300 0.59590

292 -> 300 -0.15993

292 -> 307 -0.10470

Excited State 37: Singlet-A 4.2123 eV 294.34 nm f=0.0046 <S**2>=0.000

286 -> 293 -0.12051

287 -> 294 -0.10512

288 -> 294 -0.19116

291 -> 303 0.45746

291 -> 305 0.10149

291 -> 308 -0.24743

292 -> 310 0.23948

Excited State 38: Singlet-A 4.2510 eV 291.66 nm f=0.0103 <S**2>=0.000

288 -> 294 0.30804

290 -> 305 0.21893

291 -> 303 0.27862

291 -> 304 0.14282

291 -> 308 0.12351

291 -> 309 -0.15997

292 -> 304 -0.13199

292 -> 305 0.22608

292 -> 310 -0.21810

292 -> 311 0.13719

Excited State 39: Singlet-A 4.2656 eV 290.66 nm f=0.0009 <S**2>=0.000

290 -> 298 0.54103

290 -> 299 0.23331

290 -> 300 0.10857

291 -> 298 -0.28032

291 -> 299 -0.15297

Excited State 40: Singlet-A 4.2704 eV 290.33 nm f=0.0003 <S**2>=0.000

290 -> 297 0.16376

290 -> 298 -0.26207

290 -> 299 0.50151

291 -> 298 -0.16541

291 -> 299 0.27300

Excited State 41: Singlet-A 4.2915 eV 288.90 nm f=0.0035 <S**2>=0.000

286 -> 293 0.11340

286 -> 294 0.27554

287 -> 293 0.39878

288 -> 294 0.12163

290 -> 299 0.13398

290 -> 300 -0.10828

290 -> 303 -0.26493

291 -> 310 0.16981

292 -> 308 -0.10754

292 -> 312 -0.10600

Excited State 42: Singlet-A 4.2973 eV 288.51 nm f=0.0276 <S**2>=0.000

286 -> 293 -0.10597

288 -> 294 0.54181

290 -> 305 -0.12262

291 -> 304 -0.19383

291 -> 306 -0.10201

291 -> 308 -0.10862

292 -> 305 -0.14708

292 -> 306 0.11005

292 -> 310 0.13146

Excited State 43: Singlet-A 4.3218 eV 286.88 nm f=0.0090 <S**2>=0.000

286 -> 293 0.48271

286 -> 294 -0.10767

287 -> 293 -0.13388

287 -> 294 0.35233

291 -> 303 0.16537

Excited State 44: Singlet-A 4.3573 eV 284.54 nm f=0.0565 <S**2>=0.000

286 -> 294 0.20190

287 -> 293 0.35633

290 -> 303 0.37174

291 -> 304 -0.20445

291 -> 310 -0.11295

292 -> 303 -0.11219

292 -> 308 0.11440

Excited State 45: Singlet-A 4.3854 eV 282.72 nm f=0.0150 <S**2>=0.000

286 -> 293 0.14159

288 -> 294 0.11430

290 -> 303 0.18402

290 -> 304 0.18420

291 -> 304 0.21920

291 -> 305 0.31655

291 -> 306 0.13569

292 -> 304 0.21130

292 -> 305 -0.13977

292 -> 306 -0.10934

292 -> 307 0.20816

292 -> 309 -0.17139

292 -> 310 0.10499

Excited State 46: Singlet-A 4.4157 eV 280.78 nm f=0.0049 <S**2>=0.000

290 -> 301 0.50382

290 -> 302 -0.31114

291 -> 301 -0.23335

291 -> 302 -0.20993

Excited State 47: Singlet-A 4.4237 eV 280.27 nm f=0.0047 <S**2>=0.000

290 -> 301 0.32474

290 -> 302 0.51668

291 -> 301 -0.20544

291 -> 302 0.23300

Excited State 48: Singlet-A 4.4361 eV 279.49 nm f=0.0045 <S**2>=0.000

290 -> 306 -0.22877

290 -> 307 0.15103

291 -> 303 -0.10722

291 -> 304 -0.13017

291 -> 306 -0.27610

291 -> 309 -0.25551

292 -> 304 0.11023

292 -> 307 0.14440

292 -> 311 0.32343

292 -> 312 -0.11843

Excited State 49: Singlet-A 4.4735 eV 277.15 nm f=0.0091 <S**2>=0.000

290 -> 303 -0.26778

290 -> 305 -0.14849

291 -> 304 -0.21817

291 -> 305 0.29364

292 -> 303 0.15313

292 -> 308 0.22582

292 -> 310 -0.26784

Excited State 50: Singlet-A 4.5114 eV 274.82 nm f=0.0249 <S**2>=0.000

286 -> 293 0.16017

290 -> 303 -0.11098

290 -> 305 0.14105

290 -> 307 -0.12134

290 -> 309 0.14121

291 -> 304 -0.10963

291 -> 306 0.27357

291 -> 307 0.28116

291 -> 308 -0.15594

291 -> 309 -0.19213

292 -> 307 -0.12141

292 -> 310 0.20833

292 -> 312 0.17341

Excited State 51: Singlet-A 4.5492 eV 272.54 nm f=0.0210 <S**2>=0.000

287 -> 293 -0.11901

290 -> 304 0.26330

290 -> 307 -0.12156

290 -> 308 0.13913

290 -> 312 0.10044

291 -> 305 -0.15908

291 -> 306 0.12997

291 -> 310 0.27703

291 -> 311 -0.19602

291 -> 312 0.11615

292 -> 310 -0.14700

292 -> 312 -0.16051

292 -> 313 -0.17324

Excited State 52: Singlet-A 4.5770 eV 270.88 nm f=0.0113 <S**2>=0.000

290 -> 303 0.10922

290 -> 305 -0.13277

290 -> 306 0.10305

290 -> 309 0.18671

291 -> 306 0.25120

291 -> 307 -0.23936

291 -> 313 0.11405

292 -> 306 0.11014

292 -> 307 0.11789

292 -> 309 0.24867

292 -> 311 0.28214

292 -> 312 -0.12736

292 -> 313 0.16294

Excited State 53: Singlet-A 4.5894 eV 270.15 nm f=0.0081 <S**2>=0.000

282 -> 293 -0.13006

286 -> 294 0.24272

287 -> 293 -0.21384

290 -> 303 0.11796

290 -> 305 -0.17880

290 -> 306 -0.14140

290 -> 307 -0.14848

291 -> 306 -0.15851

291 -> 307 0.10820

291 -> 311 0.22754

292 -> 309 -0.17115

292 -> 313 0.20490

Excited State 54: Singlet-A 4.6007 eV 269.49 nm f=0.0008 <S**2>=0.000

290 -> 304 0.43527

290 -> 305 0.19796

290 -> 306 0.15524

291 -> 304 -0.19269

291 -> 307 -0.12326

291 -> 311 0.14586

292 -> 304 -0.13929

292 -> 313 0.17208

Excited State 55: Singlet-A 4.6088 eV 269.01 nm f=0.0073 <S**2>=0.000

286 -> 293 -0.36272

286 -> 294 -0.17273

287 -> 293 0.12167

287 -> 294 0.49225

Excited State 56: Singlet-A 4.6177 eV 268.50 nm f=0.0284 <S**2>=0.000

282 -> 293 -0.11173

286 -> 293 -0.15319

286 -> 294 0.44387

287 -> 293 -0.25006

287 -> 294 0.26051

290 -> 305 0.15932

291 -> 312 -0.10917

Excited State 57: Singlet-A 4.6515 eV 266.55 nm f=0.0056 <S**2>=0.000

283 -> 293 0.57234

284 -> 293 -0.10887

285 -> 293 -0.38102

Excited State 58: Singlet-A 4.6731 eV 265.31 nm f=0.0005 <S**2>=0.000

282 -> 293 -0.10971

286 -> 294 -0.11463

290 -> 308 0.22224

291 -> 307 0.14558

291 -> 308 0.23026

291 -> 310 0.13215

291 -> 313 -0.10875

292 -> 306 0.11370

292 -> 308 0.28429

292 -> 309 -0.11007

292 -> 310 0.21656

292 -> 311 -0.13977

292 -> 312 -0.18571

Excited State 59: Singlet-A 4.6809 eV 264.87 nm f=0.0003 <S**2>=0.000

282 -> 293 0.23699

285 -> 293 0.10207

286 -> 294 0.13319

290 -> 305 0.13740

290 -> 306 0.14483

290 -> 310 0.13161

290 -> 311 -0.13922

291 -> 305 0.10461

291 -> 308 0.11943

291 -> 312 0.11543

291 -> 313 0.21452

292 -> 307 -0.15134

292 -> 309 -0.11021

292 -> 310 0.11692

292 -> 312 -0.18452

292 -> 314 0.22662

Excited State 60: Singlet-A 4.6928 eV 264.20 nm f=0.0188 <S**2>=0.000

284 -> 293 -0.17473

284 -> 294 -0.13156

290 -> 304 -0.19800

290 -> 306 0.13160

290 -> 308 0.10009

290 -> 310 -0.16343

290 -> 313 -0.11195

291 -> 306 -0.14282

291 -> 308 -0.13196

291 -> 310 0.30101

291 -> 311 0.10470

291 -> 313 0.14849

292 -> 305 -0.10510

292 -> 310 -0.10130

292 -> 313 0.10729

292 -> 314 0.10428

292 -> 315 -0.10049

Excited State 61: Singlet-A 4.6955 eV 264.05 nm f=0.0029 <S**2>=0.000

283 -> 293 0.16068

283 -> 294 0.10912

284 -> 293 0.50677

284 -> 294 0.29834

285 -> 294 0.12762

291 -> 310 0.11413

Excited State 62: Singlet-A 4.7003 eV 263.78 nm f=0.0079 <S**2>=0.000

284 -> 293 -0.12962

290 -> 305 -0.16082

290 -> 306 0.14257

290 -> 309 -0.13874

291 -> 305 -0.13722

291 -> 308 0.18987

291 -> 309 0.19447

292 -> 307 -0.16012

292 -> 309 -0.16985

292 -> 310 0.20717

292 -> 311 0.31294

292 -> 312 0.17017

292 -> 313 -0.12264

Excited State 63: Singlet-A 4.7036 eV 263.60 nm f=0.0064 <S**2>=0.000

282 -> 293 -0.11977

283 -> 293 0.28555

283 -> 294 -0.13752

284 -> 293 -0.17709

284 -> 294 0.17185

285 -> 293 0.43043

285 -> 294 -0.33376

Excited State 64: Singlet-A 4.7334 eV 261.93 nm f=0.0045 <S**2>=0.000

282 -> 293 0.44825

289 -> 296 0.11902

290 -> 305 -0.20409

290 -> 306 -0.18330

290 -> 308 0.13847

292 -> 309 0.11189

292 -> 312 0.16363

Excited State 65: Singlet-A 4.7479 eV 261.13 nm f=0.0005 <S**2>=0.000

282 -> 293 -0.24195

289 -> 296 -0.12470

290 -> 305 -0.17577

290 -> 307 0.12206

290 -> 311 -0.12860

291 -> 308 0.14799

291 -> 309 -0.18337

291 -> 313 0.11550

292 -> 308 0.13930

292 -> 309 0.13207

292 -> 310 0.10412

292 -> 311 -0.12296

292 -> 312 0.20262

292 -> 314 0.28573

Excited State 66: Singlet-A 4.7717 eV 259.83 nm f=0.0044 <S**2>=0.000

282 -> 293 0.12887

290 -> 305 -0.22381

290 -> 306 0.29731

290 -> 307 0.19942

291 -> 307 0.24498

291 -> 309 -0.23650

291 -> 312 -0.12177

292 -> 306 -0.13046

292 -> 310 -0.10501

292 -> 312 -0.10227

292 -> 314 -0.17163

Excited State 67: Singlet-A 4.7821 eV 259.27 nm f=0.0057 <S**2>=0.000

276 -> 293 0.10488

282 -> 294 0.32923

288 -> 296 -0.12479

289 -> 295 0.36240

290 -> 306 0.13478

290 -> 307 0.12107

291 -> 311 0.13034

291 -> 314 -0.20343

292 -> 315 0.20874

Excited State 68: Singlet-A 4.7855 eV 259.08 nm f=0.0007 <S**2>=0.000

283 -> 294 0.60998

285 -> 294 -0.32426

Excited State 69: Singlet-A 4.8109 eV 257.71 nm f=0.0034 <S**2>=0.000

288 -> 296 -0.11872

289 -> 295 0.44199

290 -> 306 -0.12840

290 -> 309 -0.12002

291 -> 306 0.11394

291 -> 311 -0.14426

291 -> 313 0.11426

291 -> 314 0.23461

292 -> 313 0.12255

292 -> 315 -0.24122

Excited State 70: Singlet-A 4.8332 eV 256.52 nm f=0.0224 <S**2>=0.000

281 -> 293 -0.12354

282 -> 293 -0.11056

289 -> 295 -0.11657

290 -> 306 -0.23250

290 -> 307 0.37114

290 -> 309 -0.16374

290 -> 311 0.11890

291 -> 306 0.15664

291 -> 309 0.17818

291 -> 315 -0.12327

292 -> 307 -0.12310

Excited State 71: Singlet-A 4.8514 eV 255.56 nm f=0.0054 <S**2>=0.000

280 -> 293 -0.12729

281 -> 293 0.12695

282 -> 293 -0.16007

282 -> 294 -0.15445

288 -> 295 -0.19934

289 -> 296 0.54955

Excited State 72: Singlet-A 4.8668 eV 254.75 nm f=0.0345 <S**2>=0.000

279 -> 293 -0.32381

281 -> 293 -0.12062

282 -> 294 0.39939

285 -> 294 0.13533

289 -> 295 -0.18577

289 -> 296 0.17730

291 -> 310 -0.10564

292 -> 315 -0.10020

Excited State 73: Singlet-A 4.8817 eV 253.98 nm f=0.0080 <S**2>=0.000

279 -> 293 0.35025

280 -> 294 -0.14863

281 -> 293 0.40703

282 -> 294 0.26822

289 -> 295 -0.17369

Excited State 74: Singlet-A 4.9044 eV 252.80 nm f=0.0359 <S**2>=0.000

279 -> 293 0.25029

280 -> 293 0.39499

280 -> 294 0.10314

281 -> 293 -0.26792

281 -> 294 -0.31407

289 -> 296 0.14487

Excited State 75: Singlet-A 4.9082 eV 252.61 nm f=0.0310 <S**2>=0.000

279 -> 293 -0.30174

280 -> 293 0.31491

280 -> 294 -0.30568

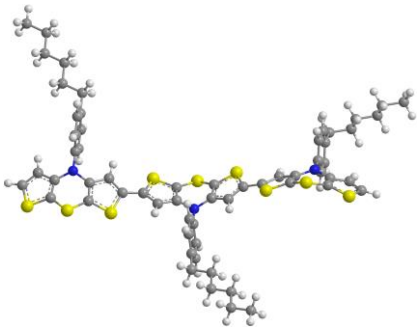
281 -> 293 0.24451

281 -> 294 -0.13616

282 -> 294 -0.13686

291 -> 310 -0.15697

11.21 Computed xyz-coordinates and excitation energies of dithienothiazine trimer **5** (all-trans conformer 2)



C	-7.285833	-2.396232	-0.642022
C	-7.359900	-1.051988	-0.359031
N	-8.569900	-0.417531	-0.009037
C	-9.768570	-0.994802	-0.483986
C	-9.882837	-2.334104	-0.769142
S	-8.624129	-3.541362	-0.430307
S	-5.687630	-2.874562	-1.136090
C	-5.080883	-1.248650	-0.871172
C	-6.095457	-0.405042	-0.484493
C	-10.973618	-0.278053	-0.777838
C	-11.956026	-1.079871	-1.278057
S	-11.440080	-2.728318	-1.439002
C	-8.556727	0.971754	0.366857
C	-8.635840	1.316705	1.715166
C	-8.621425	2.657085	2.093583
C	-8.527490	3.677401	1.140241
C	-8.445977	3.314143	-0.209710
C	-8.460717	1.977137	-0.597569
C	-3.681972	-0.945011	-1.081190
C	-2.599793	-1.790583	-1.015331
C	-1.357019	-1.151542	-1.298857
C	-1.512652	0.185303	-1.581676
S	-3.176321	0.687617	-1.481543
N	-0.090168	-1.770756	-1.240443
C	1.015687	-0.962613	-0.903168

C	1.043547	0.390539	-1.145945
S	-0.194691	1.270453	-2.062271
C	2.202999	-1.419334	-0.259064
C	3.112065	-0.419036	-0.006962
S	2.487407	1.137917	-0.526075
C	-0.000593	-3.196456	-1.064095
C	-0.199702	-3.780789	0.188715
C	-0.106188	-5.161974	0.334106
C	0.192263	-5.986906	-0.757746
C	0.388903	-5.384504	-2.005339
C	0.292931	-4.003632	-2.161665
C	4.416970	-0.513469	0.610672
S	4.805656	-1.853488	1.676510
C	6.395171	-1.206464	1.968840
C	6.618305	-0.044889	1.267063
C	5.485520	0.343933	0.493483
S	7.554293	-1.931809	3.097847
C	8.983263	-1.330957	2.228322
C	9.016466	-0.157721	1.513655
N	7.861593	0.621263	1.282921
S	10.531831	-2.125764	2.250647
C	11.238634	-0.831190	1.337379
C	10.325883	0.125663	1.006280
C	7.982262	1.908241	0.651011
C	7.903711	3.061798	1.430054
C	8.007691	4.315542	0.832676
C	8.193692	4.445729	-0.548433
C	8.270066	3.277732	-1.317043
C	8.164993	2.020045	-0.729005
C	8.341916	5.807312	-1.187985
C	9.801084	6.302888	-1.220213
C	9.951501	7.681981	-1.871496
C	11.397862	8.188421	-1.898794

C	11.552803	9.566992	-2.551645
C	13.000195	10.067012	-2.572727
C	0.336401	-7.481358	-0.582492
C	1.759255	-7.901766	-0.164278
C	1.908162	-9.415655	0.020933
C	3.316511	-9.839606	0.452549
C	3.471749	-11.353170	0.640915
C	4.879708	-11.765948	1.080077
C	-8.553824	5.131594	1.552539
C	-9.981834	5.706188	1.632366
C	-10.015272	7.183617	2.038467
C	-11.433711	7.758233	2.120586
C	-11.475554	9.238921	2.516133
C	-12.897048	9.803177	2.594900
H	-5.938283	0.641199	-0.263898
H	-11.096378	0.782939	-0.615929
H	-12.957750	-0.805051	-1.569444
H	-8.703780	0.531748	2.459235
H	-8.678781	2.913311	3.146407
H	-8.365986	4.086915	-0.967241
H	-8.394040	1.710599	-1.646325
H	-2.685264	-2.834874	-0.751436
H	2.387133	-2.457039	-0.019803
H	-0.430138	-3.154426	1.043051
H	-0.269683	-5.605968	1.310581
H	0.614588	-6.003155	-2.867664
H	0.441667	-3.544519	-3.131978
H	5.470672	1.218546	-0.141013
H	12.289772	-0.862184	1.096488
H	10.569543	1.005176	0.428310
H	7.756426	2.968790	2.499695
H	7.938434	5.205867	1.449001
H	8.406082	3.352883	-2.390988

H	8.219034	1.124725	-1.337994
H	7.730699	6.534057	-0.642634
H	7.953815	5.772978	-2.211351
H	10.190399	6.336168	-0.195770
H	10.415443	5.572394	-1.759896
H	9.324912	8.405386	-1.334256
H	9.562165	7.642231	-2.896850
H	11.786173	8.229674	-0.872897
H	12.025664	7.464026	-2.433679
H	10.924518	10.290565	-2.018226
H	11.166219	9.525128	-3.577076
H	13.646548	9.381593	-3.130114
H	13.076018	11.051517	-3.042709
H	13.403529	10.150344	-1.558482
H	0.074726	-7.985294	-1.518581
H	-0.374679	-7.829749	0.174099
H	2.023541	-7.390181	0.768756
H	2.472515	-7.551568	-0.919830
H	1.181463	-9.761406	0.767267
H	1.647996	-9.922419	-0.917143
H	3.575357	-9.331813	1.390633
H	4.044041	-9.492760	-0.292669
H	2.741903	-11.700268	1.382391
H	3.218081	-11.861013	-0.297449
H	5.147933	-11.299120	2.033121
H	4.957312	-12.849378	1.206928
H	5.628393	-11.462991	0.341219
H	-8.068558	5.243451	2.527861
H	-7.970236	5.723116	0.839428
H	-10.565853	5.115214	2.347840
H	-10.471675	5.582714	0.659123
H	-9.518561	7.304144	3.009735
H	-9.427984	7.769277	1.319678

H -12.019247 7.175596 2.843541

H -11.932314 7.630459 1.150926

H -10.977647 9.367554 3.484859

H -10.891217 9.821189 1.793384

H -12.892480 10.860174 2.875285

H -13.409554 9.716441 1.631500

H -13.494920 9.264690 3.337061

SCF Done: E(RB3LYP) = -6070.64839877 A.U. after 14 cycles

Excited State 1: Singlet-A 2.4186 eV 512.63 nm f=0.4438 <S**2>=0.000

290 -> 293 0.10717

291 -> 294 -0.12465

292 -> 293 0.68038

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -6070.55951678

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6209 eV 473.05 nm f=0.0591 <S**2>=0.000

291 -> 293 -0.35773

292 -> 294 0.58439

Excited State 3: Singlet-A 2.7238 eV 455.19 nm f=0.0016 <S**2>=0.000

290 -> 294 0.25966

291 -> 293 0.53369

292 -> 294 0.37509

Excited State 4: Singlet-A 2.7286 eV 454.39 nm f=0.0525 <S**2>=0.000

290 -> 293 0.45174

291 -> 294 0.52090

Excited State 5: Singlet-A 3.0136 eV 411.42 nm f=0.0378 <S**2>=0.000

290 -> 293 0.51793

291 -> 294 -0.44021

292 -> 293 -0.16834

Excited State 6: Singlet-A 3.1148 eV 398.05 nm f=0.0160 <S**2>=0.000

290 -> 294 0.63249

291 -> 293 -0.28148

Excited State 7: Singlet-A 3.2701 eV 379.14 nm f=0.0160 <S**2>=0.000

290 -> 295 -0.13498

291 -> 294 0.10122

291 -> 295 0.15179

291 -> 296 0.34479

292 -> 295 0.54531

Excited State 8: Singlet-A 3.2947 eV 376.32 nm f=0.0390 <S**2>=0.000

290 -> 294 -0.12131

290 -> 296 -0.15702

291 -> 295 0.38923

291 -> 296 -0.15100

292 -> 296 0.50260

Excited State 9: Singlet-A 3.5085 eV 353.38 nm f=0.0352 <S**2>=0.000

290 -> 295 0.12887

290 -> 297 0.17438

290 -> 299 -0.10076

291 -> 296 -0.13582

292 -> 295 0.10434

292 -> 297 0.60176

292 -> 299 -0.10885

Excited State 10: Singlet-A 3.5697 eV 347.33 nm f=0.0040 <S**2>=0.000

290 -> 298 -0.16037

291 -> 297 -0.16425

291 -> 298 -0.33251

291 -> 299 -0.19818

292 -> 298 0.49951

292 -> 299 0.13274

Excited State 11: Singlet-A 3.5853 eV 345.81 nm f=0.0110 <S**2>=0.000

290 -> 297 -0.13604

290 -> 299 -0.12343

291 -> 298 -0.22937

291 -> 299 0.28322

292 -> 298 -0.10585

292 -> 299 0.47460

292 -> 300 0.17965

292 -> 303 -0.10262

Excited State 12: Singlet-A 3.5922 eV 345.15 nm f=0.0566 <S**2>=0.000

290 -> 295 0.20958

291 -> 295 -0.10824

291 -> 296 -0.24049

291 -> 299 -0.17419

292 -> 295 0.23162

292 -> 297 -0.18420

292 -> 299 -0.14389

292 -> 300 0.36627

292 -> 303 -0.17130

Excited State 13: Singlet-A 3.6711 eV 337.73 nm f=0.0027 <S**2>=0.000

290 -> 296 0.20059

291 -> 295 -0.38751

291 -> 296 0.11553

291 -> 302 0.10028

292 -> 296 0.46142

292 -> 300 -0.12094

292 -> 301 0.11160

Excited State 14: Singlet-A 3.6921 eV 335.81 nm f=0.0013 <S**2>=0.000

290 -> 300	0.12559
290 -> 303	0.15661
291 -> 296	0.11850
292 -> 295	-0.10298
292 -> 297	0.11346
292 -> 300	0.48157
292 -> 302	-0.18814
292 -> 303	0.27750
292 -> 304	-0.16749

Excited State 15: Singlet-A 3.7338 eV 332.06 nm f=0.0074 <S**2>=0.000

290 -> 302	-0.14377
291 -> 295	-0.14884
291 -> 301	0.19666
291 -> 302	-0.26995
292 -> 295	0.15117
292 -> 302	0.37794
292 -> 303	0.33029

Excited State 16: Singlet-A 3.7422 eV 331.31 nm f=0.0034 <S**2>=0.000

290 -> 301	-0.16812
291 -> 295	0.16305
291 -> 301	0.31070
291 -> 302	0.23455
292 -> 301	0.47677

Excited State 17: Singlet-A 3.7536 eV 330.31 nm f=0.0074 <S**2>=0.000

290 -> 295	-0.13597
290 -> 303	-0.11647
291 -> 296	0.34129
291 -> 301	0.13751
291 -> 302	-0.11233

292 -> 295 -0.26225

292 -> 300 0.19753

292 -> 302 0.23449

292 -> 303 -0.26179

292 -> 304 0.19276

Excited State 18: Singlet-A 3.8360 eV 323.21 nm f=0.0135 <S**2>=0.000

290 -> 307 0.11653

291 -> 300 0.10416

291 -> 303 -0.11228

291 -> 304 -0.24998

292 -> 302 -0.18477

292 -> 303 0.22175

292 -> 304 0.45508

292 -> 305 0.14093

Excited State 19: Singlet-A 3.8908 eV 318.66 nm f=0.0235 <S**2>=0.000

289 -> 293 0.53862

291 -> 297 0.21267

291 -> 299 -0.10930

291 -> 300 0.10002

291 -> 305 -0.14293

292 -> 305 -0.19447

Excited State 20: Singlet-A 3.9043 eV 317.56 nm f=0.7282 <S**2>=0.000

288 -> 293 -0.21917

289 -> 293 -0.15906

289 -> 294 0.45917

290 -> 295 0.25776

291 -> 296 0.17084

292 -> 305 -0.12082

292 -> 307 -0.11505

Excited State 21: Singlet-A 3.9129 eV 316.86 nm f=0.0909 <S**2>=0.000

289 -> 293 0.33365

289 -> 294 0.18893

291 -> 297 -0.29851

291 -> 299 0.12200

291 -> 304 -0.10489

291 -> 305 0.19718

292 -> 305 0.31289

292 -> 306 -0.12002

Excited State 22: Singlet-A 3.9398 eV 314.70 nm f=0.0253 <S**2>=0.000

290 -> 298 0.18344

291 -> 297 0.42940

291 -> 299 0.10179

291 -> 305 0.14302

292 -> 298 0.31942

292 -> 305 0.21483

Excited State 23: Singlet-A 3.9600 eV 313.09 nm f=0.1233 <S**2>=0.000

288 -> 293 -0.10714

289 -> 294 0.18269

290 -> 296 -0.11111

290 -> 297 0.10378

290 -> 299 0.17604

291 -> 297 -0.11076

291 -> 298 0.36819

291 -> 300 -0.13381

292 -> 297 0.12360

292 -> 298 0.14386

292 -> 299 0.31339

292 -> 305 -0.12124

292 -> 307 0.13310

Excited State 24: Singlet-A 3.9677 eV 312.49 nm f=0.0552 <S**2>=0.000

289 -> 294 -0.21534

290 -> 295 0.43104

291 -> 295 0.11204

291 -> 296 0.20224

291 -> 297 -0.20250

291 -> 299 0.19970

292 -> 307 0.15753

Excited State 25: Singlet-A 3.9759 eV 311.84 nm f=0.0950 <S**2>=0.000

289 -> 294 -0.19703

290 -> 295 0.24353

290 -> 296 0.13801

290 -> 297 0.12485

290 -> 299 0.14644

291 -> 298 0.11787

291 -> 299 -0.29251

291 -> 300 0.16085

291 -> 305 0.14993

292 -> 299 0.30973

292 -> 304 -0.10256

292 -> 305 0.11806

Excited State 26: Singlet-A 3.9931 eV 310.50 nm f=0.0116 <S**2>=0.000

290 -> 296 0.33345

290 -> 298 0.11263

291 -> 295 0.12723

291 -> 297 -0.16373

291 -> 298 0.12884

291 -> 299 0.21359

291 -> 300 0.33491

292 -> 298 0.18696

292 -> 305 -0.13331

292 -> 306 -0.12546

292 -> 307 -0.16533

Excited State 27: Singlet-A 4.0118 eV 309.05 nm f=0.0904 <S**2>=0.000

289 -> 294 0.17312

290 -> 296 0.19931

291 -> 297 -0.13156

291 -> 298 -0.10348

291 -> 300 0.26327

291 -> 304 0.12439

291 -> 307 -0.10181

292 -> 298 -0.15395

292 -> 306 0.32623

292 -> 307 0.26590

Excited State 28: Singlet-A 4.0262 eV 307.94 nm f=0.0080 <S**2>=0.000

290 -> 296 0.39987

291 -> 295 0.17433

291 -> 300 -0.30385

291 -> 306 -0.11315

291 -> 308 0.13434

292 -> 306 -0.25525

292 -> 307 0.16002

Excited State 29: Singlet-A 4.0530 eV 305.91 nm f=0.0022 <S**2>=0.000

288 -> 293 -0.13343

290 -> 296 -0.17127

290 -> 297 0.22228

290 -> 304 0.11660

291 -> 300 0.29612

291 -> 306 -0.23388

292 -> 297 -0.10923

292 -> 306 -0.21400

292 -> 307 0.13754

292 -> 308 0.20440

292 -> 309 -0.17528

Excited State 30: Singlet-A 4.0760 eV 304.18 nm f=0.0068 <S**2>=0.000

288 -> 293 -0.12991

290 -> 296 0.16499

290 -> 297 0.18190

291 -> 300 -0.21501

291 -> 303 -0.15257

291 -> 305 0.12710

291 -> 308 -0.20775

291 -> 309 -0.12532

292 -> 301 0.10431

292 -> 305 -0.12943

292 -> 306 0.21179

292 -> 307 -0.15835

292 -> 308 0.24674

292 -> 309 -0.10631

Excited State 31: Singlet-A 4.0946 eV 302.80 nm f=0.0094 <S**2>=0.000

288 -> 293 0.32827

289 -> 294 0.12427

290 -> 305 0.10033

291 -> 301 0.17227

291 -> 306 -0.20357

291 -> 307 0.14306

291 -> 308 -0.11435

292 -> 301 -0.16786

292 -> 302 -0.18929

292 -> 308 0.20751

292 -> 309 0.24107

Excited State 32: Singlet-A 4.1137 eV 301.40 nm f=0.0095 <S**2>=0.000

288 -> 293	0.15486
290 -> 297	0.51288
290 -> 299	-0.17266
291 -> 306	0.17368
292 -> 297	-0.17661
292 -> 308	-0.22251

Excited State 33: Singlet-A 4.1214 eV 300.83 nm f=0.0227 <S**2>=0.000

288 -> 293	-0.21723
290 -> 301	-0.23796
291 -> 301	0.16114
291 -> 302	0.40573
292 -> 301	-0.37586
292 -> 302	0.14858

Excited State 34: Singlet-A 4.1279 eV 300.36 nm f=0.0260 <S**2>=0.000

288 -> 293	0.22806
290 -> 302	0.21496
291 -> 301	-0.34911
291 -> 302	0.23657
291 -> 306	-0.11322
292 -> 302	0.36127
292 -> 303	0.10879
292 -> 308	0.13829

Excited State 35: Singlet-A 4.1456 eV 299.07 nm f=0.0900 <S**2>=0.000

288 -> 293	0.36657
289 -> 294	0.17358
290 -> 305	-0.13206
291 -> 301	0.16859
291 -> 307	-0.16521
292 -> 301	-0.12031

292 -> 303 0.10608

292 -> 304 0.10536

292 -> 305 -0.10152

292 -> 309 -0.33576

Excited State 36: Singlet-A 4.1940 eV 295.62 nm f=0.0011 <S**2>=0.000

290 -> 300 0.63101

292 -> 300 -0.16157

Excited State 37: Singlet-A 4.2244 eV 293.50 nm f=0.0128 <S**2>=0.000

286 -> 293 0.12263

288 -> 294 0.27467

291 -> 303 0.46387

291 -> 307 0.10017

291 -> 308 -0.15965

291 -> 309 -0.14670

292 -> 310 -0.20521

Excited State 38: Singlet-A 4.2654 eV 290.68 nm f=0.0113 <S**2>=0.000

286 -> 293 -0.13201

287 -> 293 0.12206

288 -> 294 0.47878

290 -> 299 -0.10052

290 -> 306 -0.14838

291 -> 303 -0.26361

291 -> 304 0.10709

292 -> 306 -0.10182

292 -> 310 -0.10618

292 -> 311 0.14983

Excited State 39: Singlet-A 4.2736 eV 290.12 nm f=0.0014 <S**2>=0.000

288 -> 294 0.11425

290 -> 297 0.12586

290 -> 298 -0.24464

290 -> 299 0.50893

291 -> 298 -0.14792

291 -> 299 0.29228

Excited State 40: Singlet-A 4.2769 eV 289.90 nm f=0.0022 <S**2>=0.000

287 -> 293 -0.15951

287 -> 294 0.10929

288 -> 294 0.12537

290 -> 297 0.12671

290 -> 298 0.51937

290 -> 299 0.17622

291 -> 298 -0.25420

291 -> 299 -0.13157

Excited State 41: Singlet-A 4.2849 eV 289.35 nm f=0.0122 <S**2>=0.000

286 -> 294 0.15410

287 -> 293 0.47113

287 -> 294 -0.26866

288 -> 294 -0.13772

290 -> 298 0.15438

290 -> 299 0.17115

291 -> 298 -0.11810

Excited State 42: Singlet-A 4.3033 eV 288.12 nm f=0.0029 <S**2>=0.000

286 -> 293 0.34266

286 -> 294 0.26569

288 -> 294 0.19853

290 -> 298 -0.10391

290 -> 303 0.22433

291 -> 303 -0.15175

291 -> 305 -0.10066

291 -> 307 -0.11407

291 -> 310 0.13069

292 -> 303 -0.11720

292 -> 310 0.12426

292 -> 311 -0.10146

292 -> 312 -0.13550

Excited State 43: Singlet-A 4.3136 eV 287.43 nm f=0.0131 <S**2>=0.000

286 -> 293 0.24464

286 -> 294 0.10905

287 -> 293 -0.17974

287 -> 294 0.17147

288 -> 294 -0.23524

290 -> 305 0.11579

290 -> 306 -0.14572

291 -> 303 -0.18762

291 -> 304 0.26931

291 -> 308 -0.12903

292 -> 305 0.12413

292 -> 306 -0.16175

292 -> 310 -0.18510

292 -> 311 0.11755

Excited State 44: Singlet-A 4.3571 eV 284.56 nm f=0.0397 <S**2>=0.000

286 -> 293 -0.25133

286 -> 294 -0.16812

287 -> 293 -0.12384

290 -> 303 0.33628

291 -> 304 0.29740

291 -> 310 0.15019

292 -> 304 0.15531

292 -> 307 -0.17665

292 -> 310 0.13369

Excited State 45: Singlet-A 4.3942 eV 282.16 nm f=0.0069 <S**2>=0.000

286 -> 293	0.17976
288 -> 294	0.11432
290 -> 302	0.10114
290 -> 303	-0.20688
290 -> 304	0.15474
290 -> 306	0.10307
291 -> 304	0.14997
291 -> 305	0.25312
291 -> 307	0.12738
291 -> 308	0.11477
291 -> 309	0.17455
292 -> 303	0.11251
292 -> 304	0.10347
292 -> 306	0.12193
292 -> 307	-0.11947
292 -> 308	-0.15834
292 -> 309	0.10917
292 -> 310	0.19595
292 -> 312	0.11284

Excited State 46: Singlet-A 4.4183 eV 280.62 nm f=0.0031 <S**2>=0.000

290 -> 301	0.55615
290 -> 302	0.20181
291 -> 301	0.29843
291 -> 302	0.13413

Excited State 47: Singlet-A 4.4299 eV 279.88 nm f=0.0003 <S**2>=0.000

290 -> 301	-0.19253
290 -> 302	0.52343
291 -> 301	0.12571
291 -> 302	-0.25772
291 -> 305	-0.12142

291 -> 307 -0.13716

Excited State 48: Singlet-A 4.4482 eV 278.73 nm f=0.0286 <S**2>=0.000

290 -> 302 0.23372
290 -> 305 -0.10612
290 -> 306 0.11010
290 -> 307 0.18751
290 -> 308 0.11310
291 -> 303 -0.15398
291 -> 305 0.12235
291 -> 306 0.11877
291 -> 307 0.24313
291 -> 308 0.14823
291 -> 309 -0.11237
291 -> 311 0.10009
292 -> 304 -0.10273
292 -> 305 -0.12373
292 -> 307 0.20689
292 -> 310 -0.16759
292 -> 311 -0.21052
292 -> 312 0.10975

Excited State 49: Singlet-A 4.4660 eV 277.62 nm f=0.0231 <S**2>=0.000

287 -> 293 -0.11940
290 -> 301 -0.13561
290 -> 303 0.26150
290 -> 305 -0.15569
290 -> 308 -0.11239
291 -> 304 -0.20765
291 -> 305 0.24372
291 -> 308 -0.13897
291 -> 309 0.11825
291 -> 310 0.11473

291 -> 312 0.10704

292 -> 303 -0.10779

292 -> 305 -0.16674

292 -> 307 0.13375

292 -> 309 0.16942

292 -> 311 0.22677

Excited State 50: Singlet-A 4.5176 eV 274.45 nm f=0.0276 <S**2>=0.000

287 -> 293 -0.10893

290 -> 303 -0.10007

290 -> 306 -0.12485

290 -> 308 0.11155

290 -> 309 -0.14178

291 -> 306 0.40850

291 -> 309 0.14111

291 -> 310 0.21202

292 -> 304 -0.10810

292 -> 308 0.25239

292 -> 310 0.18297

Excited State 51: Singlet-A 4.5506 eV 272.45 nm f=0.0023 <S**2>=0.000

286 -> 293 0.13819

290 -> 303 0.23234

290 -> 304 -0.16071

290 -> 305 0.13541

291 -> 307 0.16111

291 -> 309 0.23222

291 -> 310 -0.17768

291 -> 311 0.13899

291 -> 312 -0.10091

292 -> 309 -0.23214

292 -> 312 0.23267

292 -> 313 -0.11352

Excited State 52: Singlet-A 4.5876 eV 270.26 nm f=0.0013 <S**2>=0.000

282 -> 293 0.10549

286 -> 294 -0.16830

287 -> 293 0.31218

287 -> 294 0.42513

290 -> 304 0.17979

290 -> 305 0.16216

290 -> 307 0.12128

291 -> 304 -0.14666

291 -> 311 -0.10437

Excited State 53: Singlet-A 4.5946 eV 269.85 nm f=0.0104 <S**2>=0.000

286 -> 293 -0.16241

286 -> 294 0.12438

287 -> 293 0.10297

287 -> 294 0.23364

290 -> 304 -0.16275

290 -> 305 -0.14540

290 -> 306 0.17801

290 -> 309 -0.10987

291 -> 304 0.10038

291 -> 307 0.23297

291 -> 312 0.16704

292 -> 305 0.10201

292 -> 306 0.13317

292 -> 309 -0.15480

292 -> 311 0.28462

Excited State 54: Singlet-A 4.6008 eV 269.48 nm f=0.0028 <S**2>=0.000

286 -> 293 -0.29894

286 -> 294 0.34401

287 -> 294 0.27882

290 -> 306 -0.12633

291 -> 307 -0.14024

291 -> 309 0.10680

291 -> 311 0.12043

292 -> 309 0.11465

292 -> 311 -0.19762

Excited State 55: Singlet-A 4.6025 eV 269.38 nm f=0.0095 <S**2>=0.000

286 -> 293 -0.18031

286 -> 294 0.33716

287 -> 293 -0.13382

287 -> 294 -0.11665

290 -> 304 0.32756

290 -> 305 0.13947

290 -> 307 0.12311

291 -> 304 -0.19892

292 -> 304 -0.13464

292 -> 308 -0.13421

292 -> 309 -0.12777

Excited State 56: Singlet-A 4.6294 eV 267.82 nm f=0.0305 <S**2>=0.000

286 -> 294 -0.16753

290 -> 304 0.33348

290 -> 305 -0.24696

290 -> 307 -0.10534

290 -> 309 -0.20695

291 -> 305 -0.19607

291 -> 311 0.20242

292 -> 305 0.14389

292 -> 314 -0.12566

292 -> 315 -0.14094

Excited State 57: Singlet-A 4.6423 eV 267.07 nm f=0.0004 <S**2>=0.000

283 -> 293 0.39478

285 -> 293 -0.18720

290 -> 310 -0.11741

290 -> 311 0.11150

291 -> 309 -0.13496

291 -> 310 0.10742

291 -> 311 0.11504

291 -> 312 -0.11946

291 -> 313 0.16938

292 -> 308 -0.13842

292 -> 312 0.13123

292 -> 314 -0.13736

Excited State 58: Singlet-A 4.6471 eV 266.80 nm f=0.0138 <S**2>=0.000

282 -> 293 0.12493

283 -> 293 0.45925

284 -> 293 -0.13981

285 -> 293 -0.18465

291 -> 309 0.13484

291 -> 312 0.10228

291 -> 313 -0.13627

292 -> 307 -0.10409

292 -> 308 0.13558

292 -> 314 0.11129

Excited State 59: Singlet-A 4.6589 eV 266.12 nm f=0.0110 <S**2>=0.000

290 -> 307 -0.11434

290 -> 310 -0.13667

290 -> 312 0.14785

291 -> 305 -0.14142

291 -> 307 -0.16020

291 -> 308 0.12368

292 -> 307 -0.10799

292 -> 308 0.12682

292 -> 310 -0.26528

292 -> 312 0.32288

292 -> 313 0.24719

292 -> 314 0.10009

292 -> 315 0.14304

Excited State 60: Singlet-A 4.6816 eV 264.83 nm f=0.0107 <S**2>=0.000

283 -> 293 -0.12462

285 -> 293 -0.24049

285 -> 294 0.15162

290 -> 308 0.10857

290 -> 309 0.11867

291 -> 307 -0.15477

291 -> 308 0.17146

291 -> 310 -0.10090

291 -> 315 -0.10992

292 -> 308 0.16004

292 -> 309 0.17148

292 -> 311 0.29796

292 -> 313 -0.20341

292 -> 314 -0.10634

Excited State 61: Singlet-A 4.6861 eV 264.58 nm f=0.0022 <S**2>=0.000

283 -> 293 0.20405

283 -> 294 -0.10592

285 -> 293 0.47578

285 -> 294 -0.30365

292 -> 311 0.15369

292 -> 313 -0.11033

Excited State 62: Singlet-A 4.6946 eV 264.10 nm f=0.0028 <S**2>=0.000

283 -> 293 0.15310

284 -> 293 0.54691

284 -> 294 0.40087

Excited State 63: Singlet-A 4.7202 eV 262.67 nm f=0.0007 <S**2>=0.000

282 -> 293 0.58291

286 -> 294 0.11236

289 -> 296 0.15404

Excited State 64: Singlet-A 4.7620 eV 260.36 nm f=0.0038 <S**2>=0.000

290 -> 305 0.30409

290 -> 308 0.10182

290 -> 310 -0.10552

290 -> 313 -0.10041

291 -> 305 0.12724

291 -> 308 0.18741

291 -> 310 0.11527

291 -> 311 0.16936

291 -> 314 -0.11067

292 -> 306 0.10549

292 -> 310 -0.25709

292 -> 312 -0.16472

292 -> 314 -0.16392

292 -> 315 -0.17479

Excited State 65: Singlet-A 4.7705 eV 259.90 nm f=0.0039 <S**2>=0.000

289 -> 295 0.33028

290 -> 305 0.10065

290 -> 306 0.22633

290 -> 307 0.16293

291 -> 307 -0.17352

291 -> 308 -0.17126

291 -> 311 0.17544

291 -> 314 -0.14657

292 -> 306 -0.11358

292 -> 312 0.13280

292 -> 313 0.11689

292 -> 315 -0.16753

Excited State 66: Singlet-A 4.7737 eV 259.72 nm f=0.0014 <S**2>=0.000

282 -> 294 -0.16222

283 -> 294 0.41280

285 -> 294 -0.20651

289 -> 295 0.31541

291 -> 313 0.12342

292 -> 314 -0.14172

Excited State 67: Singlet-A 4.7809 eV 259.33 nm f=0.0018 <S**2>=0.000

282 -> 294 0.27871

283 -> 294 0.47851

284 -> 294 -0.12518

285 -> 294 -0.13106

289 -> 295 -0.22069

291 -> 313 -0.10071

292 -> 314 0.11213

Excited State 68: Singlet-A 4.7894 eV 258.87 nm f=0.0011 <S**2>=0.000

289 -> 295 -0.28338

290 -> 306 0.37256

291 -> 306 0.10476

291 -> 308 -0.23790

291 -> 309 0.11074

291 -> 313 0.19781

292 -> 306 -0.14824

292 -> 314 -0.21673

Excited State 69: Singlet-A 4.8135 eV 257.57 nm f=0.0030 <S**2>=0.000

282 -> 294 -0.16860

289 -> 296 -0.14288

290 -> 305 0.18378

290 -> 306 -0.11964

290 -> 307 -0.19407

290 -> 309 0.10263

291 -> 309 -0.18260

291 -> 310 -0.21024

291 -> 312 0.12405

291 -> 313 0.17129

291 -> 314 -0.16858

292 -> 310 0.16523

292 -> 313 0.21384

Excited State 70: Singlet-A 4.8318 eV 256.60 nm f=0.0008 <S**2>=0.000

279 -> 293 -0.12336

282 -> 294 -0.20216

288 -> 295 0.10669

289 -> 296 0.31766

290 -> 305 0.15591

290 -> 307 -0.27994

290 -> 308 -0.10155

290 -> 309 -0.11368

291 -> 306 0.12140

291 -> 309 -0.17755

291 -> 310 0.15361

291 -> 314 0.14585

292 -> 313 -0.10470

Excited State 71: Singlet-A 4.8388 eV 256.23 nm f=0.0322 <S**2>=0.000

279 -> 293 0.11892

280 -> 293 0.17846

282 -> 293 -0.18461

282 -> 294 0.12841

288 -> 295 0.13274

289 -> 295 0.11982

289 -> 296 0.42387

290 -> 309 0.20374

291 -> 307 0.10497

291 -> 310 -0.13427

291 -> 314 -0.10411

Excited State 72: Singlet-A 4.8494 eV 255.67 nm f=0.0192 <S**2>=0.000

279 -> 293 -0.14692

280 -> 294 0.10598

281 -> 293 0.28021

282 -> 294 -0.16688

289 -> 295 -0.13131

289 -> 296 0.20507

290 -> 306 -0.12797

290 -> 307 0.28728

290 -> 308 0.21371

290 -> 311 -0.12151

291 -> 306 -0.16087

Excited State 73: Singlet-A 4.8770 eV 254.22 nm f=0.0239 <S**2>=0.000

280 -> 294 0.11438

281 -> 293 0.25156

282 -> 294 0.41233

285 -> 294 0.15825

289 -> 295 0.18190

290 -> 307 -0.11059

291 -> 309 -0.11905

291 -> 313 0.12156

291 -> 315 -0.11266

292 -> 314 -0.10812

292 -> 315 0.10001

292 -> 316 0.10810

Excited State 74: Singlet-A 4.8877 eV 253.67 nm f=0.0495 <S**2>=0.000

279 -> 293 0.48391

281 -> 293 -0.24523

290 -> 308 0.15327

290 -> 309 -0.15154

290 -> 311 -0.13687

291 -> 309 -0.10667

291 -> 312 0.12380

291 -> 315 -0.12092

292 -> 316 0.11610

Excited State 75: Singlet-A 4.9035 eV 252.85 nm f=0.0334 <S**2>=0.000

279 -> 293 -0.23200

280 -> 293 0.43945

280 -> 294 -0.26901

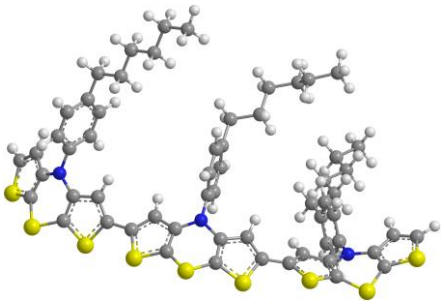
281 -> 293 -0.15879

281 -> 294 0.19337

290 -> 308 0.16661

290 -> 309 -0.17616

11.22 Computed xyz-coordinates and excitation energies of dithienothiazine trimer **5** (all-cis conformer)



C	-9.14340100	-2.25579700	-1.18067600
C	-8.55647500	-1.31027700	-0.37455600
N	-7.29774800	-1.50940200	0.23240300
C	-6.39355700	-2.37987100	-0.40989700

C	-6.81092900	-3.40956800	-1.22103900
S	-8.50507200	-3.89604700	-1.42647000
S	-10.63228900	-1.68451100	-1.87806600
C	-10.48590900	-0.18106100	-1.02479000
C	-9.34164200	-0.11544500	-0.28672000
C	-4.97199400	-2.29919900	-0.32849000
C	-4.32389000	-3.24782000	-1.08217900
S	-5.47403400	-4.24872400	-1.95233300
C	-6.80349900	-0.55718600	1.19077100
C	-6.22145000	0.64411900	0.78052400
C	-5.73066400	1.53881000	1.72807200
C	-5.80689800	1.25783100	3.09775700
C	-6.39701900	0.05125400	3.49142000
C	-6.89130600	-0.84924000	2.55123100
C	-0.58328500	-4.33058700	-1.50056000
C	-0.60041100	-2.96267400	-1.35778600
N	0.57941800	-2.18922200	-1.34148700
C	1.76595500	-2.81581600	-0.90563800
C	1.96853000	-4.17151000	-1.01698500
S	0.87085700	-5.28398700	-1.85613700
S	-2.17599300	-5.02079500	-1.38970400
C	-2.89344100	-3.42682900	-1.23012700
C	-1.92457600	-2.45269600	-1.21352100
C	2.84615400	-2.16027200	-0.24420400
C	3.85542800	-3.01196100	0.13511900
S	3.47064900	-4.67017400	-0.29453100
C	0.48950900	-0.75316900	-1.32939100
C	0.75543900	-0.04199100	-2.49881400
C	0.66721400	1.34766700	-2.50509600
C	0.30807000	2.05547600	-1.35179400
C	0.05142500	1.32706500	-0.18403800
C	0.14259900	-0.06249100	-0.16664000
C	-5.28636700	2.23828400	4.12371200

C	-6.34716900	3.25152500	4.59716100
C	-5.80486800	4.22820200	5.64608200
C	-6.84220100	5.24699500	6.13158000
C	-6.29698000	6.21706100	7.18618100
C	-7.33521100	7.23554800	7.66603200
C	0.15837800	3.55943700	-1.37857900
C	-1.23782800	4.01221000	-1.85056400
C	-1.39369900	5.53808200	-1.86530700
C	-2.78622700	6.03385400	-2.28559700
C	-3.15242500	5.75972500	-3.75000800
C	-4.51699400	6.33463200	-4.14208100
C	7.19352600	-2.62159700	2.14613600
C	7.03324600	-1.48099600	1.39357600
N	7.95037500	-0.41091100	1.43914200
C	8.69345400	-0.23805300	2.62739300
C	8.98439300	-1.28035400	3.47405300
S	8.63210400	-2.98538800	3.11894200
S	5.85964900	-3.72170100	1.95788900
C	5.10952200	-2.66562400	0.77346100
C	5.84484600	-1.51685900	0.60562600
C	9.18078200	1.01297100	3.12696300
C	9.81425000	0.89065800	4.32790000
S	9.81163600	-0.74420000	4.90852400
C	7.79860900	0.69235500	0.52832700
C	8.59935400	0.75264000	-0.61088400
C	8.46632700	1.81530000	-1.50162100
C	7.53636600	2.83627200	-1.27611600
C	6.74024200	2.76180800	-0.12619300
C	6.86548500	1.70332200	0.76927100
C	7.36962200	3.96943700	-2.26273300
C	6.27849400	3.69556700	-3.31634400
C	6.11581900	4.84027700	-4.32220900
C	5.02435300	4.58238300	-5.36689700

C	4.86306300	5.72207200	-6.37965500
C	3.76804600	5.45855800	-7.41733400
H	-11.25736400	0.56605800	-1.12748100
H	-9.06319100	0.74425000	0.30529700
H	-4.44660900	-1.58766400	0.29163700
H	-6.14614100	0.87076600	-0.27699000
H	-5.27260200	2.46521300	1.39710200
H	-6.46254100	-0.19217200	4.54679900
H	-7.33895300	-1.78531400	2.86382900
H	-2.15655900	-1.40096400	-1.13216200
H	2.86740600	-1.10006900	-0.03819900
H	1.03010800	-0.58311600	-3.39665800
H	0.87949700	1.88938400	-3.42099700
H	-0.21878200	1.85329200	0.72558300
H	-0.05454200	-0.61279100	0.74638900
H	-4.90998800	1.68709700	4.99189800
H	-4.43520300	2.78511500	3.70462400
H	-6.72253300	3.81022900	3.73161100
H	-7.20516200	2.70745900	5.00932900
H	-5.42685800	3.65954100	6.50529400
H	-4.94120900	4.76230300	5.22955900
H	-7.21744200	5.82024300	5.27396700
H	-7.70813100	4.71413900	6.54516300
H	-5.92446400	5.64353300	8.04354500
H	-5.42965400	6.74660700	6.77362100
H	-6.91591700	7.90964500	8.41815200
H	-7.69947100	7.84880300	6.83568900
H	-8.20085100	6.73605400	8.11253300
H	0.34733400	3.96344700	-0.37865900
H	0.91545700	3.99069900	-2.04219300
H	-1.42147700	3.60096800	-2.84845300
H	-1.99736100	3.57432000	-1.19135800
H	-1.16965800	5.92268700	-0.86302600

H	-0.63937500	5.97284200	-2.53400200
H	-2.84049500	7.11508300	-2.10910200
H	-3.54408300	5.58180600	-1.63213900
H	-3.15024600	4.68125000	-3.94011500
H	-2.37657800	6.18649400	-4.39775700
H	-4.75216900	6.12634300	-5.18953100
H	-4.54294900	7.42029900	-4.00440000
H	-5.31646800	5.90467900	-3.53027100
H	5.56110000	-0.73779500	-0.08703400
H	9.06657100	1.95314900	2.60719800
H	10.28231000	1.66363000	4.91723500
H	9.32427900	-0.03261700	-0.79043300
H	9.09883100	1.85323300	-2.38240600
H	6.01689800	3.54538500	0.07460400
H	6.24541100	1.66074900	1.65760800
H	7.12047400	4.88918300	-1.72273700
H	8.32129600	4.15061400	-2.77278900
H	6.52098300	2.76910900	-3.85024800
H	5.32478300	3.51625400	-2.80593100
H	5.88740700	5.76759600	-3.78127900
H	7.07237900	5.01144600	-4.83222700
H	5.24951900	3.65208900	-5.90427600
H	4.06683100	4.41573300	-4.85654500
H	4.64083600	6.65224800	-5.84267700
H	5.81898000	5.88648100	-6.89145700
H	3.67849200	6.28897900	-8.12317500
H	3.98068900	4.55296900	-7.99427400
H	2.79360700	5.32347300	-6.93720600

SCF Done: E(RB3LYP) = -6070.64506128 A.U. after 14 cycles

E(HOMO) = -4.801 eV

E(LUMO) = -1.760 eV

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5001 eV 495.91 nm f=0.3824 <S**2>=0.000

290 -> 293 0.11527

291 -> 294 0.13806

292 -> 293 0.67509

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -6070.55318352

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6890 eV 461.08 nm f=0.0380 <S**2>=0.000

290 -> 294 -0.11777

291 -> 293 0.41701

291 -> 295 0.10043

292 -> 294 0.53588

Excited State 3: Singlet-A 2.7879 eV 444.73 nm f=0.0404 <S**2>=0.000

290 -> 293 -0.39534

291 -> 293 0.25650

291 -> 294 0.43229

292 -> 294 -0.23477

292 -> 295 0.11015

Excited State 4: Singlet-A 2.8262 eV 438.70 nm f=0.0247 <S**2>=0.000

290 -> 293 0.23729

290 -> 294 -0.23953

291 -> 293 0.41438

291 -> 294 -0.25454

292 -> 294 -0.36994

Excited State 5: Singlet-A 3.0924 eV 400.93 nm f=0.0271 <S**2>=0.000

290 -> 293 0.50581

291 -> 294 0.44810

292 -> 293 -0.18533

Excited State 6: Singlet-A 3.1828 eV 389.55 nm f=0.0247 <S**2>=0.000

290 -> 294 0.60108

291 -> 293 0.28901

291 -> 295 -0.14263

292 -> 296 -0.12712

Excited State 7: Singlet-A 3.2628 eV 380.00 nm f=0.0195 <S**2>=0.000

290 -> 294 -0.10849

291 -> 294 -0.13614

291 -> 296 0.30219

292 -> 295 0.55771

292 -> 303 -0.10237

Excited State 8: Singlet-A 3.3086 eV 374.73 nm f=0.0182 <S**2>=0.000

290 -> 294 0.19538

290 -> 296 -0.14201

291 -> 295 0.39171

291 -> 296 0.17628

292 -> 296 0.45469

Excited State 9: Singlet-A 3.4743 eV 356.86 nm f=0.0779 <S**2>=0.000

290 -> 295 -0.22366

290 -> 297 0.15765

291 -> 295 -0.11065

291 -> 296 0.21045

292 -> 295 -0.11032

292 -> 297 0.55485

Excited State 10: Singlet-A 3.5582 eV 348.45 nm f=0.0649 <S**2>=0.000

290 -> 295 -0.19870

290 -> 300 0.14021

291 -> 296 0.24175

291 -> 298 0.13769

292 -> 295 -0.12822

292 -> 297 -0.19257

292 -> 298 0.26563

292 -> 299 0.15691

292 -> 300 0.34664

292 -> 303 0.18199

Excited State 11: Singlet-A 3.5706 eV 347.23 nm f=0.0029 <S**2>=0.000

290 -> 299 -0.16978

291 -> 297 0.10277

291 -> 299 -0.35937

292 -> 298 -0.22014

292 -> 299 0.47029

292 -> 300 -0.10191

Excited State 12: Singlet-A 3.5858 eV 345.77 nm f=0.0044 <S**2>=0.000

290 -> 298 -0.16436

291 -> 298 0.41933

291 -> 300 -0.12510

292 -> 298 0.34468

292 -> 299 0.12133

292 -> 300 -0.30181

Excited State 13: Singlet-A 3.6554 eV 339.18 nm f=0.0026 <S**2>=0.000

290 -> 296 0.18473

290 -> 304 0.11659

291 -> 295 -0.39936

292 -> 296 0.44739

292 -> 297 -0.12893

292 -> 301 0.10897

292 -> 304 0.11236

Excited State 14: Singlet-A 3.6782 eV 337.07 nm f=0.0078 <S**2>=0.000

291 -> 303 -0.13967

292 -> 299 -0.10228

292 -> 300 -0.21561

292 -> 301 0.13816

292 -> 302 -0.12649

292 -> 303 0.34030

292 -> 304 0.39249

Excited State 15: Singlet-A 3.6895 eV 336.05 nm f=0.0089 <S**2>=0.000

290 -> 300 0.12291

291 -> 300 -0.13590

291 -> 303 -0.21059

291 -> 304 0.17261

292 -> 300 0.20645

292 -> 302 0.12641

292 -> 303 -0.35313

292 -> 304 0.37994

Excited State 16: Singlet-A 3.6966 eV 335.40 nm f=0.0079 <S**2>=0.000

290 -> 295 0.16445

290 -> 303 -0.11556

291 -> 296 -0.19390

291 -> 297 -0.11936

291 -> 304 -0.22376

292 -> 295 0.26117

292 -> 297 0.20126

292 -> 299 0.13224

292 -> 300 0.27577

292 -> 301 -0.14361

292 -> 303 0.22398

292 -> 305 -0.11912

Excited State 17: Singlet-A 3.7325 eV 332.17 nm f=0.0096 <S**2>=0.000

290 -> 301 -0.15926

291 -> 295 0.15792

291 -> 296 -0.10873

291 -> 301 -0.34183

291 -> 303 0.11656

292 -> 299 0.11533

292 -> 301 0.46558

292 -> 302 0.15021

Excited State 18: Singlet-A 3.7529 eV 330.37 nm f=0.0128 <S**2>=0.000

290 -> 295 -0.10671

290 -> 302 -0.13662

291 -> 296 0.14595

291 -> 302 0.40709

291 -> 303 0.12870

292 -> 301 -0.11960

292 -> 302 0.41727

Excited State 19: Singlet-A 3.8377 eV 323.07 nm f=0.0265 <S**2>=0.000

290 -> 297 0.16152

290 -> 304 0.16827

291 -> 295 0.15120

291 -> 296 -0.22390

291 -> 297 0.19478

291 -> 303 0.18920

292 -> 295 0.16752

292 -> 305 0.36858

292 -> 309 -0.11768

Excited State 20: Singlet-A 3.8689 eV 320.46 nm f=0.0571 <S**2>=0.000

289 -> 294 -0.10307

290 -> 295 0.39757

290 -> 296 -0.10422

290 -> 297 -0.12512

290 -> 303 -0.12176

291 -> 296 0.30125

291 -> 297 0.13921

291 -> 304 -0.12526

292 -> 305 0.20840

Excited State 21: Singlet-A 3.9074 eV 317.30 nm f=0.0007 <S**2>=0.000

290 -> 296 -0.16427

290 -> 298 0.11064

290 -> 303 0.10403

291 -> 295 -0.10736

291 -> 297 0.52266

291 -> 298 -0.12136

291 -> 303 -0.12982

292 -> 298 0.19678

292 -> 303 0.11563

292 -> 305 -0.11075

Excited State 22: Singlet-A 3.9548 eV 313.50 nm f=0.0065 <S**2>=0.000

289 -> 293 -0.10088

290 -> 297 0.11023

290 -> 298 -0.11765

290 -> 299 -0.12570

291 -> 297 0.21701

291 -> 298 0.32635

292 -> 298 -0.26132

292 -> 299 -0.22402

292 -> 300 0.15048

292 -> 305 -0.25719

292 -> 306 -0.13234

Excited State 23: Singlet-A 3.9683 eV 312.44 nm f=0.0164 <S**2>=0.000

289 -> 293 -0.10025

290 -> 296 0.21066

290 -> 298 0.16422

290 -> 299 -0.13392

290 -> 304 0.10968

291 -> 295 0.11916

291 -> 298 -0.12652

291 -> 299 -0.29400

291 -> 300 0.18653

292 -> 298 0.35298

292 -> 299 -0.17480

Excited State 24: Singlet-A 3.9756 eV 311.86 nm f=0.0083 <S**2>=0.000

289 -> 293 -0.16111

290 -> 299 0.16015

290 -> 304 0.10706

291 -> 298 -0.10234

291 -> 299 0.34685

291 -> 300 0.25545

291 -> 306 0.10941

292 -> 299 0.27434

292 -> 300 -0.13279

292 -> 304 0.14915

292 -> 305 -0.17516

292 -> 306 -0.17910

Excited State 25: Singlet-A 3.9917 eV 310.60 nm f=0.0060 <S**2>=0.000

290 -> 296 0.41982

291 -> 295 0.16445

291 -> 297 0.13095

291 -> 298 -0.14442

291 -> 300 -0.41689

292 -> 299 0.13372

Excited State 26: Singlet-A 4.0062 eV 309.48 nm f=0.0164 <S**2>=0.000

289 -> 293 -0.19408

290 -> 295 -0.28270

290 -> 303 -0.17569

291 -> 297 0.10389

291 -> 304 -0.24405

291 -> 306 -0.20607

291 -> 308 -0.11409

292 -> 301 0.15615

292 -> 303 -0.10546

292 -> 306 0.29245

292 -> 307 0.15449

Excited State 27: Singlet-A 4.0232 eV 308.17 nm f=0.0554 <S**2>=0.000

289 -> 293 0.53536

290 -> 295 -0.12622

290 -> 303 -0.11790

291 -> 304 -0.14979

291 -> 305 0.10036

291 -> 307 0.14174

292 -> 306 -0.13894

292 -> 307 0.16043

Excited State 28: Singlet-A 4.0340 eV 307.35 nm f=0.8633 <S**2>=0.000

288 -> 293 0.36345

289 -> 294 0.48562

290 -> 295 0.15510

291 -> 300 0.10210

Excited State 29: Singlet-A 4.0386 eV 307.00 nm f=0.1164 <S**2>=0.000

288 -> 293 0.15560

289 -> 293 0.12078

289 -> 294 0.15253

290 -> 295 0.14352

290 -> 296 -0.14943

290 -> 297 0.25408

290 -> 304 0.11720

291 -> 300 -0.18687

291 -> 302 -0.11619

291 -> 303 0.19856

291 -> 305 -0.16510

291 -> 307 -0.20272

292 -> 302 0.10226

292 -> 304 0.11351

292 -> 305 -0.11324

292 -> 307 -0.15788

Excited State 30: Singlet-A 4.0529 eV 305.92 nm f=0.0596 <S**2>=0.000

289 -> 293 0.23304

290 -> 296 0.31176

290 -> 297 0.16958

291 -> 299 0.11922

291 -> 300 0.26666

291 -> 303 -0.10136

291 -> 306 -0.11152

291 -> 307 -0.18153

292 -> 306 0.20657

Excited State 31: Singlet-A 4.0817 eV 303.76 nm f=0.0666 <S**2>=0.000

289 -> 294 -0.10712

290 -> 296 -0.12056

290 -> 297 0.46869

290 -> 300 -0.11132

291 -> 297 -0.11527

291 -> 304 0.15410

291 -> 307 0.17996

292 -> 297 -0.13868

292 -> 300 0.10225

292 -> 302 -0.11991

292 -> 307 0.17560

Excited State 32: Singlet-A 4.1090 eV 301.74 nm f=0.0086 <S**2>=0.000

289 -> 293 -0.10298

290 -> 297 0.13112

290 -> 300 -0.14633

290 -> 303 -0.17656

290 -> 305 0.14243

291 -> 301 -0.14182

291 -> 302 0.28451

291 -> 303 -0.16176

291 -> 304 -0.18180

291 -> 306 0.16638

291 -> 307 -0.12228

291 -> 308 0.12711

292 -> 302 -0.18628

292 -> 305 0.10366

292 -> 307 -0.20344

Excited State 33: Singlet-A 4.1214 eV 300.83 nm f=0.0280 <S**2>=0.000

290 -> 300 -0.12076

290 -> 302 0.18481

290 -> 304 -0.10966

291 -> 302 -0.30342

291 -> 303 -0.27492

292 -> 302 0.36282

292 -> 303 0.15700

292 -> 304 -0.10486

292 -> 305 0.18511

Excited State 34: Singlet-A 4.1288 eV 300.29 nm f=0.0114 <S**2>=0.000

290 -> 301 0.23453

291 -> 301 0.46669

292 -> 301 0.37134

Excited State 35: Singlet-A 4.1653 eV 297.66 nm f=0.0109 <S**2>=0.000

288 -> 293 -0.23270

290 -> 297 0.13093

290 -> 298 0.12105

290 -> 299 0.24039

290 -> 300 0.47339

290 -> 303 -0.12515

291 -> 304 -0.10770

292 -> 300 -0.14969

Excited State 36: Singlet-A 4.1831 eV 296.39 nm f=0.0102 <S**2>=0.000

288 -> 293 0.48501

289 -> 294 -0.40821

290 -> 300 0.16577

Excited State 37: Singlet-A 4.2163 eV 294.06 nm f=0.0096 <S**2>=0.000

288 -> 294 -0.16877

290 -> 299 -0.12107

290 -> 306 -0.15205

291 -> 303 -0.13480

291 -> 308 -0.16691

292 -> 304 -0.18963

292 -> 306 -0.23852

292 -> 308 0.40463

292 -> 309 -0.17242

Excited State 38: Singlet-A 4.2314 eV 293.01 nm f=0.0069 <S**2>=0.000

290 -> 298 -0.17921

290 -> 299 0.35786

290 -> 300 -0.12711

290 -> 303 -0.10888

291 -> 299 -0.23500

291 -> 303 0.14608

291 -> 304 0.15101

291 -> 305 0.25380

291 -> 307 -0.14708

292 -> 308 0.14957

292 -> 309 0.15254

Excited State 39: Singlet-A 4.2462 eV 291.99 nm f=0.0072 <S**2>=0.000

290 -> 298 -0.15638

290 -> 299 0.36051

290 -> 300 -0.14201

290 -> 303 0.12889

291 -> 299 -0.20508

291 -> 303 -0.16405

291 -> 305 -0.25538

291 -> 307 0.14627

292 -> 309 -0.20284

Excited State 40: Singlet-A 4.2673 eV 290.55 nm f=0.0004 <S**2>=0.000

290 -> 298 0.54882

290 -> 299 0.16809

290 -> 300 -0.21531

291 -> 298 0.27663

291 -> 300 -0.10203

Excited State 41: Singlet-A 4.3151 eV 287.32 nm f=0.0077 <S**2>=0.000

287 -> 293 -0.18543

288 -> 294 0.58114

289 -> 293 -0.10885

290 -> 304 0.10628

292 -> 308 0.10026

Excited State 42: Singlet-A 4.3373 eV 285.86 nm f=0.0054 <S**2>=0.000

288 -> 294 -0.15411

290 -> 301 0.16924

290 -> 302 -0.20692

290 -> 303 0.34769

291 -> 304 -0.34345

291 -> 305 0.12189

291 -> 309 0.10963

292 -> 303 -0.16179

292 -> 309 0.17441

Excited State 43: Singlet-A 4.3579 eV 284.51 nm f=0.0151 <S**2>=0.000

286 -> 293 0.34038

286 -> 294 0.19982

287 -> 293 0.13535

287 -> 294 -0.15778

290 -> 302 0.11706

290 -> 305 -0.26943

290 -> 306 -0.12664

291 -> 303 -0.10180

291 -> 306 -0.12399

291 -> 308 0.10933

291 -> 309 0.18614

292 -> 310 -0.11778

Excited State 44: Singlet-A 4.3759 eV 283.33 nm f=0.0071 <S**2>=0.000

287 -> 293 -0.14494

287 -> 294 0.10704

288 -> 294 -0.18811

290 -> 301 0.32192

290 -> 302 0.10326

290 -> 304 0.37031

291 -> 301 -0.17117

291 -> 303 -0.13442

291 -> 304 0.10299

292 -> 304 -0.10559

292 -> 306 0.10191

292 -> 309 0.10002

292 -> 311 0.11734

Excited State 45: Singlet-A 4.3926 eV 282.26 nm f=0.0004 <S**2>=0.000

286 -> 293 0.11370

290 -> 301 0.45260

290 -> 303 -0.10943

290 -> 304 -0.27935

291 -> 301 -0.24683

291 -> 303 0.15817

292 -> 309 -0.10115

Excited State 46: Singlet-A 4.4133 eV 280.93 nm f=0.0132 <S**2>=0.000

287 -> 293 0.37555

287 -> 294 -0.25389

290 -> 302 -0.34388

290 -> 304 0.18642

291 -> 302 -0.15354

291 -> 305 0.13173

292 -> 310 0.11301

Excited State 47: Singlet-A 4.4268 eV 280.08 nm f=0.0500 <S**2>=0.000

286 -> 293 0.38084

286 -> 294 0.23166

290 -> 303 0.13471

290 -> 305 0.15821

290 -> 306 0.10635

291 -> 309 -0.17684

292 -> 305 -0.11309

292 -> 306 0.14424

292 -> 308 -0.10120

292 -> 309 -0.19252

292 -> 310 0.20057

Excited State 48: Singlet-A 4.4327 eV 279.71 nm f=0.0146 <S**2>=0.000

287 -> 293 0.23633

287 -> 294 -0.15350

290 -> 302 0.42624

290 -> 303 0.28056

290 -> 305 0.12664

291 -> 302 0.20125

292 -> 309 0.12347

Excited State 49: Singlet-A 4.4749 eV 277.07 nm f=0.0074 <S**2>=0.000

286 -> 293 -0.20924

286 -> 294 -0.10332

290 -> 305 -0.11250

290 -> 309 -0.10708

291 -> 305 0.41787

291 -> 308 0.12384

292 -> 306 0.11048

292 -> 307 -0.22680

292 -> 309 -0.29975

Excited State 50: Singlet-A 4.5081 eV 275.02 nm f=0.0057 <S**2>=0.000

290 -> 303 0.13390

290 -> 304 -0.16994

290 -> 307 0.12157

290 -> 309 0.11829

290 -> 310 -0.11186

291 -> 307 -0.10258

291 -> 308 0.12713

291 -> 309 -0.14199

291 -> 310 0.24245

291 -> 311 0.26343

292 -> 310 0.26350

292 -> 311 0.25810

Excited State 51: Singlet-A 4.5209 eV 274.25 nm f=0.0108 <S**2>=0.000

287 -> 293 0.18057

290 -> 304 -0.12475

290 -> 306 0.13768

290 -> 308 -0.13876

291 -> 306 0.22582

291 -> 308 -0.20527

291 -> 310 0.26962

291 -> 313 0.11551

292 -> 306 0.10991

292 -> 309 -0.15781

292 -> 310 -0.20460

292 -> 311 0.19301

292 -> 313 -0.12390

Excited State 52: Singlet-A 4.5987 eV 269.61 nm f=0.0019 <S**2>=0.000

290 -> 305 0.35155

290 -> 306 -0.15817

291 -> 306 -0.26769

291 -> 307 -0.10962

292 -> 306 -0.18467

292 -> 308 -0.20868

292 -> 310 -0.20219

292 -> 311 0.20788

292 -> 312 0.11473

Excited State 53: Singlet-A 4.6263 eV 268.00 nm f=0.0050 <S**2>=0.000

290 -> 307 0.19612

290 -> 309 -0.13370

291 -> 306 0.19190

291 -> 307 -0.23956

292 -> 307 0.41189

292 -> 309 -0.22919

292 -> 312 0.13314

Excited State 54: Singlet-A 4.6597 eV 266.08 nm f=0.0158 <S**2>=0.000

287 -> 293 -0.14884

287 -> 294 -0.20457

290 -> 310 -0.20404

290 -> 311 0.10076

291 -> 306 0.12829

291 -> 308 -0.17329

291 -> 311 0.21094

291 -> 313 -0.11776

292 -> 307 -0.11943

292 -> 310 -0.10286

292 -> 311 0.12237

292 -> 312 0.17548

292 -> 313 0.30808

292 -> 316 -0.15240

Excited State 55: Singlet-A 4.6810 eV 264.86 nm f=0.0086 <S**2>=0.000

283 -> 293 -0.10056

285 -> 293 -0.16742

286 -> 293 0.16691

286 -> 294 -0.15111

287 -> 293 0.25934

287 -> 294 0.40603

290 -> 305 -0.15610

291 -> 307 -0.13816

291 -> 308 -0.11954

292 -> 308 -0.15650

Excited State 56: Singlet-A 4.6911 eV 264.30 nm f=0.0204 <S**2>=0.000

286 -> 293 -0.13642

286 -> 294 0.24586

287 -> 293 0.20451

287 -> 294 0.24775

290 -> 305 0.13096

290 -> 308 0.14285

291 -> 306 0.11424

291 -> 307 0.15404

291 -> 308 0.11397

291 -> 309 0.15282

291 -> 311 0.12182

292 -> 306 0.14329

292 -> 308 0.14925

292 -> 311 0.14986

292 -> 312 0.14691

292 -> 313 0.15976

Excited State 57: Singlet-A 4.7031 eV 263.62 nm f=0.0073 <S**2>=0.000

286 -> 293 -0.27454

286 -> 294 0.46763

290 -> 308 -0.13807

291 -> 307 -0.13337

291 -> 308 -0.11001

291 -> 309 -0.11361

292 -> 308 -0.12735

292 -> 312 -0.11106

Excited State 58: Singlet-A 4.7349 eV 261.85 nm f=0.0207 <S**2>=0.000

282 -> 293 -0.10490
286 -> 294 0.12360
290 -> 306 -0.11189
290 -> 310 0.11601
291 -> 308 -0.21958
291 -> 309 0.12355
291 -> 312 0.22855
291 -> 314 -0.12773
291 -> 315 0.10291
291 -> 316 0.12144
292 -> 307 -0.10474
292 -> 308 -0.16324
292 -> 310 0.22340
292 -> 312 0.19523
292 -> 313 -0.17942
292 -> 314 -0.12956
292 -> 315 0.11353
292 -> 316 0.13146

Excited State 59: Singlet-A 4.7432 eV 261.39 nm f=0.0008 <S**2>=0.000

282 -> 293 -0.21647
283 -> 293 0.13856
285 -> 293 0.35636
287 -> 293 0.10196
287 -> 294 0.15818
288 -> 295 0.12493
289 -> 295 -0.17514
289 -> 296 0.16315
291 -> 309 -0.22006
292 -> 308 0.11848

292 -> 312 0.17131

Excited State 60: Singlet-A 4.7510 eV 260.96 nm f=0.0154 <S**2>=0.000

282 -> 293 0.53618

285 -> 293 -0.12182

290 -> 305 -0.11954

291 -> 309 -0.21150

292 -> 312 0.17984

Excited State 61: Singlet-A 4.7575 eV 260.61 nm f=0.0081 <S**2>=0.000

282 -> 293 -0.15374

285 -> 294 0.13610

287 -> 294 -0.10227

288 -> 296 0.16946

289 -> 295 0.48730

290 -> 305 -0.14651

291 -> 309 -0.14945

292 -> 312 0.10825

292 -> 313 -0.10218

Excited State 62: Singlet-A 4.7629 eV 260.31 nm f=0.0073 <S**2>=0.000

282 -> 293 0.32123

284 -> 294 0.12147

285 -> 293 0.32713

285 -> 294 0.10358

286 -> 294 -0.14114

287 -> 294 0.11739

289 -> 295 0.20112

289 -> 296 0.13518

290 -> 306 0.11493

291 -> 309 0.15612

Excited State 63: Singlet-A 4.7720 eV 259.81 nm f=0.0094 <S**2>=0.000

283 -> 293 -0.26816

283 -> 294 -0.17702

284 -> 293 0.43881

284 -> 294 0.22884

285 -> 293 0.14270

285 -> 294 0.16430

289 -> 295 -0.10762

290 -> 306 -0.14924

Excited State 64: Singlet-A 4.7785 eV 259.46 nm f=0.0031 <S**2>=0.000

283 -> 294 -0.12086

284 -> 293 0.25384

285 -> 293 -0.14563

285 -> 294 0.12906

289 -> 295 -0.12146

290 -> 306 0.36466

290 -> 308 -0.12771

291 -> 306 -0.19428

292 -> 312 0.18099

Excited State 65: Singlet-A 4.7842 eV 259.15 nm f=0.0078 <S**2>=0.000

283 -> 293 0.44635

283 -> 294 -0.22234

284 -> 293 0.24775

284 -> 294 -0.25361

290 -> 306 -0.17668

Excited State 66: Singlet-A 4.7987 eV 258.37 nm f=0.0133 <S**2>=0.000

288 -> 295 -0.10028

289 -> 296 -0.12780

290 -> 306 0.20516

290 -> 307 0.12499

290 -> 309 0.10699

291 -> 306 -0.15242

291 -> 308 0.17069

291 -> 309 -0.12874

291 -> 312 0.28193

291 -> 313 -0.10297

291 -> 316 0.13408

292 -> 308 0.12207

292 -> 310 -0.10926

292 -> 314 -0.23717

292 -> 315 0.20223

Excited State 67: Singlet-A 4.8514 eV 255.56 nm f=0.0136 <S**2>=0.000

283 -> 293 -0.23232

285 -> 293 -0.25901

288 -> 295 0.25172

289 -> 296 0.43285

Excited State 68: Singlet-A 4.8741 eV 254.37 nm f=0.0067 <S**2>=0.000

283 -> 294 0.19472

285 -> 294 0.25897

290 -> 307 0.20606

290 -> 309 0.15387

290 -> 311 0.16904

291 -> 307 0.12904

291 -> 308 -0.10312

291 -> 309 0.14238

291 -> 311 -0.13317

291 -> 313 -0.16488

292 -> 309 -0.10835

292 -> 310 0.18098

292 -> 318 0.16739

Excited State 69: Singlet-A 4.8981 eV 253.13 nm f=0.0008 <S**2>=0.000

282 -> 294 0.65802

285 -> 294 -0.12328

Excited State 70: Singlet-A 4.9057 eV 252.73 nm f=0.0019 <S**2>=0.000

279 -> 293 0.19857

282 -> 294 0.17876

290 -> 306 0.20419

290 -> 307 -0.10053

290 -> 312 -0.16311

291 -> 308 -0.12615

291 -> 313 -0.13800

291 -> 314 -0.15588

291 -> 315 0.16310

292 -> 313 0.18221

292 -> 316 0.30661

Excited State 71: Singlet-A 4.9115 eV 252.43 nm f=0.0048 <S**2>=0.000

281 -> 293 -0.14981

282 -> 294 0.14430

283 -> 294 0.28464

285 -> 294 0.39386

289 -> 295 -0.11984

290 -> 307 -0.17977

290 -> 311 -0.10587

291 -> 308 0.11904

292 -> 310 -0.10345

292 -> 311 -0.10858

Excited State 72: Singlet-A 4.9594 eV 250.00 nm f=0.0128 <S**2>=0.000

279 -> 293 0.36917

280 -> 293 0.23462

281 -> 293 0.26447

281 -> 294 0.18803

288 -> 295 0.12088

288 -> 296 -0.10944

289 -> 297 -0.12286

290 -> 307 -0.10488

291 -> 309 0.11123

292 -> 316 -0.12597

Excited State 73: Singlet-A 4.9627 eV 249.83 nm f=0.0049 <S**2>=0.000

280 -> 293 -0.11542

289 -> 297 -0.20149

290 -> 307 0.39391

290 -> 308 0.20678

290 -> 311 -0.11237

291 -> 306 -0.11453

291 -> 308 -0.25403

291 -> 311 0.13701

292 -> 311 -0.11580

292 -> 318 -0.12476

Excited State 74: Singlet-A 4.9726 eV 249.34 nm f=0.0061 <S**2>=0.000

280 -> 293 0.30240

280 -> 294 -0.26908

281 -> 293 -0.26543

288 -> 297 -0.17166

289 -> 296 -0.13455

289 -> 297 0.29358

290 -> 307 0.14930

Excited State 75: Singlet-A 4.9750 eV 249.21 nm f=0.0400 <S**2>=0.000

279 -> 293 0.43498

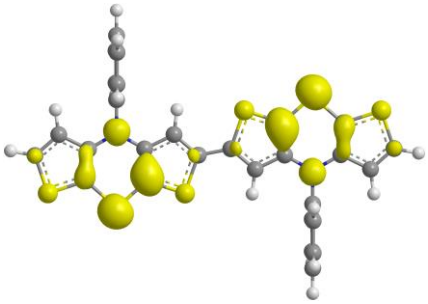
280 -> 294 -0.12582

281 -> 293 -0.27629

281 -> 294 -0.16227

289 -> 296	0.11351	
289 -> 297	-0.18844	
292 -> 311	0.13261	

11.23 Computed xyz-coordinates of the first oxidation state of dithienothiazine dimer (UB3LYP)

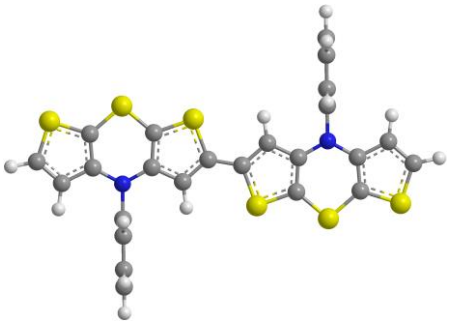


C	-2.781970	-1.552150	-0.000085
C	-3.024950	-0.175046	0.000208
N	-4.298730	0.378211	0.000469
C	-5.435320	-0.437838	0.000166
C	-5.395880	-1.816940	-0.000173
S	-3.959700	-2.837790	-0.000321
S	-1.088850	-1.920290	-0.000253
C	-0.682034	-0.207182	0.000112
C	-1.825690	0.570248	0.000340
C	-6.777850	0.057635	0.000164
C	-7.703850	-0.939375	-0.000166
S	-6.986830	-2.517140	-0.000487
C	-4.448640	1.814340	0.000328
C	-4.519920	2.498560	1.212920
C	-4.663560	3.884640	1.208480
C	-4.733980	4.576660	0.000088
C	-4.662210	3.884570	-1.208190
C	-4.518580	2.498490	-1.212390
C	0.682033	0.207186	0.000116
C	1.825690	-0.570247	0.000390
C	3.024950	0.175045	0.000267
C	2.781970	1.552150	-0.000087
S	1.088850	1.920290	-0.000291

N	4.298730	-0.378209	0.000555
C	5.435320	0.437837	0.000261
C	5.395870	1.816940	-0.000173
S	3.959700	2.837790	-0.000483
C	6.777840	-0.057635	0.000435
C	7.703850	0.939375	0.000113
S	6.986830	2.517130	-0.000383
C	4.448640	-1.814340	0.000345
C	4.519280	-2.498690	1.212910
C	4.662920	-3.884760	1.208410
C	4.733990	-4.576660	-0.000021
C	4.662880	-3.884440	-1.208270
C	4.519230	-2.498370	-1.212400
H	-1.806290	1.650350	0.000598
H	-7.028690	1.107790	0.000397
H	-8.778850	-0.850538	-0.000216
H	-4.464740	1.948600	2.144820
H	-4.721290	4.421220	2.147960
H	-4.846180	5.654450	-0.000011
H	-4.718920	4.421090	-2.147760
H	-4.462380	1.948480	-2.144200
H	1.806290	-1.650350	0.000673
H	7.028680	-1.107790	0.000773
H	8.778840	0.850537	0.000170
H	4.463600	-1.948810	2.144830
H	4.720160	-4.421430	2.147860
H	4.846200	-5.654450	-0.000168
H	4.720090	-4.420870	-2.147860
H	4.463520	-1.948260	-2.144190

SCF Done: E(UB3LYP) = -3575.43304339   A.U. after   1 cycles

11.24 Computed xyz-coordinates of the second oxidation state of dithienothiazine dimer (singlet; UB3LYP)

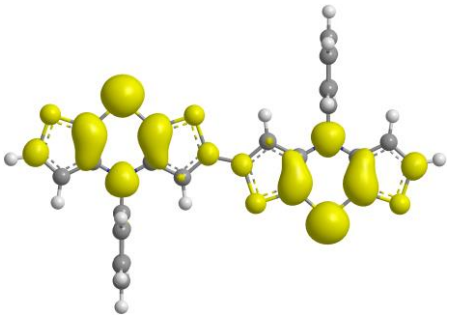


C	-0.102557	4.012690	-1.603150
C	-0.961587	2.964650	-1.181280
N	-2.337920	3.070500	-1.210630
C	-2.978400	4.218010	-1.660560
C	-2.303510	5.347380	-2.111510
S	-0.578485	5.543660	-2.199880
S	1.562500	3.599050	-1.456010
C	1.138170	2.005050	-0.820570
C	-0.240794	1.846900	-0.744141
C	-4.393420	4.386840	-1.720220
C	-4.745660	5.609830	-2.203320
S	-3.388890	6.608240	-2.606690
C	-3.132440	1.942740	-0.760905
C	-3.494500	0.958329	-1.677400
C	-4.254610	-0.124289	-1.240100
C	-4.641650	-0.213014	0.096441
C	-4.271180	0.779746	1.002610
C	-3.510440	1.866860	0.577525
C	2.158390	1.095310	-0.469011
C	3.537340	1.252520	-0.547684
C	4.258110	0.134973	-0.109936
C	3.399030	-0.911854	0.314863
S	1.734070	-0.497418	0.169650
N	5.634410	0.028130	-0.082716
C	6.274770	-1.118970	0.368503

C	5.599820	-2.246960	0.822758
S	3.874810	-2.442070	0.913689
C	7.689750	-1.288590	0.426400
C	8.041930	-2.510760	0.911628
S	6.685110	-3.507420	1.319110
C	6.429140	1.154220	-0.536231
C	6.803570	1.227460	-1.875800
C	7.564780	2.312730	-2.304720
C	7.939280	3.306330	-1.401150
C	7.555770	3.220290	-0.063413
C	6.795210	2.139550	0.377719
H	-0.716105	0.947638	-0.381155
H	-5.104240	3.633180	-1.418100
H	-5.740200	6.000870	-2.352840
H	-3.186700	1.041970	-2.712550
H	-4.544980	-0.893987	-1.944680
H	-5.234670	-1.055420	0.431744
H	-4.574880	0.711964	2.040090
H	-3.217050	2.646490	1.269920
H	4.012600	2.150800	-0.913117
H	8.400570	-0.536039	0.121545
H	9.036440	-2.902140	1.060480
H	6.507080	0.447159	-2.566140
H	7.865800	2.378370	-3.343120
H	8.532690	4.147270	-1.739390
H	7.849230	3.990670	0.639146
H	6.490230	2.058080	1.413860

SCF Done: E(UB3LYP) = -3575.23544655 A.U. after 1 cycles

11.25 Computed xyz-coordinates of the second oxidation state of dithienothiazine dimer (triplet; UB3LYP)

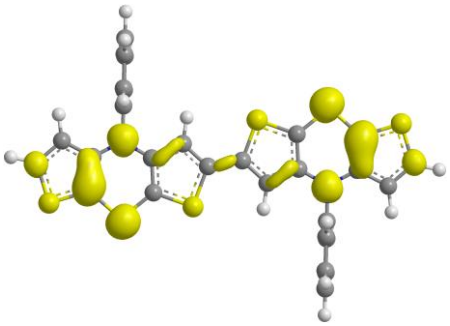


C	2.780360	1.558210	-0.001482
C	3.020940	0.182131	0.000162
N	4.287870	-0.370401	0.000749
C	5.419820	0.421117	-0.000380
C	5.381970	1.820000	-0.002227
S	3.966460	2.821490	-0.003283
S	1.086430	1.925260	-0.002279
C	0.690429	0.211495	-0.000127
C	1.815920	-0.571890	0.001042
C	6.758090	-0.077739	0.000115
C	7.677120	0.922515	-0.001374
S	6.972580	2.509440	-0.003424
C	4.431710	-1.817020	0.002372
C	4.499630	-2.489520	1.219660
C	4.638490	-3.875810	1.213900
C	4.707170	-4.567870	0.005535
C	4.638760	-3.878560	-1.204420
C	4.499910	-2.492290	-1.213370
C	-0.690432	-0.211502	-0.000125
C	-1.815920	0.571885	0.001098
C	-3.020940	-0.182134	0.000135
C	-2.780370	-1.558210	-0.001594
S	-1.086430	-1.925270	-0.002370
N	-4.287870	0.370400	0.000785
C	-5.419820	-0.421115	-0.000392

C	-5.381970	-1.820000	-0.002203
S	-3.966470	-2.821490	-0.003245
C	-6.758090	0.077743	-0.000067
C	-7.677130	-0.922508	-0.001608
S	-6.972590	-2.509440	-0.003488
C	-4.431710	1.817020	0.002402
C	-4.500400	2.489480	1.219660
C	-4.639240	3.875770	1.213850
C	-4.707150	4.567870	0.005466
C	-4.637980	3.878600	-1.204460
C	-4.499130	2.492330	-1.213370
H	1.798720	-1.651690	0.002468
H	7.009900	-1.126920	0.001511
H	8.752600	0.833534	-0.001411
H	4.446830	-1.938340	2.150640
H	4.694300	-4.411420	2.153560
H	4.816220	-5.645670	0.006781
H	4.694770	-4.416310	-2.142850
H	4.447290	-1.943260	-2.145630
H	-1.798720	1.651680	0.002630
H	-7.009900	1.126920	0.001252
H	-8.752600	-0.833526	-0.001756
H	-4.448170	1.938300	2.150670
H	-4.695620	4.411360	2.153490
H	-4.816190	5.645670	0.006669
H	-4.693410	4.416380	-2.142910
H	-4.445940	1.943310	-2.145600

SCF Done: E(UB3LYP) = -3575.24415947 A.U. after 1 cycles

11.26 Computed xyz-coordinates of the third oxidation state of dithienothiazine dimer (UB3LYP)

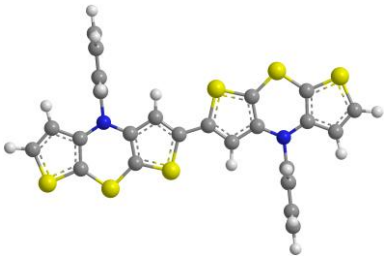


C	-2.756370	-1.564230	-0.000692
C	-3.006270	-0.165386	0.000391
N	-4.274810	0.362447	0.000655
C	-5.401490	-0.418364	-0.000097
C	-5.356760	-1.831780	-0.001699
S	-3.937620	-2.791680	-0.002660
S	-1.073930	-1.930280	-0.000894
C	-0.681702	-0.206842	0.000279
C	-1.815210	0.582300	0.000955
C	-6.737830	0.069404	0.000483
C	-7.644300	-0.943769	-0.000696
S	-6.937990	-2.531020	-0.002655
C	-4.425460	1.815470	0.001572
C	-4.495390	2.481630	1.221530
C	-4.640640	3.867090	1.212660
C	-4.712530	4.557080	0.003326
C	-4.641250	3.868590	-1.206880
C	-4.496050	2.483120	-1.217530
C	0.681683	0.206825	0.000213
C	1.815200	-0.582312	0.000938
C	3.006250	0.165376	0.000262
C	2.756350	1.564220	-0.000890
S	1.073910	1.930270	-0.001263
N	4.274800	-0.362447	0.000648
C	5.401470	0.418371	-0.000054

C	5.356730	1.831780	-0.001568
S	3.937590	2.791680	-0.002645
C	6.737820	-0.069396	0.000349
C	7.644280	0.943777	-0.000874
S	6.937960	2.531030	-0.002438
C	4.425480	-1.815470	0.001592
C	4.495580	-2.481640	1.221520
C	4.640830	-3.867120	1.212610
C	4.712620	-4.557070	0.003266
C	4.641210	-3.868550	-1.206930
C	4.495940	-2.483100	-1.217540
H	-1.798510	1.662000	0.001763
H	-7.001800	1.115250	0.001764
H	-8.721010	-0.863344	-0.000540
H	-4.441570	1.931670	2.153060
H	-4.700420	4.402840	2.151720
H	-4.827590	5.634020	0.004027
H	-4.701480	4.405480	-2.145260
H	-4.442690	1.934360	-2.149810
H	1.798490	-1.662010	0.001969
H	7.001780	-1.115240	0.001463
H	8.720990	0.863353	-0.000915
H	4.441830	-1.931740	2.153100
H	4.700700	-4.402870	2.151660
H	4.827710	-5.634010	0.003923
H	4.701390	-4.405430	-2.145320
H	4.442500	-1.934270	-2.149770

SCF Done: E(UB3LYP) = -3575.01275514 A.U. after 1 cycles

11.27 Computed xyz-coordinates of the fourth oxidation state of dithienothiazine dimer (singlet; UB3LYP)

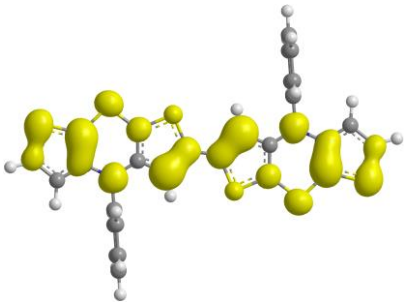


C	-2.754433	-1.573114	-0.013306
C	-3.005865	-0.170158	0.016236
N	-4.264743	0.351399	0.020628
C	-5.389141	-0.404187	-0.001127
C	-5.348579	-1.843675	-0.048850
S	-3.942539	-2.779316	-0.073664
S	-1.071897	-1.936294	-0.017763
C	-0.690320	-0.210688	0.017352
C	-1.807535	0.584189	0.034187
C	-6.721184	0.085679	0.009555
C	-7.622478	-0.928373	-0.030808
S	-6.924007	-2.527971	-0.083012
C	-4.412642	1.815321	0.043803
C	-4.473767	2.456074	1.276803
C	-4.622766	3.840991	1.285035
C	-4.705934	4.546176	0.085348
C	-4.641868	3.875767	-1.135311
C	-4.494294	2.491108	-1.169495
C	0.690310	0.210492	0.017446
C	1.807574	-0.584335	0.034368
C	3.005857	0.170082	0.016511
C	2.754349	1.573021	-0.012956
S	1.071795	1.936094	-0.017645
N	4.264765	-0.351405	0.020853
C	5.389124	0.404249	-0.001017
C	5.348468	1.843737	-0.048717

S	3.942378	2.779298	-0.073298
C	6.721209	-0.085518	0.009458
C	7.622424	0.928601	-0.031031
S	6.923838	2.528140	-0.083393
C	4.412742	-1.815317	0.043933
C	4.473857	-2.456151	1.276901
C	4.622960	-3.841049	1.285048
C	4.706211	-4.546156	0.085311
C	4.642139	-3.875679	-1.135302
C	4.494488	-2.491019	-1.169399
H	-1.793436	1.663818	0.055214
H	-6.987066	1.130208	0.045096
H	-8.700139	-0.849775	-0.032996
H	-4.412976	1.893974	2.200377
H	-4.677234	4.363233	2.231705
H	-4.824482	5.622357	0.101827
H	-4.710074	4.425237	-2.065551
H	-4.447896	1.956850	-2.110432
H	1.793556	-1.663962	0.055338
H	6.987179	-1.130024	0.044947
H	8.700091	0.850085	-0.033378
H	4.413023	-1.894096	2.200498
H	4.677446	-4.363358	2.231680
H	4.824821	-5.622331	0.101732
H	4.710405	-4.425079	-2.065579
H	4.448115	-1.956707	-2.110303

SCF Done: E(UB3LYP) = -3574.75280576 A.U. after 1 cycles

11.28 Computed xyz-coordinates of the fourth oxidation state of dithienothiazine dimer (triplet; UB3LYP)

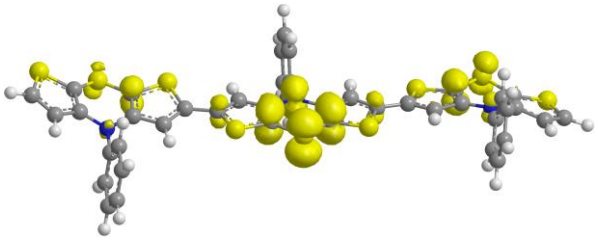


C	-2.735259	-1.574069	-0.001069
C	-2.998506	-0.169167	0.001144
N	-4.276576	0.361260	0.001425
C	-5.385931	-0.417011	-0.000712
C	-5.332723	-1.846499	-0.005614
S	-3.904096	-2.809455	-0.007922
S	-1.052821	-1.942466	-0.000339
C	-0.660872	-0.220501	0.001776
C	-1.830762	0.581082	0.002423
C	-6.729714	0.062362	0.000948
C	-7.622687	-0.954840	-0.002901
S	-6.890023	-2.548100	-0.008278
C	-4.425288	1.819055	0.003952
C	-4.492418	2.479501	1.227389
C	-4.640098	3.864588	1.218177
C	-4.716779	4.554718	0.009255
C	-4.647450	3.868462	-1.202314
C	-4.500263	2.483350	-1.216950
C	0.660897	0.220273	0.001808
C	1.830761	-0.581238	0.002629
C	2.998503	0.169089	0.001223
C	2.735189	1.573991	-0.001074
S	1.052762	1.942314	-0.000468
N	4.276566	-0.361219	0.001527
C	5.385903	0.417052	-0.000663
C	5.332640	1.846592	-0.005470

S	3.904008	2.809372	-0.007716
C	6.729672	-0.062262	0.000713
C	7.622600	0.954993	-0.003136
S	6.889933	2.548248	-0.008507
C	4.425362	-1.819025	0.004040
C	4.493252	-2.479456	1.227431
C	4.640929	-3.864550	1.218110
C	4.716977	-4.554662	0.009147
C	4.646952	-3.868397	-1.202384
C	4.499635	-2.483303	-1.216924
H	-1.816323	1.661763	0.003247
H	-6.999982	1.106667	0.004866
H	-8.700914	-0.893574	-0.002704
H	-4.437763	1.929256	2.158708
H	-4.699100	4.399238	2.157685
H	-4.834594	5.631163	0.011358
H	-4.711845	4.406151	-2.139737
H	-4.451295	1.936373	-2.150523
H	1.816380	-1.661917	0.003733
H	6.999994	-1.106552	0.004493
H	8.700830	0.893744	-0.003107
H	4.439066	-1.929279	2.158817
H	4.700421	-4.399197	2.157590
H	4.834840	-5.631103	0.011168
H	4.710885	-4.406083	-2.139838
H	4.450113	-1.936282	-2.150446

SCF Done: E(UB3LYP) = -3574.70938534 A.U. after 1 cycles

11.29 Computed xyz-coordinates of the first oxidation state of dithienothiazine trimer (UB3LYP)



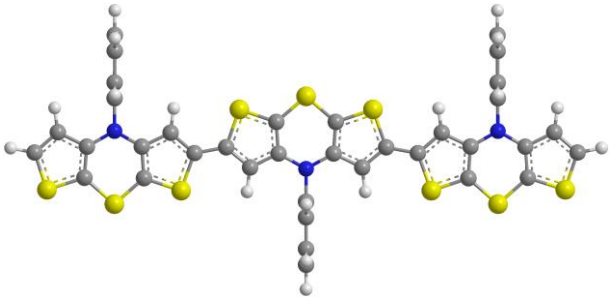
C	5.194850	-5.457370	0.440749
C	6.161190	-4.483180	0.211472
N	6.362520	-3.389790	1.048490
C	5.581100	-3.195900	2.181430
C	4.562980	-4.065930	2.570510
S	4.067240	-5.527520	1.767480
S	5.200680	-6.687400	-0.785221
C	6.540110	-5.899900	-1.611050
C	6.919950	-4.748940	-0.956597
C	5.709080	-2.098340	3.066110
C	4.813010	-2.123710	4.114470
S	3.774890	-3.543310	4.026060
C	7.404140	-2.436040	0.734157
C	8.677380	-2.610520	1.273340
C	9.677110	-1.688700	0.969578
C	9.400760	-0.606989	0.134456
C	8.123690	-0.442422	-0.400239
C	7.117050	-1.358280	-0.101362
C	7.075610	-6.469120	-2.815850
C	6.894030	-7.739110	-3.323550
C	7.578430	-7.969420	-4.544570
C	8.289850	-6.854960	-4.955900
S	8.084940	-5.508620	-3.883000
N	7.554540	-9.168310	-5.271370
C	7.872060	-9.130210	-6.644750
C	8.599770	-8.115950	-7.219080
S	9.386730	-6.791330	-6.336670
C	7.447240	-10.098600	-7.610080
C	7.855340	-9.795400	-8.874380
S	8.746590	-8.309930	-8.940980
C	6.860750	-10.310100	-4.733680
C	7.592300	-11.313900	-4.100070
C	6.933080	-12.425400	-3.577480

C	5.547540	-12.531900	-3.687430
C	4.818240	-11.526200	-4.321310
C	5.472610	-10.413600	-4.846260
C	4.658160	-1.186570	5.186270
C	3.670520	-1.133090	6.150320
C	3.820260	-0.062952	7.065440
C	4.940680	0.706547	6.780920
S	5.830940	0.099353	5.424070
S	5.399520	2.207170	7.576850
N	2.956670	0.208480	8.131070
C	1.773810	-0.594037	8.310610
C	0.548733	-0.116812	7.846330
C	-0.600936	-0.886314	8.016270
C	3.385980	1.059960	9.166100
C	4.458330	1.912930	9.051130
C	-0.524358	-2.127650	8.646040
C	0.702848	-2.601600	9.108910
C	1.855130	-1.835830	8.943450
C	2.792840	1.118240	10.467800
C	3.421760	2.000460	11.293500
S	4.770340	2.775100	10.528400
H	7.732490	-4.120010	-1.289010
H	6.431530	-1.308280	2.924290
H	8.878760	-3.456250	1.919810
H	10.669400	-1.817660	1.384670
H	10.180800	0.107620	-0.100049
H	7.908600	0.397820	-1.049380
H	6.119970	-1.241860	-0.508697
H	6.308700	-8.497450	-2.823210
H	6.869350	-10.977600	-7.364900
H	7.682540	-10.351400	-9.782500
H	8.668750	-11.217900	-4.023350
H	7.501970	-13.206300	-3.086560

H	5.036600	-13.397100	-3.281290
H	3.741200	-11.607800	-4.409550
H	4.914490	-9.628580	-5.343480
H	2.846110	-1.830670	6.191140
H	0.504029	0.849683	7.358720
H	-1.553740	-0.515495	7.657180
H	-1.419380	-2.724450	8.777450
H	0.763848	-3.565090	9.601200
H	2.813000	-2.193600	9.302950
H	1.937800	0.528945	10.764900
H	3.183370	2.242450	12.317200

SCF Done: E(UB3LYP) = -5362.63467716 A.U. after 1 cycles

11.30 Computed xyz-coordinates of the second oxidation state of dithienothiazine trimer (singlet; UB3LYP)



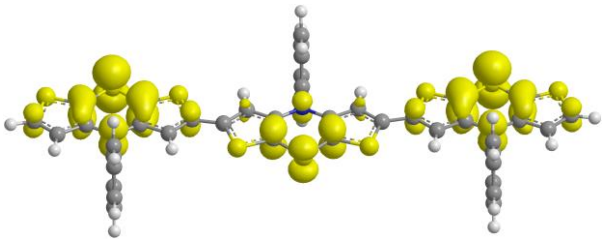
C	-1.311969	1.096971	0.000112
C	-1.214034	-0.300610	0.000293
N	-0.000008	-0.976633	0.000317
C	1.214071	-0.300672	0.000218
C	1.312085	1.096910	0.000109
S	0.000081	2.220919	0.000236
S	-2.953127	1.644874	-0.000039
C	-3.535420	-0.017120	-0.000053
C	-2.480463	-0.915818	0.000201
C	2.480470	-0.915947	0.000323
C	3.535470	-0.017315	0.000274
S	2.953267	1.644725	0.000080
C	-0.000011	-2.424713	0.000239
C	-0.000168	-3.107903	1.214791

C	-0.000113	-4.501274	1.209064
C	0.000116	-5.195923	0.000095
C	0.000254	-4.501142	-1.208803
C	0.000183	-3.107773	-1.214385
C	-4.934636	-0.278590	-0.000159
C	-5.987236	0.620732	-0.000458
C	-7.258179	0.011814	-0.000406
C	-7.163943	-1.387338	-0.000022
S	-5.526259	-1.936781	0.000404
N	-8.466221	0.695690	-0.000790
C	-9.683030	0.009183	0.000633
C	-9.791398	-1.368728	0.001354
S	-8.471710	-2.529085	0.000102
C	-10.964404	0.643222	0.001343
C	-11.989609	-0.252041	0.002520
S	-11.446177	-1.897237	0.003028
C	-8.460580	2.140828	-0.001886
C	-8.458283	2.828219	1.210861
C	-8.453616	4.221656	1.204966
C	-8.450772	4.916036	-0.004157
C	-8.452755	4.219672	-1.212142
C	-8.457441	2.826228	-1.215753
C	4.934677	-0.278811	0.000177
C	5.987225	0.620575	0.000421
C	7.258220	0.011760	0.000199
C	7.164070	-1.387394	-0.000249
S	5.526417	-1.936971	-0.000556
S	8.471944	-2.529031	-0.000825
N	8.466211	0.695747	0.000349
C	8.460395	2.140884	0.001642
C	8.458252	2.828411	-1.211024
C	8.453338	4.221848	-1.204974
C	9.683066	0.009343	-0.000842

C	9.791522	-1.368560	-0.001584
C	8.450088	4.916089	0.004227
C	8.451958	4.219586	1.212133
C	8.456905	2.826143	1.215588
C	10.964394	0.643465	-0.001280
C	11.989659	-0.251737	-0.002274
S	11.446333	-1.896961	-0.002995
H	-2.613513	-1.987728	0.000259
H	2.613450	-1.987864	0.000317
H	-0.000327	-2.554372	2.146076
H	-0.000258	-5.041279	2.148086
H	0.000196	-6.279378	0.000029
H	0.000424	-5.041053	-2.147879
H	0.000234	-2.554146	-2.145614
H	-5.852319	1.692739	-0.000808
H	-11.105224	1.713571	0.001030
H	-13.049243	-0.049891	0.003369
H	-8.463378	2.275615	2.142753
H	-8.454912	4.762223	2.143833
H	-8.449138	5.999590	-0.005036
H	-8.453381	4.758695	-2.151896
H	-8.461898	2.272085	-2.146733
H	5.852234	1.692572	0.000898
H	8.463667	2.275922	-2.142982
H	8.454754	4.762517	-2.143781
H	8.448214	5.999643	0.005242
H	8.452308	4.758503	2.151949
H	8.461358	2.271892	2.146504
H	11.105146	1.713824	-0.000842
H	13.049284	-0.049538	-0.002858

SCF Done: E(RB3LYP) = -5362.44739920 A.U. after 1 cycles

11.31 Computed xyz-coordinates of the second oxidation state of dithienothiazine trimer (triplet; UB3LYP)



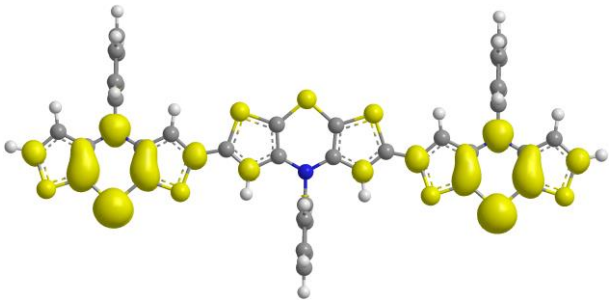
C	1.313230	1.107930	0.004320
C	1.213030	-0.275597	0.004903
N	0.000001	-0.969117	0.006447
C	-1.213020	-0.275585	0.004562
C	-1.313210	1.107940	0.003974
S	0.000014	2.277770	0.006930
S	2.954780	1.655910	0.002352
C	3.539840	0.001274	0.002647
C	2.487330	-0.892809	0.003852
C	-2.487330	-0.892787	0.003136
C	-3.539830	0.001301	0.001610
S	-2.954760	1.655940	0.001350
C	-0.000007	-2.411560	0.006429
C	0.000412	-3.101370	-1.205840
C	0.000420	-4.494940	-1.201840
C	0.000003	-5.190590	0.006639
C	-0.000423	-4.494760	1.215000
C	-0.000425	-3.101170	1.218780
C	4.946990	-0.268047	0.001471
C	5.996590	0.625573	0.000537
C	7.268260	0.004893	-0.000751
C	7.171760	-1.393280	-0.000732
S	5.524440	-1.933280	0.000891
N	8.474420	0.680854	-0.002083
C	9.686450	-0.000582	-0.003902
C	9.791350	-1.386010	-0.004301
S	8.476370	-2.531890	-0.002555

C	10.968400	0.631945	-0.005396
C	11.988200	-0.267064	-0.006894
S	11.445400	-1.914110	-0.006546
C	8.473990	2.130640	-0.001631
C	8.474090	2.812520	-1.216260
C	8.474610	4.205830	-1.209820
C	8.474860	4.900110	-0.000692
C	8.474690	4.205010	1.207960
C	8.474200	2.811700	1.213460
C	-4.946980	-0.268021	0.000360
C	-5.996590	0.625593	0.000383
C	-7.268260	0.004901	-0.001323
C	-7.171740	-1.393270	-0.002484
S	-5.524420	-1.933250	-0.001589
S	-8.476340	-2.531900	-0.004325
N	-8.474420	0.680848	-0.001803
C	-8.474010	2.130640	-0.000473
C	-8.475370	2.810970	1.215030
C	-8.475910	4.204280	1.210360
C	-9.686440	-0.000598	-0.003742
C	-9.791330	-1.386030	-0.005031
C	-8.474950	4.900100	0.002127
C	-8.473530	4.206550	-1.207420
C	-8.472980	2.813250	-1.214690
C	-10.968400	0.631915	-0.004713
C	-11.988200	-0.267102	-0.006680
S	-11.445400	-1.914150	-0.007394
H	2.617670	-1.965720	0.004102
H	-2.617680	-1.965700	0.003487
H	0.000708	-2.548320	-2.137650
H	0.000749	-5.034940	-2.141140
H	0.000008	-6.274220	0.006718
H	-0.000747	-5.034610	2.154390

H	-0.000729	-2.547930	2.150460
H	5.866960	1.697680	0.000722
H	11.112200	1.701590	-0.005361
H	13.048500	-0.067545	-0.008221
H	8.475570	2.259070	-2.147470
H	8.476360	4.745890	-2.148770
H	8.476430	5.983550	-0.000325
H	8.476520	4.744440	2.147290
H	8.475800	2.257610	2.144290
H	-5.866960	1.697710	0.001558
H	-8.477780	2.256310	2.145520
H	-8.478630	4.743140	2.150010
H	-8.476550	5.983540	0.003141
H	-8.474410	4.747180	-2.146050
H	-8.473620	2.260360	-2.146240
H	-11.112200	1.701560	-0.004016

SCF Done: E(UB3LYP) = -5362.45863266 A.U. after 1 cycles

11.32 Computed xyz-coordinates of the third oxidation state of dithienothiazine trimer (doublet; UB3LYP)



C	-1.307520	1.100470	0.037647
C	-1.207890	-0.295473	0.035648
N	-0.000014	-0.971406	0.034693
C	1.207850	-0.295458	0.034552
C	1.307470	1.100480	0.036538
S	-0.000032	2.232940	0.040103
S	-2.948820	1.643940	0.036192
C	-3.523610	-0.018395	0.032854
C	-2.481070	-0.917022	0.033080

C	2.481030	-0.916990	0.031364
C	3.523570	-0.018349	0.030759
S	2.948750	1.643980	0.034265
C	-0.000012	-2.424190	0.031129
C	-0.000610	-3.105330	1.245880
C	-0.000621	-4.498570	1.235170
C	-0.000020	-5.189300	0.023982
C	0.000586	-4.492340	-1.183640
C	0.000581	-3.099080	-1.187140
C	-4.937460	-0.283739	0.026369
C	-5.974890	0.619061	0.016606
C	-7.251540	0.003856	0.003016
C	-7.160960	-1.394300	0.004248
S	-5.520800	-1.944050	0.022918
N	-8.453610	0.686182	-0.014179
C	-9.664710	0.019490	-0.035024
C	-9.776890	-1.374260	-0.036760
S	-8.473020	-2.516640	-0.014042
C	-10.942100	0.656668	-0.055324
C	-11.962200	-0.241187	-0.071828
S	-11.431500	-1.893160	-0.063083
C	-8.442190	2.139590	-0.012355
C	-8.440610	2.815320	1.205060
C	-8.432480	4.208510	1.199710
C	-8.426530	4.904010	-0.008698
C	-8.428570	4.211680	-1.218940
C	-8.436430	2.818510	-1.227970
C	4.937410	-0.283692	0.024168
C	5.974880	0.619090	0.015545
C	7.251510	0.003855	0.001899
C	7.160890	-1.394300	0.001838
S	5.520700	-1.944020	0.019397
S	8.472920	-2.516670	-0.016736

N	8.453620	0.686151	-0.014007
C	8.442290	2.139550	-0.010184
C	8.436950	2.820220	-1.224820
C	8.429190	4.213380	-1.213810
C	9.664700	0.019433	-0.035204
C	9.776830	-1.374320	-0.038285
C	8.426850	4.903970	-0.002573
C	8.432400	4.206750	1.204840
C	8.440410	2.813550	1.208190
C	10.942100	0.656586	-0.054558
C	11.962100	-0.241285	-0.071790
S	11.431400	-1.893250	-0.064685
H	-2.610420	-1.989400	0.030278
H	2.610410	-1.989360	0.028600
H	-0.001021	-2.553370	2.177920
H	-0.001081	-5.041100	2.172490
H	-0.000023	-6.272600	0.021193
H	0.001044	-5.030020	-2.123760
H	0.000996	-2.542330	-2.116340
H	-5.841200	1.690900	0.016740
H	-11.083800	1.726350	-0.057734
H	-13.021800	-0.037707	-0.088835
H	-8.448930	2.259810	2.134890
H	-8.434050	4.747210	2.139250
H	-8.422790	5.987310	-0.007267
H	-8.426810	4.752860	-2.157050
H	-8.441600	2.265420	-2.159270
H	5.841220	1.690930	0.016628
H	8.442350	2.268470	-2.156920
H	8.427740	4.755900	-2.151140
H	8.423190	5.987270	0.000401
H	8.433740	4.744100	2.145150
H	8.448430	2.256700	2.137230

H 11.083800 1.726270 -0.055918

H 13.021800 -0.037821 -0.088439

SCF Done: E(UB3LYP) = -5362.26151293 A.U. after 1 cycles

11.33 Computed xyz-coordinates of the third oxidation state of dithienothiazine trimer (quartet; UB3LYP)

C 1.305783 1.105195 -0.036698

C 1.205523 -0.289243 -0.032208

N 0.000001 -0.965922 -0.030141

C -1.205517 -0.289235 -0.032439

C -1.305765 1.105205 -0.036934

S 0.000014 2.244361 -0.040839

S 2.950158 1.643679 -0.036667

C 3.520830 -0.020303 -0.030280

C 2.481007 -0.916030 -0.028635

C -2.481005 -0.916011 -0.028922

C -3.520820 -0.020274 -0.030577

S -2.950137 1.643699 -0.036903

C -0.000008 -2.420039 -0.022899

C -0.000419 -3.103026 -1.236314

C -0.000433 -4.496186 -1.221516

C -0.000034 -5.183546 -0.008428

C 0.000378 -4.483546 1.197413

C 0.000389 -3.090330 1.197614

C 4.939884 -0.290270 -0.024392

C 5.972966 0.612754 -0.014757

C 7.253419 -0.004267 -0.003262

C 7.164967 -1.398115 -0.005720

S 5.522747 -1.948936 -0.023011

N 8.452657 0.683812 0.013047

C 9.663999 0.020736 0.031425

C 9.779363 -1.374804 0.031762

S 8.481625 -2.524125 0.009766

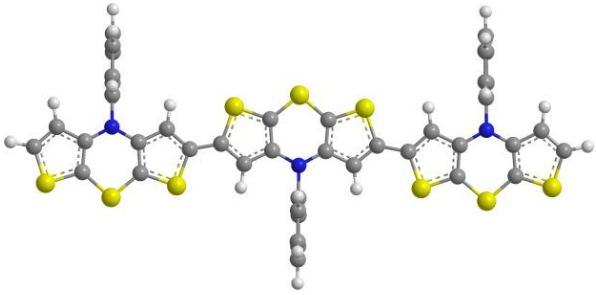
C 10.940111 0.661565 0.050502

C	11.962057	-0.233134	0.064715
S	11.434835	-1.887537	0.055138
C	8.437519	2.137652	0.012238
C	8.433813	2.813769	-1.204855
C	8.422685	4.206917	-1.198380
C	8.416168	4.901480	0.010553
C	8.420590	4.208360	1.220330
C	8.431515	2.815211	1.228501
C	-4.939875	-0.290239	-0.024661
C	-5.972964	0.612776	-0.015079
C	-7.253413	-0.004257	-0.003441
C	-7.164949	-1.398103	-0.005779
S	-5.522725	-1.948915	-0.023005
S	-8.481594	-2.524124	0.009819
N	-8.452656	0.683812	0.012901
C	-8.437535	2.137651	0.012197
C	-8.431605	2.815119	1.228512
C	-8.420704	4.208268	1.220447
C	-9.663993	0.020725	0.031383
C	-9.779343	-1.374815	0.031844
C	-8.416230	4.901480	0.010722
C	-8.422669	4.207007	-1.198263
C	-8.433774	2.813859	-1.204843
C	-10.940112	0.661542	0.050480
C	-11.962047	-0.233167	0.064821
S	-11.434807	-1.887564	0.055363
H	2.607241	-1.988703	-0.024084
H	-2.607249	-1.988684	-0.024382
H	-0.000695	-2.553407	-2.169677
H	-0.000748	-5.041150	-2.157375
H	-0.000046	-6.266800	-0.002777
H	0.000684	-5.018670	2.138942
H	0.000679	-2.530917	2.125146

H	5.839394	1.684617	-0.013662
H	11.078719	1.731630	0.053697
H	13.021317	-0.027389	0.080398
H	8.442612	2.258838	-2.135009
H	8.422135	4.746262	-2.137532
H	8.410010	5.984760	0.009894
H	8.418131	4.748852	2.158817
H	8.438586	2.261372	2.159315
H	-5.839406	1.684641	-0.014118
H	-8.438720	2.261214	2.159286
H	-8.418308	4.748686	2.158976
H	-8.410089	5.984760	0.010145
H	-8.422076	4.746423	-2.137374
H	-8.442513	2.258994	-2.135038
H	-11.078730	1.731606	0.053591
H	-13.021308	-0.027431	0.080548

SCF Done: E(UB3LYP) = -5362.25814678 A.U. after 1 cycles

11.34 Computed xyz-coordinates of the fourth oxidation state of dithienothiazine trimer (singlet; UB3LYP)



C	-1.311629	1.090149	0.080559
C	-1.210770	-0.312652	0.079567
N	-0.000013	-0.986818	0.080974
C	1.210739	-0.312646	0.079249
C	1.311593	1.090156	0.080279
S	-0.000020	2.218509	0.085246
S	-2.938946	1.646535	0.074901
C	-3.525937	-0.012530	0.072143
C	-2.476946	-0.921594	0.074782

C	2.476917	-0.921582	0.074289
C	3.525903	-0.012514	0.071572
S	2.938909	1.646549	0.074540
C	-0.000012	-2.438107	0.079025
C	-0.000410	-3.119292	1.294376
C	-0.000418	-4.512624	1.285565
C	-0.000016	-5.204708	0.075077
C	0.000389	-4.509216	-1.133467
C	0.000384	-3.115886	-1.138294
C	-4.922976	-0.265828	0.058247
C	-5.969369	0.641009	0.038704
C	-7.230888	0.030254	0.003900
C	-7.134902	-1.395276	0.002229
S	-5.502994	-1.939010	0.047228
N	-8.435714	0.683689	-0.031762
C	-9.641866	0.025486	-0.079385
C	-9.749444	-1.380626	-0.089597
S	-8.436503	-2.479817	-0.045173
C	-10.917301	0.653366	-0.121900
C	-11.927712	-0.256541	-0.163728
S	-11.396900	-1.908474	-0.151924
C	-8.434018	2.143363	-0.023605
C	-8.435492	2.807550	1.199391
C	-8.438339	4.200597	1.197823
C	-8.439369	4.900192	-0.008196
C	-8.437756	4.214181	-1.221985
C	-8.435054	2.821235	-1.239039
C	4.922940	-0.265819	0.057635
C	5.969352	0.641007	0.038498
C	7.230864	0.030237	0.003620
C	7.134848	-1.395291	0.001388
S	5.502925	-1.939006	0.046068
S	8.436425	-2.479844	-0.046398

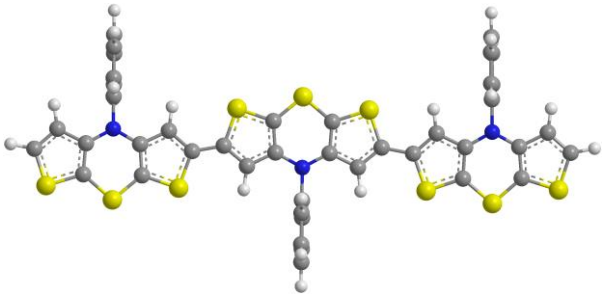
N	8.435712	0.683660	-0.031612
C	8.434085	2.143335	-0.022640
C	8.435341	2.821902	-1.237685
C	8.438137	4.214838	-1.219840
C	9.641844	0.025444	-0.079503
C	9.749390	-1.380665	-0.090393
C	8.439631	4.900160	-0.005663
C	8.438396	4.199879	1.199957
C	8.435455	2.806834	1.200735
C	10.917298	0.653311	-0.121650
C	11.927688	-0.256599	-0.163905
S	11.396837	-1.908524	-0.152886
H	-2.611854	-1.993682	0.070968
H	2.611830	-1.993668	0.070421
H	-0.000692	-2.566119	2.225820
H	-0.000726	-5.054422	2.223311
H	-0.000018	-6.288003	0.073548
H	0.000697	-5.048350	-2.072758
H	0.000670	-2.560137	-2.068231
H	-5.835297	1.712379	0.044243
H	-11.070030	1.721214	-0.122800
H	-12.988566	-0.059559	-0.201365
H	-8.439099	2.247759	2.126594
H	-8.444222	4.735433	2.139294
H	-8.444685	5.983280	-0.002129
H	-8.442180	4.759536	-2.157399
H	-8.438087	2.271602	-2.172281
H	5.835300	1.712378	0.044388
H	8.438461	2.272801	-2.171239
H	8.442723	4.760725	-2.154943
H	8.445020	5.983244	0.001017
H	8.444199	4.734181	2.141733
H	8.438925	2.246526	2.127626

H 11.070054 1.721155 -0.122026

H 12.988547 -0.059626 -0.201427

SCF Done: E(RB3LYP) = -5362.02082059 A.U. after 1 cycles

11.35 Computed xyz-coordinates of the fourth oxidation state of dithienothiazine trimer (triplet; UB3LYP)



C 1.312390 1.101400 -0.181117

C 1.208740 -0.311235 -0.148456

N 0.002155 -0.967989 -0.119255

C -1.202330 -0.306644 -0.106865

C -1.301180 1.106500 -0.134507

S 0.007189 2.201350 -0.182331

S 2.950450 1.638840 -0.203959

C 3.516970 -0.032709 -0.147990

C 2.473420 -0.933835 -0.132711

C -2.468810 -0.923721 -0.068277

C -3.509260 -0.018459 -0.063327

S -2.936610 1.650150 -0.109359

C 0.000399 -2.428140 -0.095089

C 0.007955 -3.118370 -1.303750

C 0.006955 -4.511060 -1.271780

C -0.001062 -5.184100 -0.050744

C -0.008035 -4.472080 1.147980

C -0.007286 -3.079030 1.135200

C 4.924340 -0.296849 -0.113664

C 5.955250 0.613763 -0.031408

C 7.230230 0.006944 -0.005149

C 7.146630 -1.397580 -0.066883

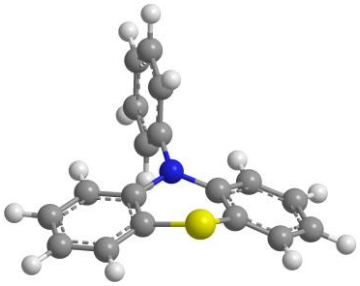
S 5.516670 -1.955030 -0.162230

N	8.426780	0.689172	0.075962
C	9.637720	0.037919	0.094589
C	9.759020	-1.364330	0.037831
S	8.464990	-2.499140	-0.050400
C	10.908800	0.677796	0.169330
C	11.929800	-0.218935	0.164864
S	11.412000	-1.874620	0.070525
C	8.401170	2.145120	0.148245
C	8.409450	2.880420	-1.033690
C	8.386450	4.271100	-0.954089
C	8.355980	4.901800	0.288900
C	8.347970	4.147460	1.461330
C	8.370470	2.755960	1.398880
C	-4.916120	-0.281929	-0.023019
C	-5.955280	0.623974	-0.038262
C	-7.225300	0.009427	0.028877
C	-7.129240	-1.395030	0.091964
S	-5.494500	-1.943720	0.072963
S	-8.437120	-2.503610	0.185915
N	-8.429200	0.683136	0.037903
C	-8.423120	2.139330	-0.037918
C	-8.425250	2.876290	1.142980
C	-8.427240	4.266990	1.061020
C	-9.633680	0.024425	0.114325
C	-9.741790	-1.378500	0.186009
C	-8.427870	4.895940	-0.183213
C	-8.426520	4.139870	-1.354570
C	-8.424630	2.748280	-1.289910
C	-10.910900	0.656000	0.129461
C	-11.923100	-0.247066	0.209299
S	-11.389800	-1.899090	0.269183
H	2.600940	-2.005560	-0.098313
H	-2.601210	-1.995000	-0.044883

H	0.014238	-2.578800	-2.242820
H	0.012248	-5.066350	-2.201270
H	-0.001671	-6.267040	-0.033375
H	-0.013532	-4.997170	2.094890
H	-0.011732	-2.509550	2.056520
H	5.813320	1.683130	0.017399
H	11.047900	1.746420	0.222067
H	12.988500	-0.013245	0.209652
H	8.438990	2.377320	-1.992200
H	8.397040	4.858180	-1.863970
H	8.341920	5.983520	0.343941
H	8.327990	4.638410	2.426360
H	8.368680	2.156350	2.300850
H	-5.825080	1.695060	-0.093698
H	-8.429650	2.374090	2.102410
H	-8.432190	4.855340	1.970110
H	-8.433140	5.977630	-0.240037
H	-8.432280	4.629450	-2.320470
H	-8.430180	2.147310	-2.190930
H	-11.060000	1.723510	0.084441
H	-12.983700	-0.047840	0.238043

SCF Done: E(UB3LYP) = -5362.02293052 A.U. after 1 cycles

11.36 Computed xyz-coordinates of phenothiazine monomer



C	-1.795086	-1.354131	0.177201
C	-0.417541	-1.235818	-0.084426
N	0.249618	-0.000063	0.116058
C	-0.417161	1.235822	-0.084449

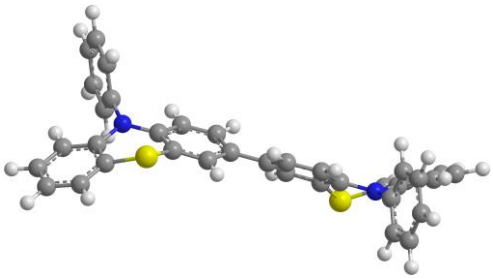
C	-1.794687	1.354597	0.177146
S	-2.669348	0.000356	0.937962
C	0.262716	2.376695	-0.535866
C	-0.407428	3.583307	-0.725414
C	-1.776496	3.678023	-0.497557
C	-2.467224	2.552430	-0.054375
C	-2.467953	-2.551796	-0.054271
C	-1.777566	-3.677614	-0.497412
C	-0.408465	-3.583298	-0.725290
C	0.262023	-2.376874	-0.535801
C	1.691163	-0.000235	0.156030
C	2.325591	-0.000074	1.397794
C	3.717824	-0.000183	1.468792
C	4.477561	-0.000457	0.300315
C	3.843037	-0.000610	-0.941664
C	2.451680	-0.000492	-1.016144
H	1.324469	2.325910	-0.730362
H	0.151667	4.447741	-1.064508
H	-2.303008	4.611220	-0.656813
H	-3.532816	2.603810	0.138031
H	-3.533565	-2.602865	0.138124
H	-2.304347	-4.610656	-0.656614
H	0.150368	-4.447918	-1.064348
H	1.323786	-2.326383	-0.730305
H	1.723432	0.000130	2.298659
H	4.206591	-0.000060	2.436180
H	5.560000	-0.000542	0.356275
H	4.429894	-0.000816	-1.852913
H	1.953830	-0.000584	-1.978849

SCF Done: E(RB3LYP) = -1146.88908691 A.U. after 7 cycles

E (HOMO) = -5.354 eV

E (LUMO) = -0.967 eV

11.37 Computed xyz-coordinates of phenothiazine dimer



C	7.242412	3.447151	-0.365240
C	5.965356	3.364064	-0.915579
C	5.244661	2.173298	-0.857517
C	5.763751	1.046202	-0.193696
C	7.048658	1.147486	0.359631
C	7.781238	2.328341	0.261602
S	3.709389	2.047100	-1.755483
C	2.862417	0.889826	-0.695527
C	3.592109	-0.124522	-0.049180
N	5.006689	-0.149329	-0.103600
C	1.475228	0.938871	-0.618718
C	0.742607	-0.047006	0.058535
C	1.470757	-1.072651	0.673582
C	2.859957	-1.106125	0.633320
C	5.682752	-1.361775	0.287903
C	-2.887841	-1.146795	0.165052
C	-3.587575	0.072326	0.207657
N	-5.003586	0.093988	0.242741
C	-5.771394	-0.910887	-0.399123
C	-5.283580	-2.226611	-0.503610
S	-3.776136	-2.683013	0.332160
C	-7.036071	-0.637777	-0.941046
C	-7.779322	-1.636230	-1.566649
C	-7.271081	-2.924992	-1.693503
C	-6.013749	-3.210581	-1.166401
C	-1.499959	-1.177700	0.087230
C	-0.737333	-0.001013	0.111890

C	-1.435951	1.209788	0.193389
C	-2.825510	1.248960	0.225747
C	-5.659905	1.323554	0.613803
C	6.086103	-2.253426	-0.705292
C	6.738298	-3.435162	-0.356775
C	6.987947	-3.726977	0.983041
C	6.584561	-2.834807	1.976191
C	5.932245	-1.652709	1.631492
C	-6.103717	1.473498	1.927101
C	-6.742220	2.649929	2.316357
C	-6.937908	3.676916	1.394613
C	-6.494134	3.526533	0.081032
C	-5.855613	2.351920	-0.311613
H	7.803762	4.371208	-0.431564
H	5.528467	4.220142	-1.417007
H	7.484377	0.294873	0.860556
H	8.775710	2.367508	0.690828
H	0.956076	1.735627	-1.138613
H	0.952221	-1.846822	1.226501
H	3.378948	-1.907959	1.138676
H	-7.447464	0.358574	-0.864743
H	-8.757760	-1.392595	-1.964214
H	-7.840970	-3.700433	-2.190810
H	-5.600070	-4.209392	-1.246346
H	-1.007646	-2.139821	0.008415
H	-0.891611	2.145246	0.246095
H	-3.320714	2.207539	0.287157
H	5.885678	-2.014672	-1.743019
H	7.050098	-4.125680	-1.131788
H	7.494868	-4.646077	1.253356
H	6.776482	-3.058017	3.019310
H	5.615739	-0.956161	2.399178
H	-5.945367	0.667049	2.633219

H -7.085488 2.762458 3.338217

H -7.434350 4.591457 1.697833

H -6.644439 4.322716 -0.638867

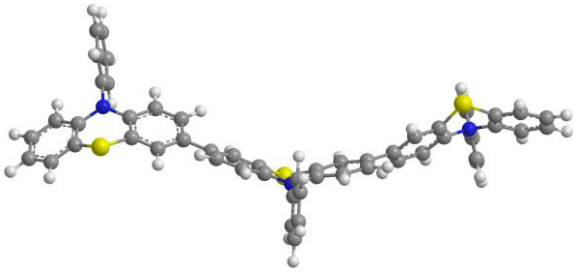
H -5.509480 2.229727 -1.331388

SCF Done: E(RB3LYP) = -2292.57861641 A.U. after 6 cycles

E (HOMO) = -5.143 eV

E (LUMO) = -1.263 eV

11.38 Computed xyz-coordinates of phenothiazine trimer



C -9.672262 -0.257675 1.695500

C -9.813419 -1.147948 0.614987

N -8.672235 -1.725835 0.002516

C -7.439073 -1.033094 -0.059966

C -7.069232 -0.126900 0.950665

S -8.066338 0.009092 2.422976

C -6.533008 -1.224349 -1.112577

C -5.324016 -0.539413 -1.157918

C -4.968687 0.389311 -0.172106

C -5.876916 0.584004 0.878783

C -10.786169 0.343319 2.277571

C -12.070462 0.032045 1.836896

C -12.224607 -0.873063 0.791838

C -11.112700 -1.445929 0.178554

C -8.865029 -2.858467 -0.869549

C -8.671985 -4.139734 -0.354658

C -8.852809 -5.253519 -1.173248

C -9.225612 -5.088328 -2.506039

C -9.418277 -3.806526 -3.020751

C -9.239593 -2.691073 -2.205128

C	-3.690249	1.135992	-0.228124
C	-2.524143	0.540476	-0.730351
C	-1.326848	1.242435	-0.814553
C	-1.222063	2.562002	-0.339133
C	-2.386240	3.155088	0.169286
C	-3.591167	2.462519	0.209059
S	0.055616	0.486505	-1.648517
C	1.383231	1.248427	-0.733602
C	1.246765	2.571389	-0.275131
N	0.012253	3.255005	-0.387002
C	2.580686	0.557522	-0.590201
C	3.716461	1.164276	-0.034069
C	3.586808	2.492909	0.388390
C	2.381004	3.177029	0.283561
C	0.002351	4.684778	-0.195294
C	7.429812	0.384737	0.078140
C	7.454596	-0.998188	0.333117
N	8.683644	-1.694659	0.437776
C	9.821082	-1.296257	-0.309955
C	10.025959	0.057879	-0.633094
S	8.955568	1.306291	0.055936
C	10.779114	-2.224180	-0.744244
C	11.891368	-1.817169	-1.477672
C	12.064121	-0.480274	-1.821095
C	11.118616	0.452806	-1.401855
C	6.227619	1.068316	-0.067959
C	4.992988	0.423199	0.094524
C	5.022345	-0.945947	0.386742
C	6.220163	-1.644158	0.489400
C	8.671510	-3.017103	1.013374
C	0.033725	5.510460	-1.318291
C	0.024865	6.895706	-1.163672
C	-0.015444	7.456675	0.111642

C	-0.046681	6.630220	1.234590
C	-0.037624	5.244977	1.083963
C	9.017929	-3.165212	2.355846
C	9.015484	-4.430966	2.939826
C	8.667495	-5.549013	2.184002
C	8.320816	-5.400570	0.841290
C	8.321891	-4.136834	0.254361
H	-6.772058	-1.916723	-1.907028
H	-4.665004	-0.712041	-2.000533
H	-5.632988	1.267721	1.683460
H	-10.641461	1.039835	3.095532
H	-12.932326	0.489126	2.307702
H	-13.214517	-1.134223	0.435962
H	-11.257532	-2.137953	-0.638730
H	-8.381878	-4.253854	0.683074
H	-8.702035	-6.247777	-0.769014
H	-9.365924	-5.954674	-3.142059
H	-9.708698	-3.673727	-4.056479
H	-9.389399	-1.692764	-2.599681
H	-2.544323	-0.489628	-1.065982
H	-2.358406	4.176830	0.520093
H	-4.470590	2.977182	0.577713
H	2.638829	-0.458488	-0.962878
H	4.429709	3.000695	0.842057
H	2.323693	4.194782	0.642311
H	10.661354	-3.269986	-0.499080
H	12.617380	-2.559823	-1.787717
H	12.920855	-0.162186	-2.402671
H	11.236117	1.501385	-1.650455
H	6.258755	2.123851	-0.311137
H	4.095952	-1.483044	0.552017
H	6.192517	-2.700563	0.715193
H	0.064471	5.061644	-2.303931

H 0.049258 7.534340 -2.039020

H -0.022436 8.533929 0.230919

H -0.078014 7.062259 2.228076

H -0.061634 4.597641 1.952941

H 9.286484 -2.287900 2.932183

H 9.285453 -4.541779 3.983633

H 8.666023 -6.532864 2.638746

H 8.049176 -6.267334 0.249959

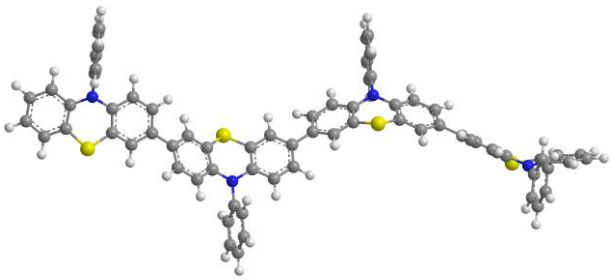
H 8.053094 -4.015313 -0.788563

SCF Done: E(RB3LYP) = -3438.26798310 A.U. after 5 cycles

E (HOMO) = -5.064 eV

E (LUMO) = -1.372 eV

11.39 Computed xyz-coordinates of phenothiazine tetramer



C 14.128677 -0.037314 -0.822311

C 14.181667 -0.660192 0.438551

N 13.005817 -1.184685 1.033644

C 11.739074 -0.595620 0.803401

C 11.450708 0.037366 -0.419456

S 12.615767 -0.071970 -1.765092

C 10.720879 -0.624479 1.766668

C 9.481501 -0.042681 1.524494

C 9.203157 0.618478 0.322041

C 10.223208 0.651030 -0.640113

C 15.271123 0.517572 -1.394809

C 16.504367 0.416937 -0.754771

C 16.576030 -0.229147 0.475060

C 15.429866 -0.749214 1.072181

C 13.147924 -2.084627 2.151793

C	5.468321	1.295845	0.335123
C	5.357228	2.465019	-0.438471
N	4.091156	3.044647	-0.697786
C	2.926042	2.247836	-0.804854
C	2.799320	1.053401	-0.072621
S	4.027937	0.632252	1.150031
C	1.853133	2.610937	-1.630748
C	0.716936	1.816114	-1.728534
C	0.600677	0.609651	-1.026832
C	1.675431	0.245880	-0.201968
C	6.702059	0.692283	0.552916
C	7.890282	1.255463	0.065296
C	7.779259	2.442037	-0.669956
C	6.544590	3.026332	-0.928694
C	4.045330	4.395078	-1.202670
C	13.348866	-1.604874	3.448508
C	13.483010	-2.500883	4.507086
C	13.417568	-3.874369	4.274135
C	13.217606	-4.351267	2.979800
C	13.082768	-3.457666	1.918389
C	3.806482	5.435927	-0.306179
C	3.755487	6.751228	-0.764848
C	3.942931	7.027526	-2.118127
C	4.181820	5.986027	-3.014335
C	4.233177	4.669916	-2.559557
C	-0.600167	-0.249994	-1.144644
C	-1.873585	0.303397	-1.343604
C	-3.001607	-0.496859	-1.486685
C	-2.920705	-1.896193	-1.370111
C	-1.648830	-2.449335	-1.164766
C	-0.518100	-1.645968	-1.070654
S	-4.543208	0.269787	-1.948433
C	-5.669434	-0.858679	-1.149756

C	-5.351489	-2.226793	-1.069967
N	-4.080017	-2.703307	-1.470588
C	-6.903086	-0.380915	-0.723175
C	-7.900767	-1.244410	-0.247549
C	-7.593276	-2.609462	-0.202346
C	-6.347467	-3.089453	-0.590557
C	-3.907432	-4.125399	-1.641316
C	-11.635500	-0.983643	0.378015
C	-11.766703	0.276605	0.988389
N	-13.039601	0.768449	1.369236
C	-14.206474	0.434708	0.635080
C	-14.312353	-0.809892	-0.012919
S	-13.056892	-2.050497	0.239682
C	-15.291116	1.318466	0.533422
C	-16.430383	0.975736	-0.191372
C	-16.508215	-0.243503	-0.856593
C	-15.437045	-1.129776	-0.770226
C	-10.396356	-1.455062	-0.041541
C	-9.220239	-0.724505	0.181055
C	-9.349889	0.511577	0.826109
C	-10.591028	1.008066	1.208295
C	-13.095118	1.900075	2.261868
C	-3.993335	-4.662248	-2.925019
C	-3.829428	-6.033203	-3.117903
C	-3.580113	-6.867373	-2.029500
C	-3.494728	-6.329254	-0.745547
C	-3.657695	-4.959653	-0.548989
C	-13.318402	1.671327	3.618962
C	-13.379521	2.745656	4.505253
C	-13.217313	4.048389	4.037076
C	-12.993464	4.276726	2.679530
C	-12.932623	3.205416	1.790790
H	10.895852	-1.106690	2.717789

H	8.732995	-0.078858	2.307150
H	10.044866	1.121664	-1.599879
H	15.192197	1.008765	-2.357924
H	17.391496	0.834187	-1.215549
H	17.526005	-0.324898	0.988039
H	15.509356	-1.237058	2.033122
H	1.904329	3.524063	-2.206490
H	-0.076181	2.132849	-2.395255
H	1.621222	-0.661818	0.387526
H	6.732915	-0.234093	1.114254
H	8.670848	2.932530	-1.042196
H	6.508118	3.940294	-1.504237
H	13.399379	-0.536451	3.623392
H	13.638412	-2.125811	5.512029
H	13.522202	-4.569765	5.098918
H	13.166518	-5.417871	2.794220
H	12.927579	-3.815035	0.907326
H	3.662165	5.207417	0.743095
H	3.569554	7.557682	-0.065035
H	3.903113	8.050527	-2.474014
H	4.328051	6.196550	-4.067415
H	4.418070	3.856211	-3.251193
H	-1.994822	1.379059	-1.392320
H	-1.534606	-3.521928	-1.098577
H	0.445692	-2.125981	-0.949680
H	-7.104247	0.680606	-0.808850
H	-8.323329	-3.315885	0.174587
H	-6.150272	-4.149532	-0.519185
H	-15.251019	2.276729	1.031336
H	-17.253968	1.678707	-0.239659
H	-17.387148	-0.507398	-1.432118
H	-15.477489	-2.088984	-1.273632
H	-10.351600	-2.410848	-0.550226

H -8.467644 1.099752 1.049275

H -10.640672 1.968444 1.701204

H -4.187315 -4.002459 -3.762278

H -3.896570 -6.447067 -4.117319

H -3.452769 -7.933121 -2.180201

H -3.301078 -6.974566 0.103438

H -3.592101 -4.535340 0.446169

H -13.442949 0.653741 3.969710

H -13.553328 2.563393 5.559417

H -13.264810 4.883188 4.726736

H -12.867013 5.288173 2.311121

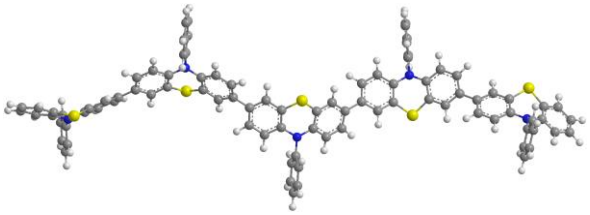
H -12.760273 3.377307 0.734648

SCF Done: E(RB3LYP) = -4583.95751812 A.U. after 4 cycles

E (HOMO) = -5.025 eV

E (LUMO) = -1.427 eV

11.40 Computed xyz-coordinates of phenothiazine pentamer



C -18.391413 -0.815609 1.071411

C -18.457406 -1.050435 -0.314464

N -17.280939 -1.332998 -1.054536

C -16.029241 -0.784242 -0.685453

C -15.729289 -0.517394 0.662873

S -16.852425 -1.055579 1.939390

C -15.036759 -0.495478 -1.632627

C -13.811706 0.041729 -1.253357

C -13.524009 0.342811 0.083512

C -14.517946 0.056385 1.030829

C -19.536316 -0.498611 1.799023

C -20.782741 -0.462302 1.178063

C -20.865669 -0.727108 -0.185060

C	-19.718836	-1.003698	-0.926062
C	-17.422229	-1.883380	-2.380162
C	-9.822155	1.176001	0.190514
C	-9.733329	2.081335	1.263227
N	-8.486796	2.634611	1.645640
C	-7.278377	1.916455	1.481430
C	-7.127586	0.985525	0.437466
S	-8.388279	0.848179	-0.816421
C	-6.183355	2.104609	2.336521
C	-5.001537	1.393102	2.163296
C	-4.860165	0.440525	1.146839
C	-5.957236	0.249676	0.293793
C	-11.036347	0.598360	-0.164139
C	-12.229606	0.938464	0.489519
C	-12.142394	1.867703	1.533352
C	-10.924989	2.415202	1.921975
C	-8.486452	3.782767	2.518710
C	-1.180854	-0.492826	1.092764
C	-1.198199	-1.815820	0.616313
N	0.006137	-2.537983	0.431365
C	1.212098	-1.884488	0.081922
C	1.463515	-0.562940	0.494102
S	0.352394	0.234780	1.638826
C	2.205971	-2.519962	-0.675624
C	3.383532	-1.864479	-1.016396
C	3.620456	-0.536528	-0.640849
C	2.626448	0.098986	0.117720
C	-2.356892	0.235780	1.234099
C	-3.610339	-0.334833	0.968878
C	-3.625616	-1.665263	0.532614
C	-2.450805	-2.384646	0.346078
C	-0.076807	-3.965640	0.241549
C	-17.305063	-3.262576	-2.547710

C	-17.438812	-3.823725	-3.816780
C	-17.689770	-3.008136	-4.918813
C	-17.807009	-1.628594	-4.750789
C	-17.673868	-1.064326	-3.483723
C	-8.622613	3.642366	3.902030
C	-8.618129	4.772199	4.717492
C	-8.477676	6.040867	4.155524
C	-8.341274	6.178644	2.775280
C	-8.345785	5.050702	1.956228
C	0.140206	-4.800807	1.336619
C	0.066555	-6.184249	1.181601
C	-0.223295	-6.733426	-0.066147
C	-0.440576	-5.897252	-1.161041
C	-0.368105	-4.514083	-1.009919
C	4.862299	0.173282	-1.026283
C	6.087137	-0.503659	-1.116820
C	7.250243	0.145420	-1.515756
C	7.257301	1.525786	-1.785083
C	6.035189	2.205325	-1.681799
C	4.866740	1.541046	-1.326136
S	8.716750	-0.825914	-1.802783
C	9.949739	0.397657	-1.400184
C	9.717293	1.752872	-1.698731
N	8.451642	2.189864	-2.157268
C	11.177299	-0.029839	-0.907825
C	12.251598	0.856658	-0.744646
C	12.029596	2.197099	-1.081337
C	10.791100	2.639246	-1.533190
C	8.346956	3.514767	-2.718370
C	15.996416	0.476121	-0.259527
C	16.086954	-0.534554	0.714189
N	17.349374	-0.989141	1.169053
C	18.471951	-1.021293	0.302942

C	18.612967	-0.062846	-0.717349
S	17.475456	1.307605	-0.807224
C	19.475219	-1.992975	0.431370
C	20.570910	-2.009825	-0.428767
C	20.681470	-1.077492	-1.455398
C	19.689919	-0.109798	-1.599829
C	14.763796	0.901493	-0.743196
C	13.561875	0.382663	-0.240972
C	13.654987	-0.597747	0.754362
C	14.884992	-1.055888	1.212974
C	17.403290	-1.755735	2.389320
C	8.364449	3.658461	-4.104957
C	8.261898	4.926876	-4.674134
C	8.141912	6.051196	-3.859167
C	8.124536	5.906491	-2.472133
C	8.226885	4.640305	-1.899605
C	17.753025	-1.104127	3.571559
C	17.816269	-1.817240	4.767567
C	17.530052	-3.181206	4.784158
C	17.179941	-3.832791	3.601840
C	17.116499	-3.123191	2.404301
H	-15.220218	-0.691979	-2.679337
H	-13.083650	0.260656	-2.025461
H	-14.330533	0.239651	2.082441
H	-19.447802	-0.303601	2.861705
H	-21.670841	-0.234014	1.754738
H	-21.825521	-0.710114	-0.688193
H	-19.807979	-1.194589	-1.985976
H	-6.252790	2.814301	3.148596
H	-4.189968	1.564740	2.860400
H	-5.885480	-0.451836	-0.529189
H	-11.048277	-0.128250	-0.967929
H	-13.040126	2.185424	2.050232

H	-10.906889	3.126826	2.735100
H	2.060046	-3.538414	-1.006086
H	4.111997	-2.394432	-1.618455
H	2.777554	1.115314	0.462341
H	-2.290053	1.267546	1.558349
H	-4.570117	-2.161510	0.343818
H	-2.512333	-3.408104	0.004606
H	-17.110226	-3.885344	-1.682719
H	-17.347107	-4.896318	-3.942547
H	-17.793682	-3.444902	-5.905325
H	-18.002117	-0.990766	-5.605100
H	-17.764754	0.007020	-3.347023
H	-8.730870	2.653975	4.333496
H	-8.723587	4.660639	5.790400
H	-8.474284	6.918312	4.791788
H	-8.231593	7.162587	2.334262
H	-8.240977	5.143521	0.881779
H	0.364882	-4.360922	2.300983
H	0.235761	-6.830434	2.035097
H	-0.279959	-7.809161	-0.185914
H	-0.666468	-6.320466	-2.132922
H	-0.536349	-3.859181	-1.856983
H	6.140956	-1.558889	-0.876450
H	5.989473	3.262131	-1.903030
H	3.941222	2.103885	-1.297871
H	11.310913	-1.083907	-0.693711
H	12.824060	2.923620	-0.957806
H	10.661011	3.687758	-1.760010
H	19.405570	-2.735471	1.213591
H	21.333510	-2.768267	-0.294545
H	21.525621	-1.096064	-2.133986
H	19.758473	0.631745	-2.387561
H	14.744049	1.650969	-1.525758

H 12.753450 -1.007930 1.194000

H 14.907068 -1.814656 1.982247

H 8.457703 2.776250 -4.727003

H 8.275739 5.034714 -5.752478

H 8.061979 7.037064 -4.302360

H 8.031099 6.778238 -1.834942

H 8.213412 4.521296 -0.822383

H 17.972876 -0.043504 3.544906

H 18.088566 -1.306656 5.684009

H 17.579141 -3.735185 5.714463

H 16.956438 -4.893315 3.610263

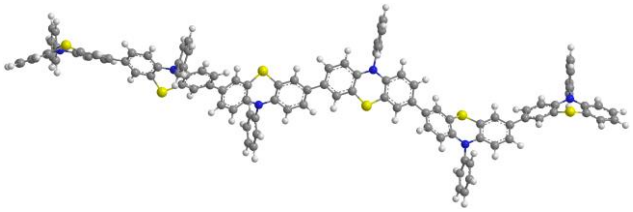
H 16.846263 -3.624980 1.482410

SCF Done: E(RB3LYP) = -5729.64703181 A.U. after 5 cycles

E (HOMO) = -5.004 eV

E (LUMO) = -1.449 eV

11.41 Computed xyz-coordinates of phenothiazine hexamer



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C 7.233910 -3.271313 0.865235

C 6.162179 -2.425644 0.587789

C 6.333707 -1.279386 -0.210010

C 7.626014 -0.992158 -0.673257

C 8.701468 -1.819497 -0.357586

S 4.588470 -2.736507 1.366094

C 3.519607 -2.095106 0.090758

C 3.923262 -0.973641 -0.656574

N 5.229443 -0.445080 -0.520053

C 2.252858 -2.645382 -0.064539

C 1.306153 -2.075993 -0.928698

C 1.698628 -0.937646 -1.643229

C	2.977759	-0.405783	-1.522144
C	5.492524	0.874160	-1.040021
C	5.755635	1.081731	-2.396367
C	6.005161	2.369801	-2.865664
C	5.993502	3.450651	-1.984427
C	5.731642	3.241763	-0.631475
C	5.481061	1.954573	-0.158605
C	-2.445018	-2.393226	-1.418515
C	-2.660410	-3.779159	-1.313720
N	-3.965210	-4.320721	-1.417548
C	-5.100067	-3.592018	-0.986514
C	-5.122506	-2.186853	-1.050915
S	-3.795037	-1.317764	-1.865741
C	-6.244930	-4.229744	-0.488601
C	-7.349672	-3.500751	-0.063620
C	-7.361266	-2.100824	-0.091050
C	-6.215889	-1.462885	-0.589883
C	-1.174213	-1.849094	-1.267204
C	-0.047978	-2.660603	-1.067850
C	-0.261061	-4.043233	-1.007196
C	-1.534715	-4.590231	-1.112761
C	-4.100550	-5.744381	-1.607772
C	-10.931799	-1.087848	0.705947
C	-10.774129	0.165905	1.323618
N	-11.896388	0.900136	1.777936
C	-13.156713	0.797402	1.142588
C	-13.547050	-0.390418	0.497570
S	-12.539841	-1.854609	0.646442
C	-14.070806	1.860523	1.136358
C	-15.307711	1.745707	0.512021
C	-15.686178	0.576373	-0.158683
C	-14.769300	-0.485051	-0.157586
C	-9.835831	-1.794762	0.223608

C	-8.526057	-1.320916	0.388475
C	-8.370998	-0.088947	1.035582
C	-9.465581	0.644678	1.478760
C	-11.670616	2.007198	2.674743
C	-19.375744	0.975520	-0.952086
C	-19.533120	0.206012	-2.118629
N	-20.801338	0.076546	-2.735267
C	-21.995165	0.102284	-1.975066
C	-22.079113	0.856212	-0.790527
S	-20.740621	1.945476	-0.339714
C	-23.138844	-0.607566	-2.366442
C	-24.304164	-0.572359	-1.609261
C	-24.381579	0.150962	-0.412538
C	-23.235392	0.857719	-0.019262
C	-18.144588	1.068235	-0.312503
C	-16.998124	0.452689	-0.835725
C	-17.150822	-0.278931	-2.019962
C	-18.388146	-0.412590	-2.639801
C	-20.859028	-0.419538	-4.088337
C	-4.315335	-6.230795	-2.896593
C	-4.451111	-7.601897	-3.108859
C	-4.371929	-8.486923	-2.035147
C	-4.156776	-7.999649	-0.746165
C	-4.021090	-6.629955	-0.530050
C	-11.304212	3.266531	2.193650
C	-11.092519	4.315241	3.086352
C	-11.246367	4.109635	4.457149
C	-11.612155	2.852444	4.934979
C	-11.824366	1.800764	4.044997
C	-20.954849	0.499806	-5.132403
C	-21.012030	0.051900	-6.450998
C	-20.973527	-1.313701	-6.727619
C	-20.877363	-2.232727	-5.683110

C	-20.820015	-1.788657	-4.363526
C	-25.614921	0.175753	0.407891
C	-26.884745	0.122173	-0.185542
C	-28.046268	0.117841	0.578926
C	-27.996035	0.234960	1.979719
C	-26.726948	0.292582	2.572825
C	-25.568571	0.248179	1.805519
S	-29.607222	-0.165497	-0.234439
C	-30.664940	0.773434	0.851978
C	-30.381384	0.828664	2.228758
N	-29.184132	0.280252	2.748686
C	-31.822392	1.341863	0.332490
C	-32.779744	1.945052	1.161226
C	-32.509059	1.969588	2.534671
C	-31.335420	1.437800	3.056183
C	-29.081355	0.103055	4.176765
C	-36.400426	3.021672	0.799890
C	-36.423903	3.636763	-0.464646
N	-37.625462	4.175540	-0.986772
C	-38.885471	3.603574	-0.676003
C	-39.101479	2.979838	0.566826
S	-37.851055	3.070326	1.834399
C	-39.955764	3.643807	-1.581768
C	-41.187764	3.077342	-1.262482
C	-41.377495	2.431875	-0.044862
C	-40.322859	2.379084	0.863592
C	-35.234907	2.454128	1.302630
C	-34.022544	2.525452	0.601247
C	-34.041324	3.171395	-0.640853
C	-35.213321	3.701342	-1.169181
C	-37.538310	5.067713	-2.116730
C	-29.353085	-1.152546	4.718307
C	-29.265817	-1.349321	6.095670

C	-28.907227	-0.293345	6.931599
C	-28.634520	0.962128	6.388843
C	-28.721010	1.162687	5.012790
C	-37.571796	6.442518	-1.886859
C	-37.487699	7.329724	-2.958769
C	-37.370018	6.844546	-4.260059
C	-37.336120	5.469297	-4.489531
C	-37.419599	4.579610	-3.420447
H	9.344499	-3.621274	0.639488
H	7.063974	-4.157368	1.466226
H	7.795469	-0.111055	-1.275611
H	9.688706	-1.561494	-0.723068
H	1.985840	-3.506641	0.536670
H	1.009629	-0.470587	-2.337034
H	3.240655	0.462442	-2.109514
H	5.763862	0.238273	-3.077004
H	6.208569	2.527974	-3.918440
H	6.188088	4.451656	-2.351722
H	5.721706	4.078751	0.057030
H	5.276040	1.778127	0.890611
H	-6.275213	-5.308278	-0.428756
H	-8.202472	-4.040658	0.330274
H	-6.188056	-0.381986	-0.663485
H	-1.064764	-0.771712	-1.306174
H	0.580707	-4.714702	-0.885756
H	-1.649339	-5.663282	-1.055920
H	-13.816022	2.789934	1.625310
H	-15.972257	2.601464	0.523834
H	-15.029072	-1.423099	-0.634149
H	-10.010779	-2.735225	-0.285488
H	-7.378268	0.306482	1.214448
H	-9.296298	1.591351	1.971724
H	-23.121012	-1.196076	-3.272696

H	-25.154858	-1.151986	-1.947284
H	-23.254000	1.459224	0.881998
H	-18.082134	1.632743	0.610363
H	-16.289334	-0.748061	-2.480283
H	-18.458201	-0.990617	-3.550365
H	-4.374861	-5.532185	-3.722609
H	-4.618263	-7.976411	-4.112085
H	-4.477171	-9.552801	-2.201237
H	-4.094629	-8.684466	0.091593
H	-3.854447	-6.245414	0.469507
H	-11.186355	3.420486	1.127264
H	-10.807837	5.291209	2.710668
H	-11.081173	4.926770	5.149786
H	-11.732357	2.688187	5.999514
H	-12.108513	0.818404	4.403092
H	-20.983667	1.558409	-4.903195
H	-21.086386	0.769592	-7.259749
H	-21.017995	-1.661433	-7.753226
H	-20.847022	-3.295420	-5.893948
H	-20.745613	-2.498334	-3.547731
H	-26.976974	0.080511	-1.264409
H	-26.639159	0.352376	3.648274
H	-24.612600	0.258208	2.315354
H	-32.000229	1.270187	-0.734262
H	-33.207644	2.442270	3.214769
H	-31.161835	1.498589	4.121008
H	-39.829224	4.129900	-2.538483
H	-41.996172	3.136443	-1.982026
H	-42.330048	1.978540	0.201172
H	-40.449748	1.889180	1.822240
H	-35.276523	1.949839	2.260854
H	-33.124301	3.278427	-1.208157
H	-35.178490	4.189458	-2.132769

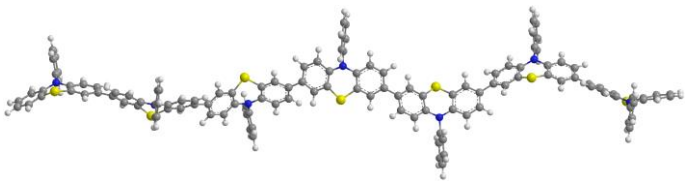
H	-29.631545	-1.964918	4.057673
H	-29.478071	-2.326636	6.513364
H	-28.840186	-0.447275	8.002372
H	-28.355160	1.785893	7.035424
H	-28.511976	2.136310	4.584896
H	-37.662847	6.805864	-0.870146
H	-37.513844	8.397709	-2.775987
H	-37.304718	7.534922	-5.093078
H	-37.244782	5.087994	-5.499972
H	-37.393653	3.509841	-3.592558

SCF Done: E(RB3LYP) = -6875.33646642 A.U. after 7 cycles

E (HOMO) = -4.992 eV

E (LUMO) = -1.464 eV

11.42 Computed xyz-coordinates of phenothiazine heptamer



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C	26.94996	1.28367	0.43155
N	25.74056	2.00342	0.25561
C	24.51516	1.33595	0.01675
C	24.27314	0.05996	0.55727
S	25.43306	-0.64055	1.71663
C	23.49303	1.91264	-0.75009
C	22.29442	1.24462	-0.97391
C	22.06469	-0.04066	-0.46808
C	23.08880	-0.61921	0.29594
C	28.12022	-0.72424	1.16180
C	29.34186	-0.17973	0.77250
C	29.36688	1.09710	0.22093
C	28.18711	1.81532	0.03914
C	25.81763	3.41492	-0.03034

C	20.79705	-0.76425	-0.72176
C	19.57340	-0.08263	-0.78885
C	18.38246	-0.74938	-1.05462
C	18.34936	-2.14724	-1.20661
C	19.57203	-2.82956	-1.13197
C	20.76517	-2.15143	-0.90933
S	16.90338	0.20925	-1.31970
C	15.70040	-0.96112	-0.71729
C	15.90296	-2.33909	-0.91764
N	17.12708	-2.82629	-1.43517
C	14.52027	-0.48103	-0.16169
C	13.46149	-1.33967	0.16817
C	13.64890	-2.70552	-0.07544
C	14.84260	-3.19679	-0.59220
C	17.18381	-4.19875	-1.87601
C	17.36545	-5.24305	-0.96605
C	17.41739	-6.55861	-1.42165
C	17.28888	-6.83347	-2.78303
C	17.10809	-5.79003	-3.68920
C	17.05555	-4.47235	-3.23698
C	25.65588	4.31925	1.01863
C	25.72515	5.68968	0.77351
C	25.95572	6.15795	-0.51888
C	26.11692	5.25328	-1.56796
C	26.04832	3.88265	-1.32658
C	9.78324	-0.91175	1.00500
C	9.78716	0.18327	1.88753
N	8.57982	0.67629	2.44022
C	7.35712	0.59802	1.73213
C	7.11574	-0.44660	0.82117
S	8.26896	-1.80211	0.70019
C	6.33608	1.54198	1.91068
C	5.13938	1.45228	1.20899

C	4.90947	0.43418	0.27570
C	5.93254	-0.50803	0.09406
C	10.96182	-1.37739	0.43193
C	12.20560	-0.81492	0.75322
C	12.20848	0.25443	1.65697
C	11.02974	0.75173	2.20077
C	8.66092	1.56964	3.56980
C	1.23057	0.67138	-0.62462
C	1.19532	0.18803	-1.94484
N	-0.02664	0.10559	-2.65669
C	-1.25344	-0.13567	-1.99311
C	-1.45524	0.29727	-0.66986
S	-0.24472	1.34553	0.11486
C	-2.31657	-0.80071	-2.62022
C	-3.51518	-1.03353	-1.95494
C	-3.70389	-0.64088	-0.62457
C	-2.64016	0.02351	0.00313
C	2.42088	0.71951	0.09244
C	3.64251	0.34726	-0.48707
C	3.60848	-0.10129	-1.81297
C	2.41538	-0.19320	-2.52100
C	0.02752	-0.08432	-4.08563
C	-7.39861	-1.09932	0.11490
C	-7.40935	-1.40456	1.48788
N	-8.62919	-1.63389	2.17089
C	-9.82306	-0.97830	1.78524
C	-10.04521	-0.61505	0.44439
S	-8.91496	-1.16683	-0.82021
C	-10.83170	-0.67165	2.70932
C	-11.99653	-0.02233	2.31628
C	-12.20273	0.37719	0.99035
C	-11.19359	0.07059	0.06584
C	-6.20880	-0.82957	-0.55280

C	-4.96937	-0.90759	0.09826
C	-4.98128	-1.24893	1.45607
C	-6.17005	-1.47932	2.13905
C	-8.57850	-2.24918	3.47471
C	8.49894	1.04481	4.85122
C	8.57462	1.88430	5.96152
C	8.81213	3.24727	5.79258
C	8.97382	3.77158	4.51036
C	8.89879	2.93554	3.39821
C	0.20294	-1.35369	-4.64192
C	0.25303	-1.50332	-6.02632
C	0.12830	-0.38913	-6.85582
C	-0.04711	0.87642	-6.29882
C	-0.09768	1.03000	-4.91426
C	-8.81991	-3.61840	3.57847
C	-8.77856	-4.23941	4.82584
C	-8.49600	-3.49396	5.96908
C	-8.25511	-2.12426	5.86463
C	-8.29637	-1.49995	4.61961
C	-13.42988	1.09515	0.57392
C	-14.67499	0.79702	1.14594
C	-15.82581	1.48955	0.78561
C	-15.79601	2.47951	-0.21314
C	-14.55255	2.77049	-0.79182
C	-13.39844	2.10343	-0.39700
S	-17.32860	1.18985	1.69614
C	-18.51139	1.52397	0.40385
C	-18.24347	2.52485	-0.54804
N	-16.97789	3.15622	-0.60268
C	-19.73646	0.86741	0.43170
C	-20.77424	1.21351	-0.44584
C	-20.51846	2.23941	-1.36348
C	-19.28149	2.87110	-1.42450

C	-16.84794	4.35898	-1.38862
C	-24.50810	0.55850	-0.62251
C	-24.60258	-0.81308	-0.32679
N	-25.86140	-1.46175	-0.29064
C	-27.03151	-0.77556	0.12213
C	-27.17349	0.60354	-0.11899
S	-25.96609	1.45868	-1.11438
C	-28.08389	-1.43797	0.77091
C	-29.22768	-0.74948	1.16894
C	-29.34079	0.62072	0.95652
C	-28.30165	1.29408	0.31830
C	-23.27972	1.21032	-0.62867
C	-22.08188	0.51837	-0.39874
C	-22.17699	-0.85328	-0.13435
C	-23.40581	-1.50207	-0.08504
C	-25.88881	-2.90301	-0.33330
C	-16.90905	5.59239	-0.74160
C	-16.78712	6.77034	-1.47708
C	-16.60415	6.71696	-2.85779
C	-16.54313	5.48267	-3.50425
C	-16.66457	4.30323	-2.77240
C	-26.11572	-3.52987	-1.55801
C	-26.14644	-4.92140	-1.63302
C	-25.95027	-5.68777	-0.48544
C	-25.72291	-5.06071	0.73931
C	-25.69171	-3.66974	0.81802
H	23.63222	2.89527	-1.17785
H	21.54142	1.72740	-1.58550
H	22.94566	-1.59866	0.73730
H	28.07710	-1.71436	1.60104
H	30.30652	1.54312	-0.08385
H	28.23093	2.80136	-0.40085
H	19.54245	0.98927	-0.63284

H	19.59723	-3.90126	-1.26842
H	21.68764	-2.71979	-0.89521
H	14.40969	0.58862	-0.02653
H	12.86617	-3.41160	0.17558
H	14.94886	-4.26177	-0.74124
H	17.46512	-5.02283	0.09048
H	17.55831	-7.36726	-0.71388
H	17.32974	-7.85761	-3.13550
H	17.00799	-5.99926	-4.74790
H	16.91571	-3.65164	-3.93051
H	25.47716	3.94208	2.01852
H	25.59890	6.38908	1.59181
H	26.00928	7.22370	-0.70886
H	26.29595	5.61318	-2.57452
H	26.17275	3.17529	-2.13830
H	6.47431	2.35806	2.60552
H	4.38791	2.21556	1.37273
H	5.78996	-1.33473	-0.59223
H	10.90551	-2.19634	-0.27560
H	13.14695	0.70422	1.95864
H	11.08137	1.57944	2.89369
H	-2.20898	-1.14193	-3.63999
H	-4.30174	-1.56424	-2.47834
H	-2.75113	0.37798	1.02131
H	2.39104	1.05636	1.12196
H	4.52914	-0.37387	-2.31516
H	2.43925	-0.54654	-3.54207
H	-10.70726	-0.94082	3.74850
H	-12.73955	0.20697	3.07094
H	-11.32185	0.32911	-0.97885
H	-6.25297	-0.55322	-1.59977
H	-4.04694	-1.35137	1.99519
H	-6.12961	-1.73897	3.18721

H	8.31520	-0.01658	4.96849
H	8.44828	1.47255	6.95608
H	8.87123	3.89930	6.65635
H	9.15869	4.83086	4.37460
H	9.02432	3.33715	2.39936
H	0.29918	-2.21572	-3.99207
H	0.38953	-2.48911	-6.45559
H	0.16752	-0.50774	-7.93246
H	-0.14460	1.74491	-6.93981
H	-0.23302	2.00814	-4.46828
H	-9.03833	-4.18654	2.68214
H	-8.96678	-5.30401	4.90258
H	-8.46374	-3.97771	6.93846
H	-8.03552	-1.54073	6.75117
H	-8.11094	-0.43565	4.53231
H	-14.75418	0.01229	1.88914
H	-14.47914	3.54208	-1.54482
H	-12.45576	2.38953	-0.84826
H	-19.89804	0.10378	1.18370
H	-21.28319	2.53228	-2.07311
H	-19.12357	3.64226	-2.16479
H	-28.01406	-2.50017	0.95709
H	-30.02649	-1.29488	1.65806
H	-30.22305	1.16149	1.27684
H	-28.37127	2.36002	0.13378
H	-23.25990	2.27686	-0.81971
H	-21.27743	-1.43666	0.02270
H	-23.42993	-2.56238	0.12265
H	-17.05179	5.62002	0.33211
H	-16.83522	7.72738	-0.97068
H	-16.50938	7.63334	-3.42876
H	-16.40108	5.43658	-4.57773
H	-16.61785	3.34107	-3.26916

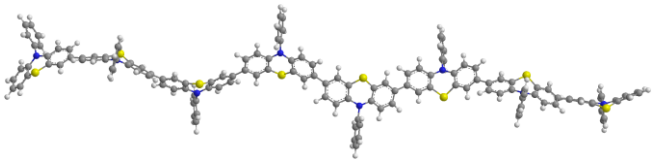
H	-26.26639	-2.92199	-2.44218
H	-26.32326	-5.40454	-2.58697
H	-25.97401	-6.76977	-0.54439
H	-25.56961	-5.65290	1.63403
H	-25.51503	-3.17722	1.76720
H	30.25573	-0.74640	0.90329

SCF Done: E(RB3LYP) = -8021.02589567 A.U. after 5 cycles

E (HOMO) = -4.989 eV

E (LUMO) = -1.462 eV

11.43 Computed xyz-coordinates of phenothiazine octamer



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C	-30.73344	-2.50698	0.77095
N	-29.98086	-2.41031	-0.42714
C	-28.77652	-1.66620	-0.48034
C	-28.60292	-0.51944	0.31501
S	-29.96835	0.10390	1.27697
C	-27.71846	-2.02613	-1.32680
C	-26.54477	-1.28210	-1.37179
C	-26.35527	-0.16017	-0.55584
C	-27.41016	0.19512	0.29715
C	-31.44833	-1.54817	2.89348
C	-32.20070	-2.68535	3.17843
C	-32.22540	-3.72682	2.25661
C	-31.49199	-3.64704	1.07490
C	-30.23964	-3.36398	-1.47791
C	-22.67885	0.73858	-0.84438
C	-22.67829	2.13247	-0.65545
N	-21.46828	2.86812	-0.67714
C	-20.24612	2.29336	-0.25302
C	-20.00887	0.91382	-0.39353

S	-21.16974	-0.09815	-1.29296
C	-19.22156	3.06675	0.31083
C	-18.02371	2.49093	0.71866
C	-17.79740	1.11352	0.61072
C	-18.82486	0.33854	0.05331
C	-23.85847	0.00488	-0.78224
C	-25.10051	0.62731	-0.59091
C	-25.09987	2.01944	-0.44155
C	-23.91950	2.75387	-0.45889
C	-21.54214	4.30436	-0.79112
C	-16.52845	0.49376	1.05861
C	-15.30334	1.15784	0.90176
C	-14.10994	0.59632	1.34223
C	-14.07757	-0.68967	1.91054
C	-15.30169	-1.35633	2.06139
C	-16.49663	-0.77166	1.65712
S	-12.62391	1.57959	1.28591
C	-11.43495	0.27279	1.04111
C	-11.63933	-0.97934	1.64914
N	-12.85223	-1.27252	2.31747
C	-10.26397	0.55270	0.34637
C	-9.21682	-0.37725	0.26793
C	-9.40915	-1.60868	0.90625
C	-10.59336	-1.90945	1.56949
C	-12.89779	-2.43174	3.17467
C	-13.10333	-3.71148	2.65338
C	-13.14112	-4.81105	3.50835
C	-12.97408	-4.63593	4.88184
C	-12.76947	-3.35829	5.39996
C	-12.73097	-2.25586	4.54770
C	-31.06905	-2.98718	-2.53350
C	-31.33637	-3.88673	-3.56438
C	-30.77591	-5.16261	-3.54156

C	-29.94654	-5.53933	-2.48547
C	-29.67701	-4.64274	-1.45360
C	-21.35634	4.88708	-2.04397
C	-21.41854	6.27276	-2.18271
C	-21.66664	7.07616	-1.07113
C	-21.85258	6.49245	0.18182
C	-21.79047	5.10784	0.32449
C	-5.54894	-0.27449	-0.70326
C	-5.54707	0.54389	-1.84715
N	-4.33902	0.85082	-2.51945
C	-3.10710	0.93266	-1.82692
C	-2.87086	0.15791	-0.67661
S	-4.04887	-1.08865	-0.18850
C	-2.07124	1.77366	-2.25766
C	-0.86455	1.84322	-1.57062
C	-0.63878	1.09897	-0.40638
C	-1.67696	0.26154	0.02741
C	-6.72537	-0.54110	-0.01159
C	-7.96504	-0.06150	-0.45883
C	-7.96419	0.71923	-1.62108
C	-6.78585	1.02748	-2.29153
C	-4.41923	1.43051	-3.83799
C	3.06055	1.45036	0.36779
C	3.10403	1.31952	1.76758
N	4.33641	1.37263	2.46383
C	5.53949	0.92190	1.86882
C	5.73303	1.00554	0.47790
S	4.54226	1.86807	-0.53139
C	6.58683	0.38602	2.63144
C	7.76321	-0.05260	2.03438
C	7.94463	-0.00411	0.64691
C	6.89554	0.52851	-0.11649
C	1.85999	1.35121	-0.32691

C	0.63826	1.18070	0.34021
C	0.68119	1.09350	1.73702
C	1.88280	1.14701	2.43419
C	4.30642	1.53752	3.89681
C	11.60365	-0.81095	0.04317
C	11.58699	-1.42696	-1.22111
N	12.78615	-1.87713	-1.82611
C	14.02090	-1.22595	-1.59114
C	14.27383	-0.57629	-0.36904
S	13.11907	-0.74480	0.97961
C	15.04168	-1.20593	-2.55193
C	16.24873	-0.56011	-2.30936
C	16.48928	0.11944	-1.10906
C	15.46742	0.10125	-0.14852
C	10.43535	-0.32991	0.62395
C	9.18756	-0.49148	0.00468
C	9.17066	-1.13679	-1.23781
C	10.34024	-1.58181	-1.84356
C	12.68780	-2.76735	-2.95700
C	-4.26429	0.59918	-4.94646
C	-4.33791	1.13325	-6.23206
C	-4.56618	2.49651	-6.41076
C	-4.72020	3.32754	-5.30134
C	-4.64668	2.79749	-4.01490
C	4.08060	0.45144	4.74615
C	4.06146	0.64242	6.12619
C	4.26855	1.91425	6.65982
C	4.49401	2.99630	5.81078
C	4.51278	2.80926	4.42947
C	12.83275	-4.13773	-2.74549
C	12.74223	-5.02078	-3.82036
C	12.50747	-4.53590	-5.10585
C	12.36244	-3.16489	-5.31656

C	12.45214	-2.27930	-4.24464
C	17.76528	0.82808	-0.85485
C	18.98342	0.32373	-1.33258
C	20.18212	0.99649	-1.12213
C	20.22790	2.18147	-0.36585
C	19.01054	2.68299	0.11596
C	17.80999	2.02842	-0.13533
S	21.65578	0.39957	-1.92862
C	22.86307	0.91474	-0.72122
C	22.67041	2.11162	-0.00742
N	21.45893	2.83582	-0.11588
C	24.03536	0.17959	-0.59007
C	25.09438	0.62370	0.21536
C	24.91183	1.83252	0.89818
C	23.72713	2.55344	0.80102
C	21.42605	4.18925	0.38225
C	28.76817	-0.24691	0.60533
C	28.76969	-1.65170	0.53752
N	29.98075	-2.38048	0.62911
C	31.20094	-1.84596	0.14221
C	31.43663	-0.45901	0.17079
S	30.27736	0.62126	0.98815
C	32.21234	-2.67037	-0.37276
C	33.40679	-2.13096	-0.84490
C	33.61372	-0.75537	-0.84265
C	32.61624	0.07739	-0.34072
C	27.58989	0.47921	0.47146
C	26.34828	-0.15725	0.32895
C	26.34916	-1.55726	0.30350
C	27.52898	-2.28775	0.39005
C	29.90677	-3.79936	0.87780
C	21.60154	5.23876	-0.51860
C	21.57499	6.55656	-0.06483

C	21.37323	6.82650	1.28761
C	21.19807	5.77611	2.18821
C	21.22454	4.45762	1.73844
C	30.08968	-4.26003	2.18102
C	30.02442	-5.62580	2.45246
C	29.77624	-6.53205	1.42308
C	29.59262	-6.07095	0.11973
C	29.65755	-4.70648	-0.15523
H	-27.81849	-2.88521	-1.97469
H	-25.77065	-1.58046	-2.06881
H	-27.30586	1.04603	0.96008
H	-31.42096	-0.72020	3.59266
H	-32.80910	-4.61847	2.45415
H	-31.51769	-4.47409	0.37995
H	-19.35869	4.13165	0.43306
H	-17.26813	3.12953	1.16072
H	-18.68413	-0.72776	-0.08044
H	-23.80459	-1.07227	-0.88797
H	-26.03662	2.55062	-0.32174
H	-23.96903	3.82660	-0.33848
H	-15.27335	2.13232	0.42876
H	-15.32661	-2.33588	2.51733
H	-17.42004	-1.31311	1.82586
H	-10.15057	1.53292	-0.10192
H	-8.63791	-2.36833	0.85964
H	-10.70316	-2.88155	2.02857
H	-13.23185	-3.84170	1.58510
H	-13.30060	-5.80276	3.10119
H	-13.00380	-5.49255	5.54520
H	-12.63980	-3.21755	6.46675
H	-12.57252	-1.25732	4.93742
H	-31.49799	-1.99219	-2.53898
H	-31.98153	-3.58977	-4.38308

H	-30.98424	-5.86163	-4.34328
H	-29.50879	-6.53061	-2.46393
H	-29.03287	-4.93006	-0.63065
H	-21.16401	4.25087	-2.89965
H	-21.27332	6.72230	-3.15815
H	-21.71467	8.15350	-1.17974
H	-22.04518	7.11376	1.04875
H	-21.93256	4.64846	1.29581
H	-2.20674	2.38184	-3.14059
H	-0.10103	2.51941	-1.93662
H	-1.53846	-0.35942	0.90479
H	-6.66982	-1.13691	0.89175
H	-8.89949	1.08771	-2.02545
H	-6.83543	1.63627	-3.18302
H	6.48424	0.30899	3.70442
H	8.53682	-0.47273	2.66620
H	7.00163	0.61745	-1.19143
H	1.88191	1.40905	-1.40876
H	-0.23873	0.99354	2.30069
H	1.86597	1.07297	3.51210
H	14.89345	-1.69894	-3.50202
H	16.99985	-0.56018	-3.09035
H	15.61958	0.58401	0.80980
H	10.50327	0.17843	1.57852
H	8.22818	-1.31128	-1.74333
H	10.27743	-2.07380	-2.80372
H	-4.08749	-0.45884	-4.79358
H	-4.21712	0.48404	-7.09145
H	-4.62361	2.91093	-7.41062
H	-4.89734	4.38828	-5.43605
H	-4.76542	3.43832	-3.14889
H	3.92216	-0.53487	4.32567
H	3.88596	-0.20171	6.78294

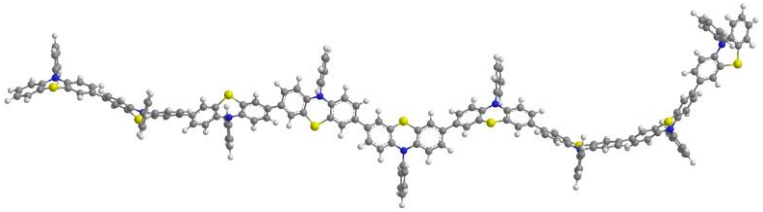
H	4.25406	2.06051	7.73367
H	4.65513	3.98633	6.22129
H	4.68708	3.64181	3.75837
H	13.01468	-4.50151	-1.74120
H	12.85486	-6.08551	-3.65202
H	12.43720	-5.22319	-5.94097
H	12.17955	-2.78362	-6.31450
H	12.34064	-1.21281	-4.40233
H	19.00383	-0.61040	-1.88138
H	18.99554	3.60562	0.67839
H	16.89222	2.47472	0.22891
H	24.13986	-0.73333	-1.16472
H	25.69217	2.20912	1.54879
H	23.62540	3.47129	1.36228
H	32.07063	-3.74140	-0.39595
H	34.17121	-2.79846	-1.22550
H	34.53593	-0.33161	-1.22129
H	32.75805	1.15195	-0.32194
H	27.64539	1.56135	0.48123
H	25.41277	-2.09700	0.22697
H	27.47892	-3.36695	0.36333
H	21.75766	5.01509	-1.56723
H	21.71177	7.36992	-0.76797
H	21.35271	7.85145	1.63949
H	21.04121	5.98163	3.24075
H	21.08959	3.63701	2.43351
H	30.28150	-3.54508	2.97221
H	30.16704	-5.97957	3.46695
H	29.72566	-7.59385	1.63473
H	29.39901	-6.77219	-0.68370
H	29.51621	-4.34276	-1.16640
H	-32.75922	-2.74962	4.10436

SCF Done: E(RB3LYP) = -9166.71541847 A.U. after 7 cycles

E (HOMO) = -4.982 eV

E (LUMO) = -1.471 eV

11.44 Computed xyz-coordinates of phenothiazine nonamer



C	32.77446	6.16107	-1.06983
C	32.06155	6.91443	-0.11884
N	31.18154	6.27680	0.79256
C	30.47673	5.10248	0.43407
C	31.03208	4.17622	-0.46745
S	32.71791	4.37981	-1.01283
C	29.21235	4.80507	0.96153
C	28.53247	3.64818	0.59783
C	29.06630	2.74215	-0.32689
C	30.33100	3.04039	-0.85538
C	33.61045	6.78275	-1.99475
C	33.80182	8.16217	-1.96122
C	33.12970	8.91382	-1.00290
C	32.26034	8.30274	-0.10204
C	30.73064	7.02035	1.94332
C	26.83582	-0.32591	-0.20165
C	26.90263	-0.81935	-1.51731
N	26.17654	-1.97400	-1.89654
C	24.93803	-2.29576	-1.28959
C	24.68368	-1.95411	0.05072
S	25.98911	-1.26881	1.05350
C	23.92340	-2.96855	-1.98457
C	22.71173	-3.27398	-1.37500
C	22.43971	-2.89965	-0.05342
C	23.45376	-2.22375	0.64067
C	27.51498	0.82885	0.16900

C	28.33367	1.52112	-0.73542
C	28.42392	1.00756	-2.03518
C	27.71841	-0.12602	-2.42230
C	26.52160	-2.62187	-3.13827
C	18.71986	-3.45657	0.45127
C	18.62646	-3.74582	1.82454
N	17.37045	-3.99734	2.42903
C	16.18798	-3.38093	1.95361
C	16.04408	-3.04758	0.59445
S	17.27275	-3.58306	-0.58230
C	15.11341	-3.08505	2.80389
C	13.95977	-2.47584	2.32367
C	13.82779	-2.10887	0.97883
C	14.90337	-2.40449	0.12829
C	19.94321	-3.16057	-0.13966
C	21.13952	-3.19877	0.59132
C	21.04701	-3.52887	1.94883
C	19.82208	-3.78234	2.55570
C	17.35049	-4.58961	3.74427
C	12.61147	-1.43365	0.46954
C	11.34293	-1.73035	0.98909
C	10.20105	-1.07451	0.54216
C	10.26543	-0.12878	-0.49702
C	11.53238	0.16030	-1.02339
C	12.67557	-0.46611	-0.54051
S	8.66254	-1.35729	1.39688
C	7.53116	-1.08550	0.04542
C	7.83371	-0.13043	-0.94250
N	9.09559	0.50947	-0.97582
C	6.30525	-1.74090	0.06065
C	5.30051	-1.44107	-0.87072
C	5.59327	-0.46638	-1.83225
C	6.83120	0.16452	-1.87727

C	9.24938	1.67167	-1.81669
C	9.49764	1.54586	-3.18565
C	9.64301	2.68698	-3.97183
C	9.54112	3.95247	-3.39449
C	9.29334	4.07561	-2.02846
C	9.14737	2.93613	-1.23865
C	31.38010	6.82617	3.16184
C	30.96648	7.53064	4.29135
C	29.90395	8.42852	4.20509
C	29.25409	8.62206	2.98638
C	29.66549	7.92036	1.85508
C	27.37226	-3.72598	-3.10192
C	27.72589	-4.37138	-4.28578
C	27.23032	-3.91454	-5.50581
C	26.37910	-2.81044	-5.54146
C	26.02368	-2.16255	-4.36011
C	17.14181	-5.96353	3.85669
C	17.11643	-6.56247	5.11522
C	17.29931	-5.79023	6.26100
C	17.50778	-4.41593	6.14785
C	17.53357	-3.81369	4.89161
C	1.57035	-2.08022	-1.14464
C	1.44786	-3.42217	-0.74187
N	0.18012	-4.05244	-0.69081
C	-0.99496	-3.32118	-0.39353
C	-1.10801	-1.96372	-0.74561
S	0.14535	-1.20551	-1.76277
C	-2.09207	-3.91029	0.25063
C	-3.23613	-3.17658	0.54396
C	-3.33467	-1.81473	0.23398
C	-2.23847	-1.22644	-0.41374
C	2.80592	-1.44279	-1.15655
C	3.98664	-2.12427	-0.82774

C	3.86529	-3.47061	-0.46278
C	2.62757	-4.10176	-0.40701
C	0.13756	-5.49008	-0.58134
C	-6.95102	-0.85185	0.87405
C	-6.85712	0.50457	1.23373
N	-8.01490	1.25580	1.55143
C	-9.26973	0.96823	0.96342
C	-9.59867	-0.33958	0.56198
S	-8.51800	-1.69539	0.98005
C	-10.23866	1.96244	0.76681
C	-11.46920	1.66750	0.19120
C	-11.78517	0.37476	-0.24326
C	-10.81442	-0.61908	-0.05167
C	-5.82092	-1.58312	0.52452
C	-4.53765	-1.01983	0.57407
C	-4.44492	0.32091	0.96683
C	-5.57475	1.06986	1.27497
C	-7.84289	2.53306	2.19979
C	-15.49325	0.41974	-1.04603
C	-15.60503	-0.52600	-2.08091
N	-16.86188	-0.81713	-2.66655
C	-18.06052	-0.73740	-1.91787
C	-18.18638	0.17263	-0.85231
S	-16.91208	1.38790	-0.56938
C	-19.16965	-1.54530	-2.20563
C	-20.33834	-1.46006	-1.45731
C	-20.45121	-0.58642	-0.36915
C	-19.34247	0.22317	-0.08231
C	-14.26901	0.68278	-0.44140
C	-13.08853	0.06221	-0.87445
C	-13.19828	-0.85473	-1.92677
C	-14.42578	-1.15266	-2.50808
C	-16.88122	-1.54258	-3.91329

C	-0.04804	-6.24465	-1.73894
C	-0.09214	-7.63589	-1.66275
C	0.04914	-8.27333	-0.43135
C	0.23529	-7.51777	0.72611
C	0.27987	-6.12706	0.65383
C	-7.53778	3.68164	1.46551
C	-7.37866	4.90139	2.11993
C	-7.52409	4.97670	3.50496
C	-7.82870	3.82955	4.23562
C	-7.98788	2.60730	3.58435
C	-17.00953	-0.82667	-5.10278
C	-17.02897	-1.50181	-6.32226
C	-16.92073	-2.89100	-6.35394
C	-16.79318	-3.60647	-5.16359
C	-16.77272	-2.93510	-3.94288
C	-21.68274	-0.51633	0.45138
C	-22.95154	-0.66360	-0.12732
C	-24.10957	-0.63411	0.64216
C	-24.05676	-0.39506	2.02719
C	-22.78863	-0.23842	2.60395
C	-21.63230	-0.31142	1.83557
S	-25.66611	-1.02881	-0.13239
C	-26.74465	-0.03200	0.87974
C	-26.45803	0.14096	2.24616
N	-25.24254	-0.32860	2.79872
C	-27.91923	0.46103	0.32312
C	-28.89048	1.10070	1.10715
C	-28.61720	1.23975	2.47331
C	-27.42683	0.78469	3.02879
C	-25.13098	-0.41218	4.23444
C	-32.54131	2.04222	0.67651
C	-32.58209	2.56470	-0.62861
N	-33.79845	3.03089	-1.18548

C	-35.04205	2.44812	-0.83224
C	-35.24065	1.90804	0.45190
S	-33.99309	2.12205	1.70748
C	-36.11358	2.39571	-1.73595
C	-37.33003	1.82117	-1.37419
C	-37.50183	1.25846	-0.11368
C	-36.44535	1.29739	0.79335
C	-31.35983	1.54613	1.21638
C	-30.15004	1.60178	0.50921
C	-30.18727	2.15559	-0.77615
C	-31.37385	2.61310	-1.33839
C	-33.73758	3.84254	-2.37615
C	-25.35252	-1.64247	4.85199
C	-25.25262	-1.75312	6.23794
C	-24.93149	-0.63598	7.00704
C	-24.70992	0.59424	6.38866
C	-24.80895	0.70876	5.00351
C	-33.82025	5.22831	-2.24591
C	-33.76429	6.03858	-3.37887
C	-33.62530	5.46587	-4.64190
C	-33.54214	4.07976	-4.77173
C	-33.59823	3.26678	-3.64153
H	28.75062	5.48390	1.66418
H	27.55019	3.47369	1.02069
H	30.80309	2.35364	-1.54813
H	34.12955	6.17517	-2.72718
H	33.26790	9.98775	-0.95442
H	31.74116	8.90945	0.62601
H	24.08636	-3.27504	-3.00804
H	21.97193	-3.82458	-1.94389
H	23.28702	-1.89911	1.66099
H	27.43796	1.16631	1.19590
H	29.02696	1.51720	-2.77721

H	27.80374	-0.47300	-3.44222
H	15.17707	-3.33069	3.85433
H	13.16527	-2.25213	3.02554
H	14.83688	-2.17084	-0.92793
H	19.95995	-2.89572	-1.19026
H	21.94562	-3.60271	2.54965
H	19.80062	-4.03003	3.60740
H	11.23729	-2.48361	1.76097
H	11.63209	0.89983	-1.80498
H	13.63484	-0.17908	-0.95441
H	6.11513	-2.46425	0.84502
H	4.85738	-0.21239	-2.58591
H	7.01696	0.89680	-2.64983
H	9.57614	0.55969	-3.62843
H	9.83591	2.58686	-5.03365
H	9.65481	4.83888	-4.00774
H	9.21355	5.05707	-1.57564
H	8.95482	3.01775	-0.17549
H	32.20439	6.12498	3.21552
H	31.47413	7.37666	5.23649
H	29.58245	8.97545	5.08390
H	28.42702	9.31892	2.91500
H	29.16422	8.06750	0.90546
H	27.75046	-4.07023	-2.14668
H	28.38741	-5.22929	-4.25332
H	27.50565	-4.41667	-6.42604
H	25.99134	-2.45225	-6.48808
H	25.36364	-1.30316	-4.38210
H	17.00107	-6.55248	2.95826
H	16.95402	-7.63079	5.19873
H	17.27946	-6.25686	7.23907
H	17.65012	-3.81170	7.03628
H	17.69401	-2.74591	4.79755

H	-2.05398	-4.95362	0.52960
H	-4.04968	-3.67419	1.05848
H	-2.28070	-0.18409	-0.70732
H	2.84462	-0.39480	-1.42943
H	4.75090	-4.04896	-0.22730
H	2.58379	-5.14207	-0.11741
H	-10.03237	2.97976	1.06716
H	-12.17945	2.47355	0.04959
H	-11.02538	-1.64212	-0.34088
H	-5.94782	-2.61239	0.21010
H	-3.47366	0.79399	1.05009
H	-5.45263	2.10164	1.57207
H	-19.12212	-2.25121	-3.02246
H	-21.16152	-2.11794	-1.70972
H	-19.39320	0.94098	0.72816
H	-14.23825	1.38698	0.38174
H	-12.31077	-1.33995	-2.31564
H	-14.46119	-1.86713	-3.31814
H	-0.15612	-5.73623	-2.68966
H	-0.23652	-8.21925	-2.56468
H	0.01501	-9.35508	-0.37290
H	0.34623	-8.00973	1.68547
H	0.42428	-5.53433	1.54963
H	-7.42695	3.61669	0.38929
H	-7.14192	5.79112	1.54807
H	-7.40017	5.92647	4.01226
H	-7.94216	3.88359	5.31212
H	-8.22446	1.70812	4.14063
H	-17.09285	0.25290	-5.06381
H	-17.12875	-0.94206	-7.24496
H	-16.93600	-3.41523	-7.30247
H	-16.70927	-4.68685	-5.18409
H	-16.67355	-3.48536	-3.01443

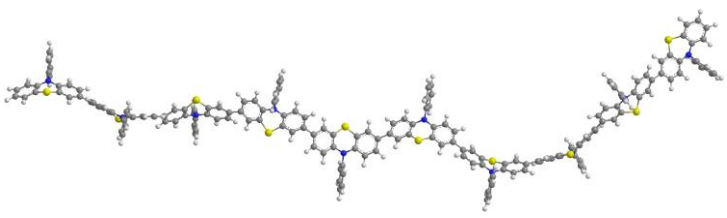
H	-23.04432	-0.80765	-1.19739
H	-22.69976	-0.07862	3.66906
H	-20.67426	-0.22036	2.33362
H	-28.09875	0.30017	-0.73359
H	-29.32771	1.74373	3.11771
H	-27.25149	0.93319	4.08475
H	-36.00088	2.81556	-2.72526
H	-38.14021	1.80820	-2.09408
H	-38.44191	0.79876	0.16619
H	-36.55843	0.87325	1.78454
H	-31.38663	1.11146	2.20864
H	-29.27373	2.24774	-1.35157
H	-31.35288	3.03197	-2.33437
H	-25.60167	-2.50275	4.24219
H	-25.42570	-2.71102	6.71453
H	-24.85431	-0.72272	8.08466
H	-24.46015	1.46533	6.98323
H	-24.63845	1.66234	4.51736
H	-33.92795	5.66066	-1.25819
H	-33.82861	7.11534	-3.27325
H	-33.58149	6.09653	-5.52231
H	-33.43397	3.63020	-5.75200
H	-33.53515	2.18897	-3.73670
H	34.46861	8.63587	-2.67143

SCF Done: E(RB3LYP) = -10312.4049228 A.U. after 7 cycles

E (HOMO) = -4.976 eV

E (LUMO) = -1.476 eV

11.45 Computed xyz-coordinates of phenothiazine decamer



C	34.79300	9.29837	-0.61893

C	35.75367	8.42661	-1.16402
N	35.38967	7.11816	-1.57226
C	34.36075	6.40165	-0.91504
C	33.26780	7.07539	-0.34026
S	33.07309	8.82790	-0.60777
C	34.37568	5.00323	-0.81769
C	33.35519	4.31403	-0.17238
C	32.28320	4.98353	0.43041
C	32.27093	6.38309	0.33730
C	35.14955	10.57160	-0.18004
C	36.45734	11.02967	-0.32306
C	37.40872	10.18933	-0.89214
C	37.06743	8.90010	-1.29481
C	36.29648	6.38704	-2.42260
C	29.77214	2.29364	1.36197
C	29.12430	2.84060	2.48398
N	28.08495	2.13535	3.13799
C	27.23224	1.25262	2.43277
C	27.69088	0.55372	1.30125
S	29.41645	0.62191	0.85557
C	25.90690	1.02833	2.83172
C	25.08063	0.15528	2.13338
C	25.52435	-0.51810	0.98869
C	26.84801	-0.28871	0.58568
C	30.76393	2.99901	0.68935
C	31.20390	4.25367	1.13561
C	30.58288	4.77782	2.27584
C	29.55934	4.09788	2.92623
C	27.67436	2.57976	4.44745
C	22.88054	-3.12150	0.19539
C	22.93597	-3.21290	-1.20741
N	22.07671	-4.08855	-1.91351
C	20.78824	-4.41497	-1.42501

C	20.52779	-4.45124	-0.04340
S	21.86589	-4.26077	1.11887
C	19.72628	-4.72487	-2.28622
C	18.46694	-5.04724	-1.79302
C	18.19401	-5.04725	-0.41965
C	19.25465	-4.72935	0.44133
C	23.69552	-2.23663	0.89169
C	24.64291	-1.43858	0.23377
C	24.71907	-1.55732	-1.15934
C	23.88009	-2.41198	-1.86544
C	22.37545	-4.37235	-3.29592
C	14.42165	-5.33928	-0.11157
C	14.25478	-5.98621	1.12623
N	12.96161	-6.27064	1.62866
C	11.85535	-5.43894	1.33129
C	11.78835	-4.73354	0.11601
S	13.00596	-5.03569	-1.15157
C	10.78192	-5.28798	2.22046
C	9.70213	-4.46718	1.91549
C	9.64795	-3.73724	0.72183
C	10.72346	-3.88599	-0.16625
C	15.68682	-5.01395	-0.58800
C	16.84912	-5.37304	0.11026
C	16.67939	-6.05438	1.32179
C	15.41621	-6.34135	1.82646
C	12.84392	-7.19677	2.72834
C	8.50924	-2.84533	0.40172
C	7.20305	-3.16233	0.80227
C	6.13340	-2.31589	0.53209
C	6.30979	-1.13512	-0.21118
C	7.61428	-0.82219	-0.61868
C	8.68646	-1.65006	-0.30588
S	4.54397	-2.68552	1.24950

C	3.49617	-1.98077	-0.00959
C	3.90710	-0.82299	-0.69530
N	5.20977	-0.29809	-0.51919
C	2.23202	-2.52331	-0.20813
C	1.29541	-1.91277	-1.05496
C	1.69522	-0.74050	-1.70778
C	2.97184	-0.21442	-1.54427
C	5.48016	1.03737	-0.99270
C	5.77430	1.28437	-2.33581
C	6.03252	2.58590	-2.76113
C	5.99819	3.64031	-1.84894
C	5.70498	3.39165	-0.50921
C	5.44592	2.09087	-0.08006
C	36.06081	6.37507	-3.79694
C	36.91891	5.67638	-4.64461
C	38.01249	4.98931	-4.12054
C	38.24833	5.00191	-2.74608
C	37.39256	5.69912	-1.89571
C	28.17832	1.91927	5.56714
C	27.79770	2.32644	6.84485
C	26.91425	3.39257	7.00468
C	26.40987	4.05215	5.88416
C	26.78763	3.64768	4.60545
C	23.06100	-5.54634	-3.60513
C	23.36287	-5.84661	-4.93248
C	22.98052	-4.97507	-5.95075
C	22.29471	-3.80097	-5.64058
C	21.99129	-3.49740	-4.31497
C	12.51230	-8.52298	2.45448
C	12.39167	-9.43958	3.49783
C	12.60208	-9.03237	4.81409
C	12.93364	-7.70553	5.08728
C	13.05480	-6.78646	4.04711

C	-2.45003	-2.20413	-1.59872
C	-2.66521	-3.59378	-1.57195
N	-3.96861	-4.12897	-1.71758
C	-5.10742	-3.42596	-1.25556
C	-5.13070	-2.01941	-1.24338
S	-3.79708	-1.10617	-1.99769
C	-6.25500	-4.09053	-0.80093
C	-7.36376	-3.38647	-0.34544
C	-7.37718	-1.98701	-0.29806
C	-6.22858	-1.32235	-0.75271
C	-1.18113	-1.66887	-1.40568
C	-0.05649	-2.48992	-1.23932
C	-0.26892	-3.87385	-1.25562
C	-1.54106	-4.41444	-1.40405
C	-4.10127	-5.53879	-1.99331
C	-10.95444	-1.02288	0.53044
C	-10.80366	0.20383	1.20199
N	-11.93014	0.91504	1.68182
C	-13.18882	0.83252	1.04017
C	-13.57233	-0.32880	0.34480
S	-12.55873	-1.79336	0.43352
C	-14.10826	1.89050	1.07742
C	-15.34425	1.79550	0.44796
C	-15.71592	0.65363	-0.27190
C	-14.79332	-0.40182	-0.31557
C	-9.85418	-1.70416	0.02171
C	-8.54652	-1.23400	0.21234
C	-8.39836	-0.03145	0.91415
C	-9.49714	0.67873	1.38415
C	-11.71124	1.98971	2.61894
C	-19.41083	1.05460	-1.03646
C	-19.56260	0.34913	-2.24344
N	-20.83057	0.24247	-2.86573

C	-22.02293	0.21005	-2.10347
C	-22.11121	0.89049	-0.87537
S	-20.78605	1.97073	-0.36715
C	-23.16033	-0.48714	-2.53414
C	-24.32234	-0.51303	-1.77126
C	-24.40154	0.13210	-0.53090
C	-23.26290	0.82871	-0.09980
C	-18.17918	1.12608	-0.39511
C	-17.02774	0.55175	-0.95285
C	-17.17549	-0.11745	-2.17400
C	-18.41266	-0.22959	-2.79860
C	-20.88382	-0.18302	-4.24282
C	-4.29991	-5.94742	-3.31139
C	-4.43060	-7.30345	-3.60722
C	-4.36295	-8.25120	-2.58754
C	-4.16452	-7.84165	-1.26915
C	-4.03359	-6.48727	-0.96966
C	-11.34156	3.26495	2.18452
C	-11.13724	4.28220	3.11449
C	-11.30259	4.02954	4.47607
C	-11.67238	2.75676	4.90723
C	-11.87663	1.73622	3.97985
C	-20.98543	0.78797	-5.23839
C	-21.03779	0.40791	-6.57843
C	-20.98884	-0.94135	-6.92447
C	-20.88683	-1.91203	-5.92835
C	-20.83414	-1.53595	-4.58770
C	-25.62848	0.08561	0.29815
C	-26.90291	0.07189	-0.28737
C	-28.05743	-0.00189	0.48440
C	-27.99442	-0.00152	1.88936
C	-26.72072	0.01879	2.47481
C	-25.56921	0.04641	1.69655

S	-29.62565	-0.22364	-0.33437
C	-30.67617	0.61540	0.83774
C	-30.37938	0.55447	2.21153
N	-29.17557	-0.03227	2.66982
C	-31.84064	1.22087	0.37973
C	-32.79088	1.75011	1.26545
C	-32.50611	1.65942	2.63346
C	-31.32661	1.08803	3.09669
C	-29.05849	-0.34886	4.07225
C	-36.40910	2.87351	1.04100
C	-36.45077	3.56821	-0.18094
N	-37.65634	4.14871	-0.64524
C	-38.91652	3.57121	-0.34539
C	-39.11514	2.87152	0.85946
S	-37.83934	2.86640	2.10477
C	-40.00450	3.68151	-1.22393
C	-41.23669	3.10930	-0.91591
C	-41.40987	2.38956	0.26185
C	-40.33777	2.26675	1.14267
C	-35.23972	2.26589	1.48432
C	-34.03906	2.37375	0.76753
C	-34.07546	3.09864	-0.43004
C	-35.25259	3.66854	-0.90218
C	-37.57974	5.10836	-1.71936
C	-29.29996	-1.65854	4.48503
C	-29.19063	-1.99402	5.83359
C	-28.84064	-1.02246	6.76964
C	-28.59952	0.28745	6.35609
C	-28.70774	0.62655	5.00894
C	-37.58187	6.46653	-1.40397
C	-37.50608	7.41759	-2.42032
C	-37.42898	7.01316	-3.75181
C	-37.42650	5.65454	-4.06695

C	-37.50079	4.70114	-3.05353
H	35.19231	4.44378	-1.25138
H	33.42087	3.23421	-0.11170
H	31.44602	6.94538	0.75906
H	34.38947	11.21134	0.25372
H	36.72209	12.02807	0.00331
H	38.43102	10.52662	-1.01831
H	37.82650	8.26154	-1.72371
H	25.51370	1.54074	3.69810
H	24.05989	0.02748	2.47365
H	27.24883	-0.81217	-0.27447
H	31.20102	2.55656	-0.19803
H	30.90712	5.72984	2.67908
H	29.10904	4.54421	3.80145
H	19.88824	-4.73567	-3.35466
H	17.68992	-5.31516	-2.49900
H	19.09175	-4.69958	1.51220
H	23.62108	-2.20703	1.97250
H	25.42170	-0.94867	-1.71614
H	23.96315	-2.45462	-2.94205
H	10.78725	-5.81600	3.16336
H	8.90567	-4.37222	2.64397
H	10.71355	-3.36806	-1.11825
H	15.76350	-4.47246	-1.52346
H	17.54565	-6.38227	1.88383
H	15.33558	-6.86639	2.76752
H	7.01004	-4.08424	1.33811
H	7.80002	0.08905	-1.16922
H	9.68023	-1.34520	-0.61167
H	1.95820	-3.41357	0.34598
H	1.01445	-0.24059	-2.38660
H	3.24159	0.68128	-2.08532
H	5.79978	0.46091	-3.04010

H	6.26039	2.77516	-3.80370
H	6.19968	4.65188	-2.18197
H	5.67750	4.20810	0.20304
H	5.21713	1.88338	0.95851
H	35.20693	6.91325	-4.19097
H	36.73206	5.66971	-5.71218
H	38.67930	4.44597	-4.78003
H	39.09771	4.46901	-2.33461
H	37.57142	5.71202	-0.82681
H	28.86408	1.09186	5.42877
H	28.19162	1.81061	7.71283
H	26.61896	3.70868	7.99849
H	25.72223	4.88129	6.00408
H	26.39766	4.15555	3.73101
H	23.35280	-6.21490	-2.80393
H	23.89605	-6.76010	-5.16896
H	23.21564	-5.20915	-6.98259
H	21.99555	-3.12057	-6.42941
H	21.45890	-2.58621	-4.06800
H	12.35113	-8.82643	1.42693
H	12.13358	-10.46966	3.28100
H	12.50802	-9.74564	5.62474
H	13.09777	-7.38466	6.10943
H	13.31183	-5.75393	4.25342
H	-6.28419	-5.17076	-0.79910
H	-8.21843	-3.94782	0.01281
H	-6.20134	-0.23909	-0.76751
H	-1.07181	-0.59096	-1.38516
H	0.57209	-4.55072	-1.16208
H	-1.65572	-5.48899	-1.40661
H	-13.85865	2.80002	1.60495
H	-16.01383	2.64610	0.49570
H	-15.04764	-1.32008	-0.83209

H	-10.02440	-2.62168	-0.52912
H	-7.40784	0.35912	1.11470
H	-9.33261	1.60326	1.91891
H	-23.13968	-1.01838	-3.47506
H	-25.16831	-1.08046	-2.14058
H	-23.28507	1.37242	0.83741
H	-18.12039	1.64002	0.55706
H	-16.31015	-0.55287	-2.65957
H	-18.47900	-0.75842	-3.73888
H	-4.35045	-5.20055	-4.09472
H	-4.58477	-7.61721	-4.63311
H	-4.46432	-9.30534	-2.81833
H	-4.11155	-8.57533	-0.47317
H	-3.87927	-6.16334	0.05305
H	-11.21564	3.45545	1.12499
H	-10.84968	5.27052	2.77502
H	-11.14333	4.82234	5.19779
H	-11.80173	2.55601	5.96441
H	-12.16378	0.74226	4.30166
H	-21.02237	1.83314	-4.95500
H	-21.11652	1.16555	-7.34943
H	-21.02959	-1.23648	-7.96660
H	-20.84823	-2.96222	-6.19354
H	-20.75513	-2.28589	-3.80924
H	-27.00381	0.11636	-1.36543
H	-26.62414	-0.00811	3.55086
H	-24.60812	0.02346	2.19635
H	-32.02929	1.23734	-0.68736
H	-33.19774	2.07162	3.35851
H	-31.14278	1.05868	4.16119
H	-39.89166	4.22730	-2.14961
H	-42.05871	3.22357	-1.61303
H	-42.36285	1.93209	0.49844

H	-40.45141	1.71775	2.07046
H	-35.26969	1.70087	2.40843
H	-33.16834	3.23684	-1.00647
H	-35.23145	4.21627	-1.83362
H	-29.57059	-2.40431	3.74711
H	-29.37860	-3.01318	6.15087
H	-28.75586	-1.28431	7.81797
H	-28.32702	1.04587	7.08080
H	-28.52097	1.64266	4.68128
H	-37.64226	6.76777	-0.36494
H	-37.50785	8.47228	-2.17065
H	-37.37083	7.75309	-4.54168
H	-37.36636	5.33554	-5.10105
H	-37.49812	3.64401	-3.29271

SCF Done: E(RB3LYP) = -11458.0944859 A.U. after 5 cycles

E (HOMO) = -4.973 eV

E (LUMO) = -1.484 eV

12 References

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