Supplementary Material for: Photoisomerization Action Spectroscopy: Flicking the Protonated Merocyanine-Spiropyran Switch in the Gas Phase

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Additional results of the quantum-chemical calculations

Table S1: DFT results for SPH^+ and MCH^+ isomers. Diagonal elements are isomer energies (kJ/-mol) with respect to that of the TTT form of MCH^+. Blue off-diagonal elements are isomerization barriers for rotation around single bonds in MCH^+ or inversion of the five-membered ring in SPH^+. Yellow cells are estimated barriers for isomerization around the central double bond in MCH^+. Red cells show proton-exchange barriers between MCH^+ and SPH^+ (O and N protonation). All values are electronic energies (ZPE-uncorrected) obtained at DSD-PBEP86-D3(BJ)/def2-QZVP (upper row in each cell) and PW6B95-D3(BJ)/def2-TZVP (lower row) levels of theory.

	TTT	TTC	CTT	CTC	CCT	TCT	TCC	CCC	$SP(S)_1$	$SP(S)_2$	$SP(R)_1$	$SP(R)_2$
TTT	0.0 (0.0)	37.6 (43.5)	30.2 (36.8)			- (179.6)						
TTC	37.3 (41.1)	0.3 (2.4)		27.3 (32.8)			- (188.9)					
CTT	24.7 (30.0)		5.6 (6.8)	34.4 (40.0)	- (176.0)							
CTC		19.6 (24.8)	32.1 (36.4)	8.0 (10.4)				- (187.4)				
CCT			- (160.9)		13.0 (21.9)			20.1 (21.5)				
TCT	- (149.0)					21.3 (30.6)	30.0 (29.4)					
TCC		- (152.3)				20.6 (21.0)	30.7 (39.0)					
CCC				- (173.3)	15.1 (18.9)			18.0 (24.5)	175.4 (189.9)			
$SP(S)_1$								148.1 (149.0)	45.3 (65.4)	16.2 (14.9)		
$SP(S)_2$									26.0 (25.6)	35.5 (54.7)		
$SP(R)_1$											42.4 (63.3)	13.8 (11.9)
$SP(R)_2$											12.8 (11.6)	43.4 (63.6)

Table S2: DFT results for SPH^+ and MCH^+ isomers. Diagonal elements are isomer energies (kJ/-mol) with respect to that of the TTT form of MCH^+. Blue off-diagonal elements are isomerization barriers for rotation around single bonds in MCH^+ or inversion of the five-membered ring in SPH^+. Yellow cells are estimated barriers for isomerization around the central double bond in MCH^+. Red cells show proton-exchange barriers between MCH^+ and SPH^+ (O and N protonation). All values are Gibbs free energies at 298.15K obtained at the DSD-PBEP86-D3(BJ)/def2-QZVP (upper row in each cell) and PW6B95-D3(BJ)/def2-TZVP (lower row) levels of theory.

	TTT	TTC	CTT	CTC	CCT	TCT	TCC	CCC	$SP(S)_1$	$SP(S)_2$	$SP(R)_1$	$SP(R)_2$
TTT	0.0 (0.0)	33.9 (39.8)	24.9 (31.4)			- (170.4)						
TTC	34.2 (38.0)	−0.3 (1.8)		23.3 (28.8)			- (179.5)					
CTT	21.6 (26.9)		3.3 (4.5)	36.0 (41.5)	- (169.1)							
CTC		16.8 (21.9)	32.9 (37.3)	6.2 (8.7)				- (175.9)				
CCT			- (149.3)		15.4 (24.3)			18.2 (19.6)				
TCT	- (140.4)					20.7 (30.0)	30.8 (30.2)					
TCC		- (140.8)				19.3 (19.7)	32.2 (40.5)					
CCC				- (159.1)	14.6 (18.4)			19.0 (25.5)	168.7 (183.1)			
$SP(S)_1$								134.9 (135.8)	52.8 (72.8)	22.6 (21.4)		
$SP(S)_2$									34.3 (33.9)	41.1 (60.3)		
$SP(R)_1$											51.7 (72.5)	14.5 (12.7)
$SP(R)_2$											14.5 (13.2)	51.7 (72.0)

Table S3: Excitation energies ΔE (nm) and oscillator strengths f_{osc}in length form for the first 10 transitions in the *trans* merocyanine isomers calculated at the TDA-B2GP-PLYP/def2-TZVP level of theory.

	TTT		TTC		CTT		CTC	
	ΔE	f_{osc}	ΔE	f_{osc}	ΔE	f_{osc}	ΔE	f_{osc}
1	394.4	1.07438	381.0	1.12257	389.8	1.06666	379.2	1.06913
2	336.6	0.01912	330.3	0.02043	335.1	0.01610	330.6	0.02443
3	302.9	0.00001	303.1	0.00233	303.4	0.00211	303.2	0.00280
4	327.0	0.05044	322.9	0.07372	324.0	0.06236	320.1	0.06101
5	269.2	0.00022	268.9	0.00026	269.0	0.00022	269.0	0.00034
6	284.5	0.06049	277.9	0.08202	285.5	0.05863	280.0	0.08332
7	244.1	0.30891	239.4	0.45599	240.6	0.33421	238.9	0.47702
8	239.4	0.03642	231.6	0.07651	238.2	0.03242	231.2	0.05157
9	232.9	0.10312	234.2	0.01539	231.4	0.07532	234.7	0.01029
10	210.2	0.09465	203.6	0.18292	207.9	0.10579	203.8	0.12781

Table S4: Excitation energies ΔE (nm) and oscillator strengths f_{osc}in length form for the first 10 transitions in the *cis* merocyanine isomers calculated at the TDA-B2GP-PLYP/def2-TZVP level of theory.

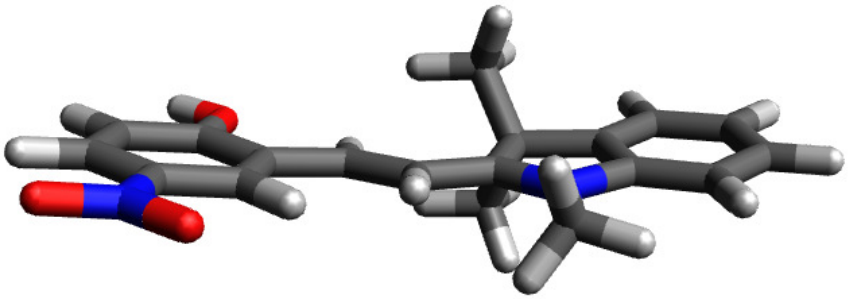
	TCT		TCC		CCT		CCC	
	ΔE	f_{osc}	ΔE	f_{osc}	ΔE	f_{osc}	ΔE	f_{osc}
1	319.4	0.33773	325.5	0.33565	348.5	0.27145	344.6	0.53448
2	303.0	0.00614	304.3	0.00226	303.9	0.00032	303.6	0.00083
3	293.1	0.03013	297.8	0.10669	308.5	0.03437	310.7	0.06654
4	275.6	0.00667	270.6	0.00052	283.5	0.01347	270.4	0.00073
5	273.9	0.00852	277.0	0.02206	284.6	0.01420	296.5	0.02110
6	282.1	0.02659	276.5	0.05015	275.8	0.03432	276.1	0.05651
7	244.9	0.15739	234.2	0.14971	246.9	0.20259	232.5	0.35404
8	249.9	0.21916	251.3	0.10391	255.9	0.01817	245.2	0.02633
9	231.3	0.17144	226.6	0.15037	231.5	0.04973	228.6	0.05479
10	224.7	0.08858	216.2	0.59248	225.7	0.14707	208.4	0.22456

Table S5: Excitation energies ΔE (nm) and oscillator strengths f_{osc}in length form for the first 10 transitions in the spyropyran isomers calculated at the TDA-B2GP-PLYP/def2-TZVP level of theory.

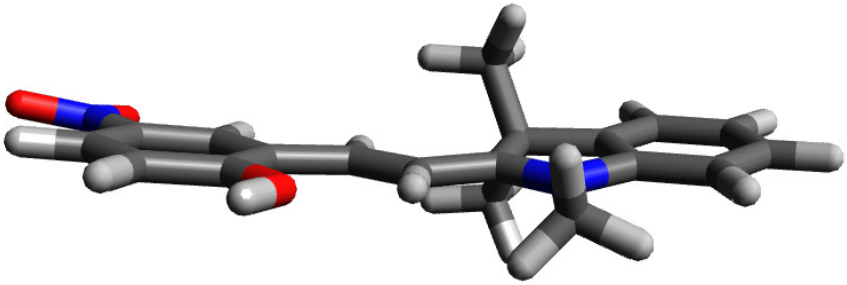
	$SP(S)_1$		$SP(S)_2$		$SP(R)_1$		$SP(R)_2$	
	ΔE	f_{osc}	ΔE	f_{osc}	ΔE	f_{osc}	ΔE	f_{osc}
1	305.0	0.00007	305.8	0.00004	304.8	0.00059	305.3	0.00019
2	271.5	0.00026	271.3	0.00023	271.2	0.00457	272.0	0.00027
3	266.4	0.12639	260.9	0.13489	267.3	0.11049	262.8	0.10712
4	254.9	0.03062	255.2	0.02943	259.7	0.01282	250.6	0.04966
5	230.3	0.02226	230.9	0.00964	230.4	0.01037	230.6	0.02140
6	222.6	1.08876	220.9	1.23163	223.1	1.09227	220.2	1.21177
7	194.7	0.00276	196.8	0.00430	195.4	0.00509	195.9	0.00222
8	215.6	0.35006	211.7	0.34707	211.2	0.36902	212.2	0.35471
9	220.6	0.00209	214.6	0.00420	208.6	0.01023	213.3	0.01073
10	199.9	0.00925	204.6	0.01291	214.4	0.00709	201.4	0.00132

Images of all optimised structures

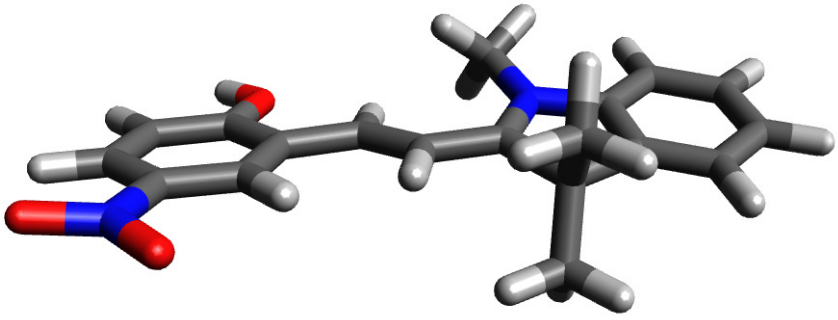
merocyanine TTT



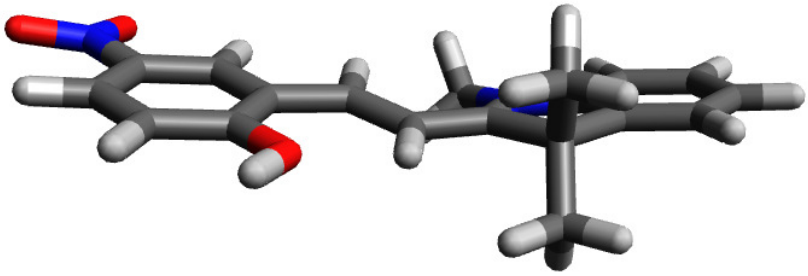
merocyanine TTC



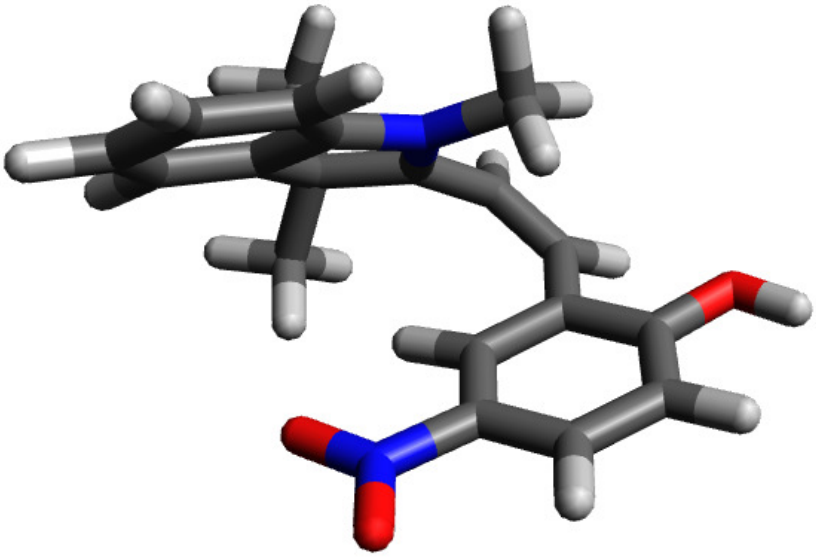
merocyanine CTT



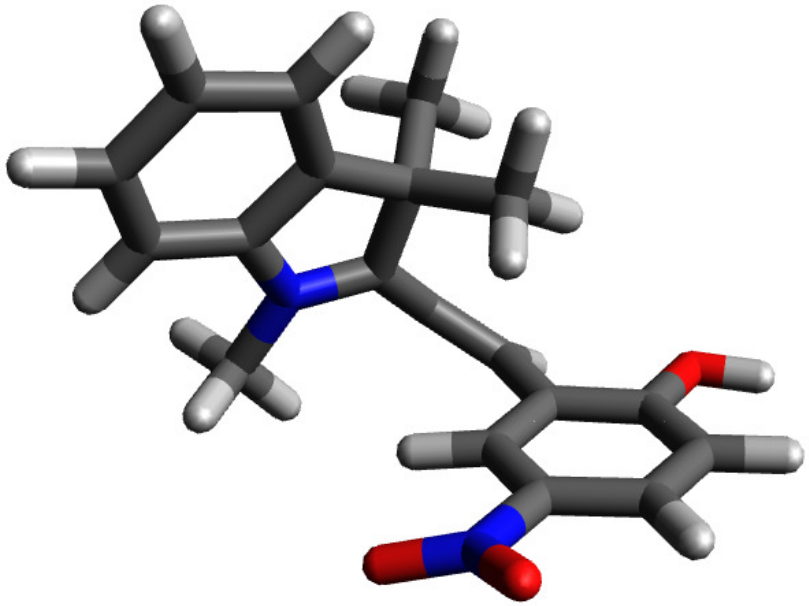
merocyanine CTC



merocyanine CCT



merocyanine TCT



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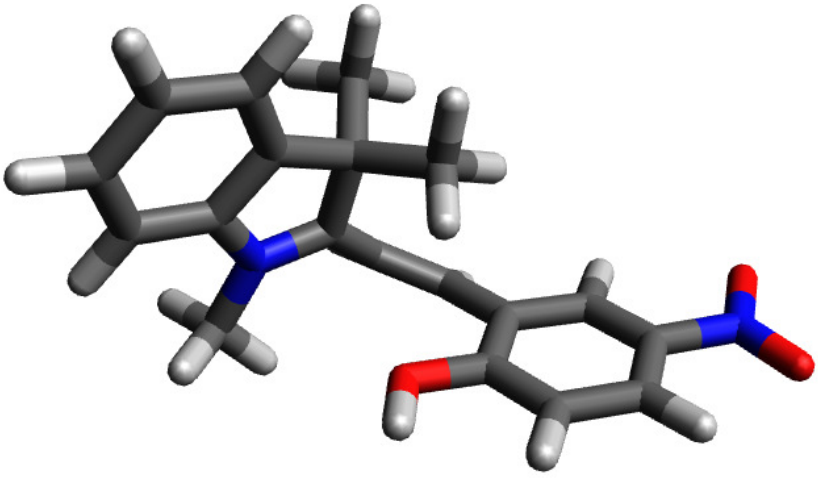
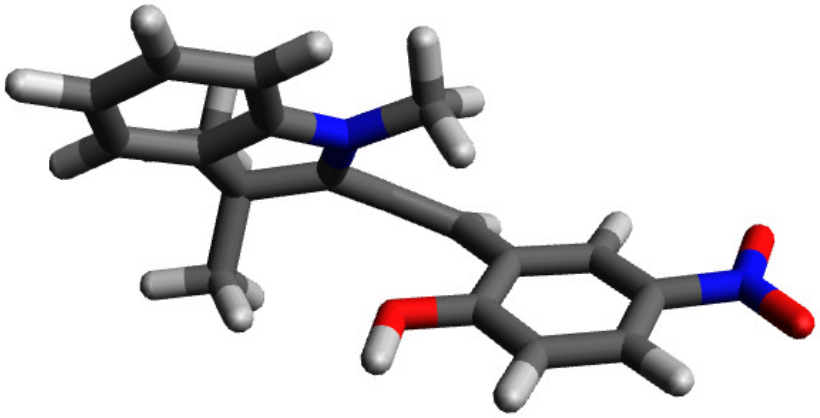
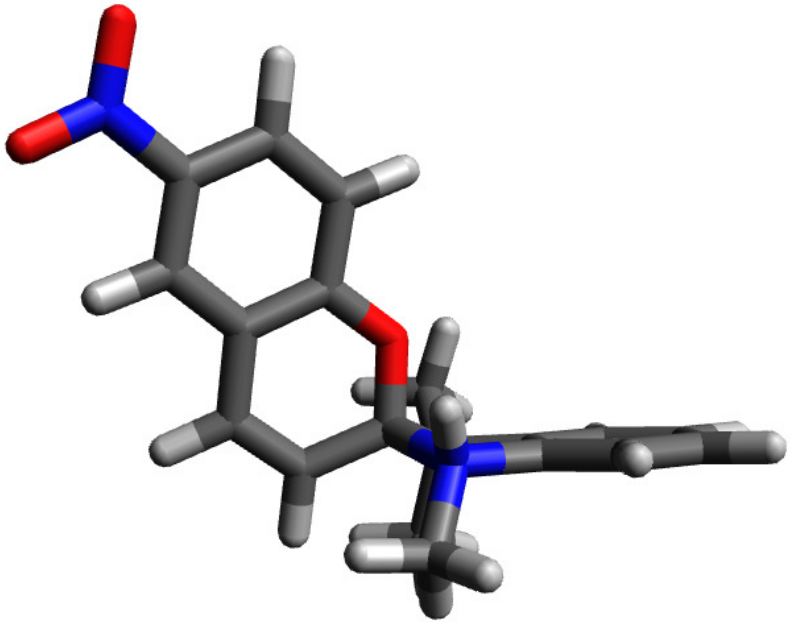


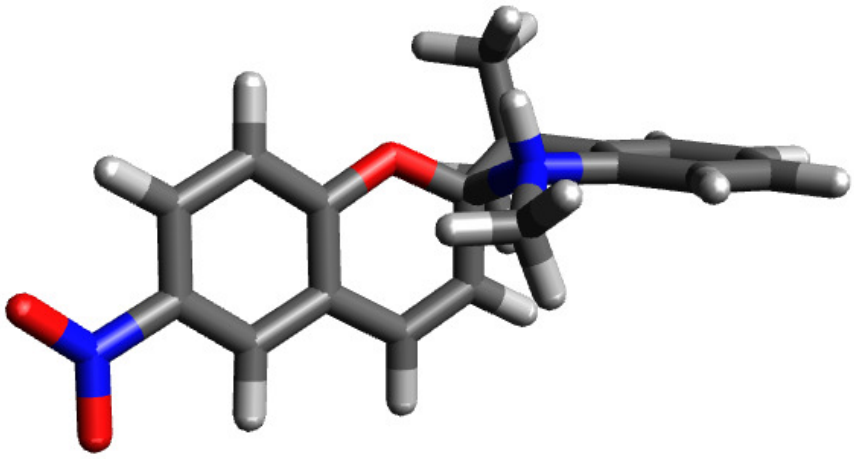
merocyanine CCC



spiropyran SP(S)$_1$



spiropyran SP(S)$_2$



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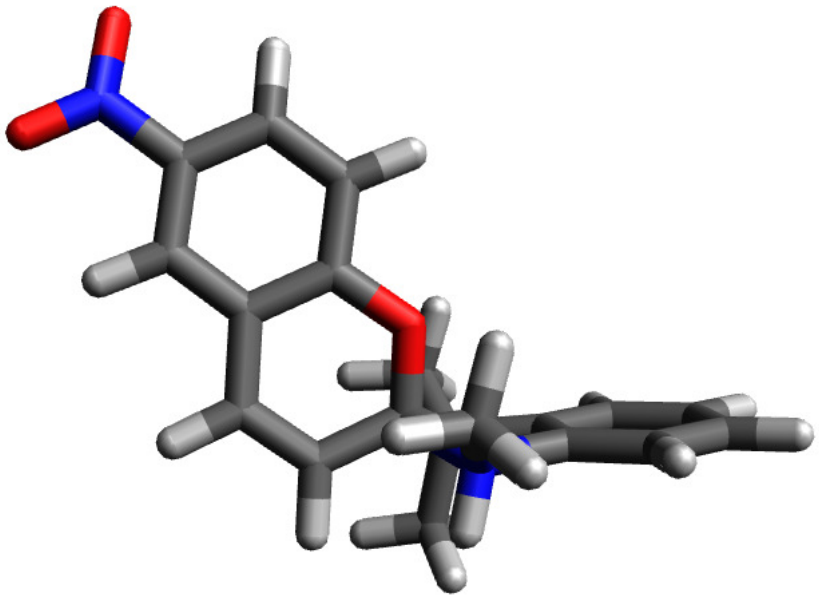
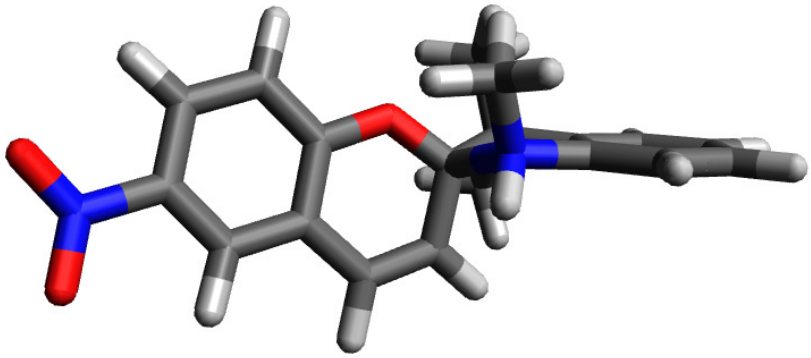
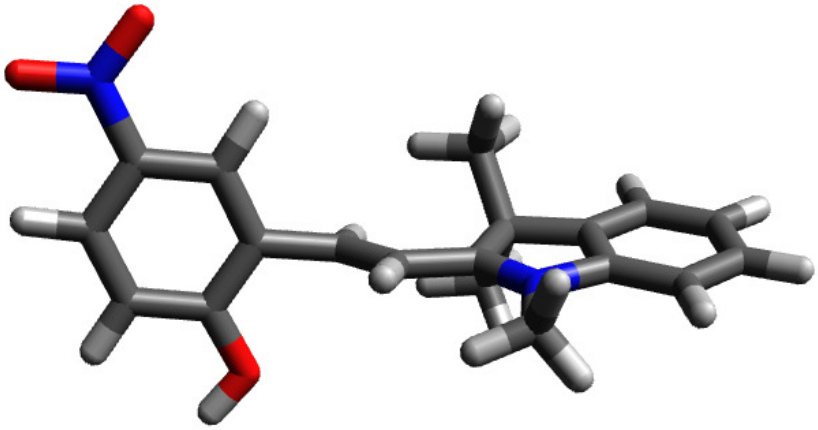


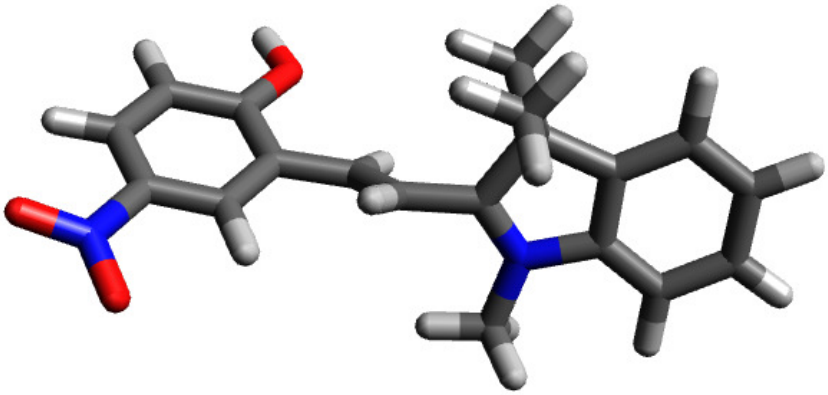
spiropyran $SP(R)_2$



TS for rotation from TTT to TTC



TS for rotation from TTT to CTT



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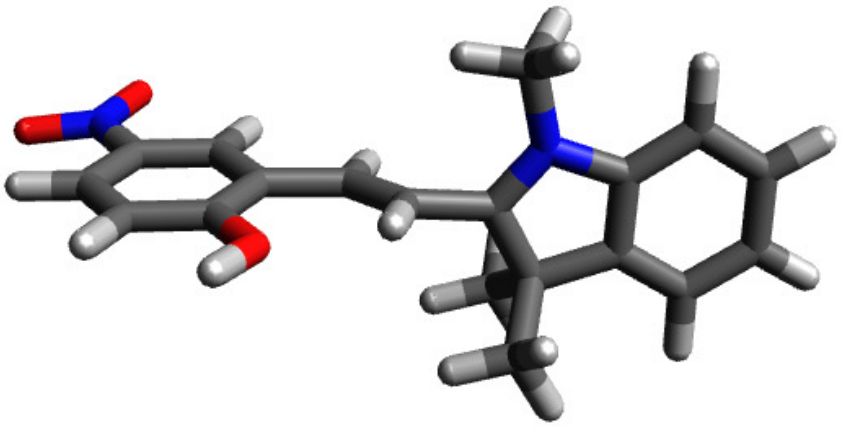

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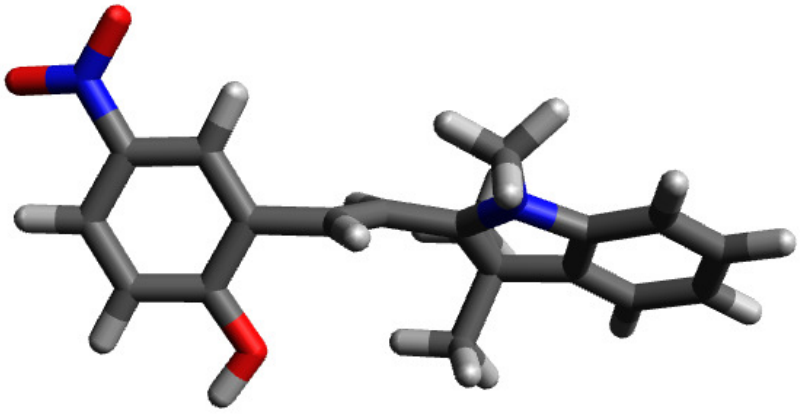
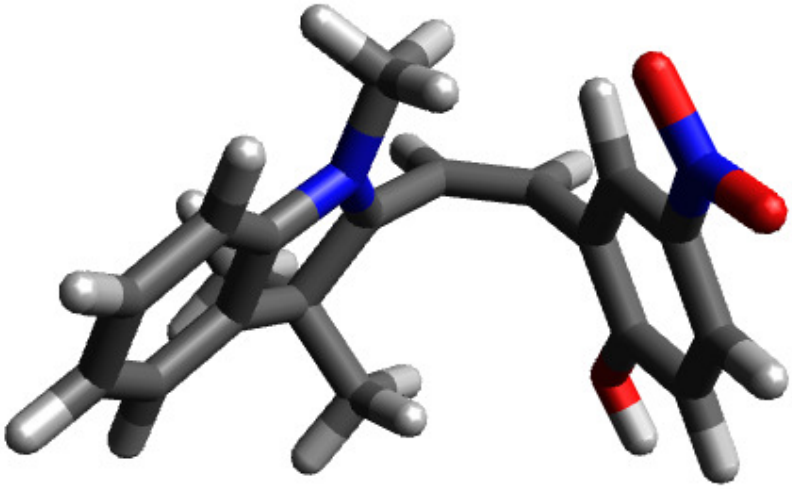


TS for rotation from CCT to CCC



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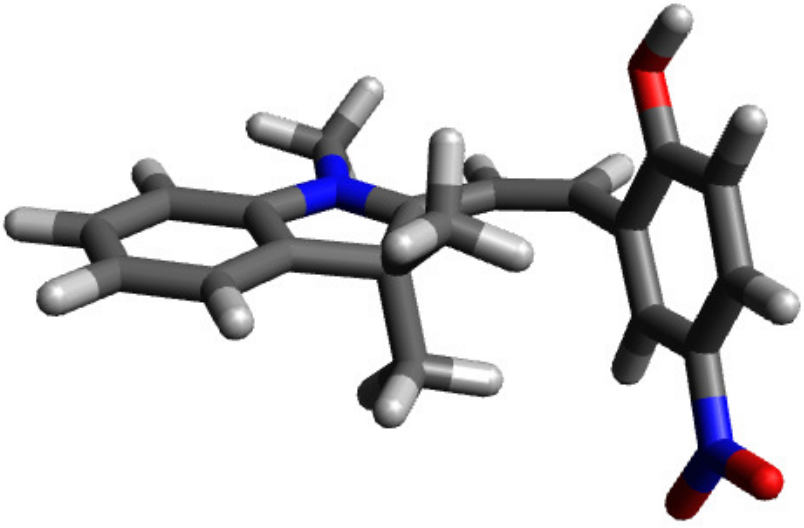

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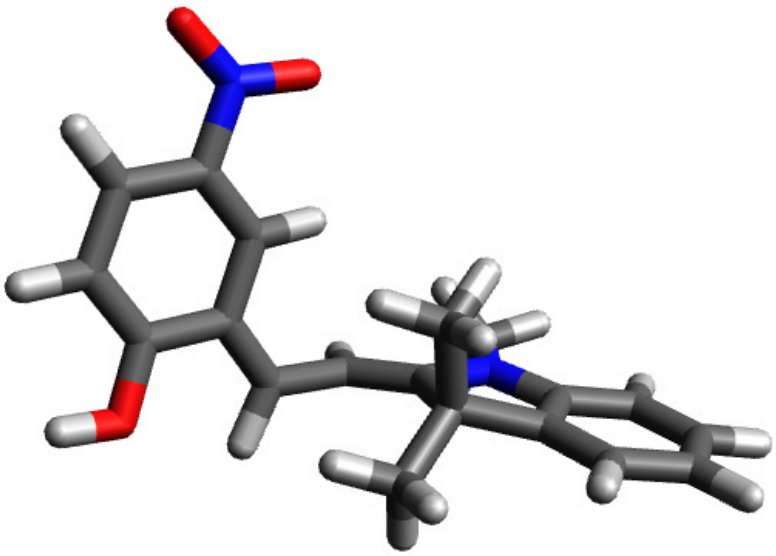

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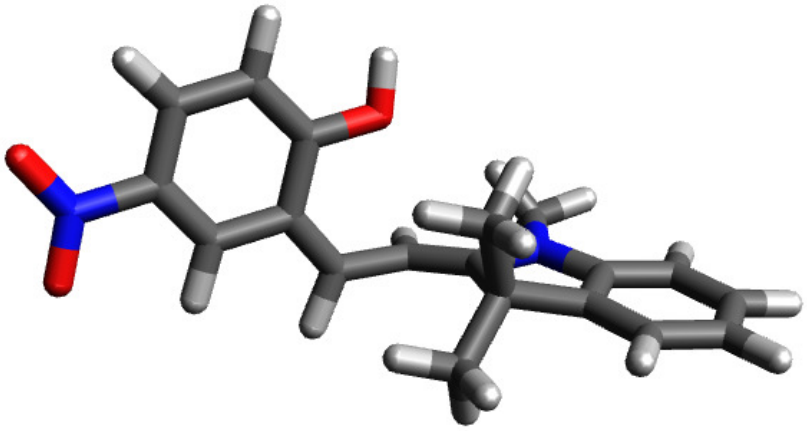

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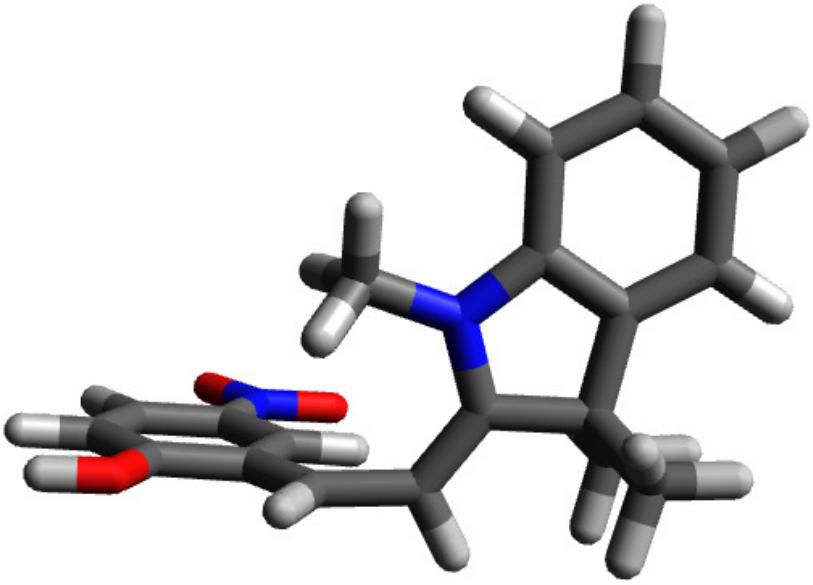
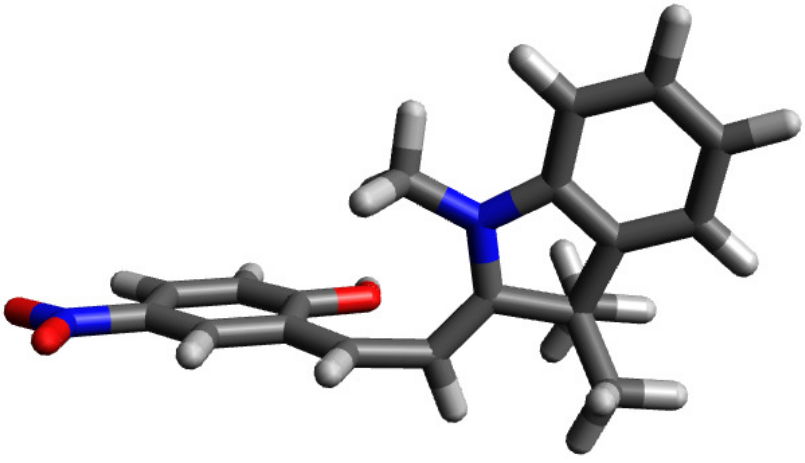
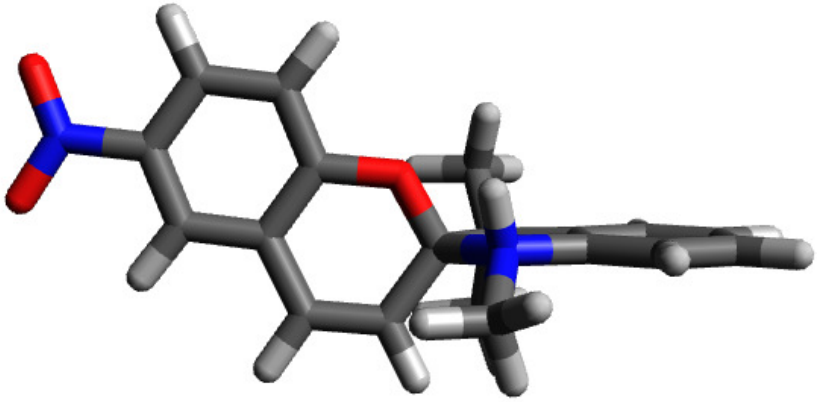


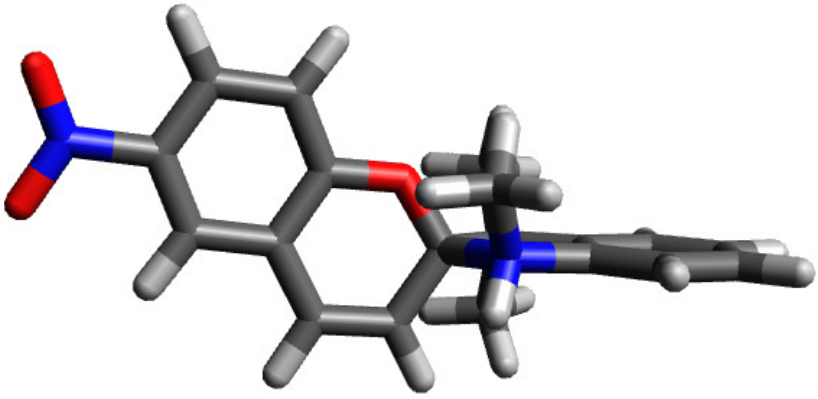
TS for rotation from CTC to CCC



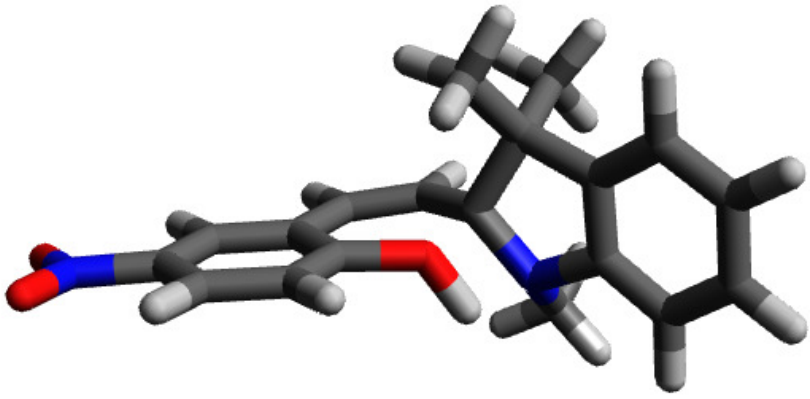
TS for inversion between $SP(S)_1$ and $SP(S)_2$



TS for inversion between $SP(R)_1$ and $SP(R)_2$



TS between SP(S) and merocyanine CCC



Cartesian coordinates of all optimised structures in Å

merocyanine (TTT)

C	-2.763838	-1.065217	0.999564
C	-2.939364	-0.691320	-0.321344
C	-4.051958	-1.131866	-1.003844
C	-4.964232	-1.938140	-0.336011
C	-4.776758	-2.283617	0.993962
C	-3.661916	-1.849960	1.691412
C	-0.926499	0.152909	0.498872
C	0.368758	0.679278	0.706624
C	1.061126	1.422884	-0.186750
C	2.413407	1.875590	-0.025780
C	3.144935	1.674734	1.145637
C	3.055117	2.518059	-1.104990
C	4.444274	2.092393	1.226600
C	4.373258	2.943612	-0.994016
C	5.073232	2.732550	0.169964
N	-1.542892	-0.522237	1.450242
N	5.191957	1.847236	2.463102
O	6.337598	2.227621	2.499849
O	4.609441	1.274463	3.356618
C	-1.788188	0.183650	-0.746472
C	-1.072577	-0.370802	-1.980765
C	-2.283409	1.617099	-1.011866
C	-1.038575	-0.724749	2.797654
O	2.350924	2.677703	-2.233218
H	2.867362	3.141326	-2.897740
H	-4.218282	-0.869959	-2.036819
H	-5.832414	-2.304286	-0.858742
H	-5.501487	-2.904258	1.494280
H	-3.520535	-2.134667	2.720463
H	0.840880	0.407613	1.636922
H	0.596481	1.705431	-1.116220
H	2.716503	1.192968	2.007383
H	4.848508	3.434029	-1.829849
H	6.095886	3.051649	0.279750
H	-0.677883	-1.366988	-1.804940
H	-1.784364	-0.421390	-2.798668
H	-0.257732	0.271370	-2.293049
H	-2.739495	2.048544	-0.125756
H	-3.033566	1.589586	-1.796113
H	-1.472195	2.257594	-1.340881
H	-1.821180	-1.154550	3.404732
H	-0.191266	-1.404094	2.788520
H	-0.741040	0.224211	3.228681

merocyanine (TTC)

C	-2.942701	0.320170	-0.285590
C	-3.010387	1.667387	-0.582580
C	-4.234292	2.264247	-0.780562
C	-5.373320	1.477104	-0.694859
C	-5.284192	0.120262	-0.418202
C	-4.057265	-0.488266	-0.205403
C	-0.788836	1.017305	-0.292772
C	0.620732	0.879798	-0.239210
C	1.486704	1.910377	-0.402904
C	2.921470	1.895523	-0.470401
C	3.563083	3.122966	-0.681668
C	3.733668	0.744121	-0.385836
C	4.924411	3.187808	-0.820341
C	5.112581	0.838646	-0.512279
C	5.715047	2.054758	-0.736517
N	-1.584645	-0.018061	-0.099115
N	5.561392	4.481227	-1.089137
O	6.738218	4.464233	-1.365417
O	4.865265	5.468130	-1.025045
C	-1.623488	2.240862	-0.613910
C	-1.319661	2.784805	-2.016222
C	-1.491649	3.311979	0.477448
C	-1.160109	-1.357309	0.268302
O	3.141574	-0.444183	-0.191600
H	3.803580	-1.140239	-0.148947
H	-4.312781	3.316325	-1.007426
H	-6.340737	1.925438	-0.850732
H	-6.182238	-0.472256	-0.363415
H	-3.997589	-1.541244	0.014086
H	1.007661	-0.111797	-0.096468
H	1.073208	2.900832	-0.519985
H	2.988949	4.032499	-0.754150
H	5.713977	-0.055667	-0.441913
H	6.781850	2.143489	-0.854745
H	-1.446420	2.009562	-2.766167
H	-2.018534	3.584736	-2.240262
H	-0.313986	3.183093	-2.095555
H	-1.750257	2.902878	1.449507
H	-2.182863	4.119664	0.257803
H	-0.492685	3.729955	0.530587
H	-1.998611	-1.874837	0.713349
H	-0.818040	-1.900927	-0.607037
H	-0.364083	-1.306391	1.000290

merocyanine (CTT)

C	-3.035150	1.022841	0.763566
C	-3.164450	-0.341358	0.939284
C	-4.409008	-0.888563	1.152722
C	-5.504814	-0.038509	1.190632
C	-5.353362	1.330284	1.024445
C	-4.104533	1.892127	0.807207
C	-0.928508	0.227995	0.604357
C	0.475810	0.094582	0.464420
C	1.419183	1.063691	0.532619
C	2.837564	0.884097	0.383561
C	3.442546	-0.353081	0.146097
C	3.667547	2.021727	0.459362
C	4.799408	-0.431726	-0.020805
C	5.043569	1.913739	0.301636
C	5.614163	0.688041	0.056112
N	-1.667162	1.317295	0.536333
N	5.413512	-1.732571	-0.309823
O	6.586250	-1.730974	-0.602283
O	4.704944	-2.711080	-0.244236
C	-1.814885	-0.976180	0.819560
C	-1.425362	-1.748068	2.079985
C	-1.744707	-1.873317	-0.426309
C	-1.230111	2.654628	0.194927
O	3.072839	3.204627	0.673317
H	3.725243	3.908350	0.722657
H	-4.537103	-1.951168	1.289630
H	-6.487379	-0.448590	1.356672
H	-6.218627	1.970606	1.066676
H	-3.994755	2.956815	0.685383
H	0.790664	-0.929389	0.331602
H	1.127372	2.076593	0.749488
H	2.868980	-1.261655	0.080548
H	5.662115	2.796252	0.365257
H	6.676068	0.577174	-0.085009
H	-1.496900	-1.118777	2.961712
H	-2.103673	-2.586526	2.205361
H	-0.415567	-2.141890	2.006392
H	-2.012884	-1.322138	-1.322709
H	-2.446948	-2.692468	-0.306752
H	-0.752627	-2.297171	-0.551679
H	-2.068028	3.191417	-0.228876
H	-0.871770	3.180597	1.075027
H	-0.441466	2.599720	-0.546067

merocyanine (CTC)

C	-3.283942	0.285137	0.332531
C	-3.402288	-1.091448	0.297129
C	-4.646938	-1.668818	0.198185
C	-5.754718	-0.835906	0.133775
C	-5.614997	0.544469	0.164683
C	-4.366013	1.137352	0.266282
C	-1.157668	-0.470558	0.385668
C	0.257539	-0.585116	0.376368
C	1.155212	0.385275	0.076953
C	2.587541	0.302885	-0.018676
C	3.271932	1.502241	-0.245252
C	3.354977	-0.877093	0.081582
C	4.636990	1.522948	-0.355699
C	4.738781	-0.829081	-0.025576
C	5.387277	0.365165	-0.243961
N	-1.906485	0.611657	0.424263
N	5.316279	2.796364	-0.614992
O	6.498117	2.747278	-0.862780
O	4.645897	3.802912	-0.568914
C	-2.037422	-1.698892	0.377032
C	-1.845529	-2.447424	1.707009
C	-1.741682	-2.608628	-0.813316
C	-1.468238	1.978649	0.606475
O	2.714330	-2.041918	0.265328
H	3.346294	-2.765608	0.305401
H	-4.766421	-2.740547	0.166147
H	-6.738374	-1.267909	0.049780
H	-6.490597	1.168965	0.101622
H	-4.264572	2.209904	0.272119
H	0.610393	-1.584854	0.557529
H	0.790640	1.373001	-0.157632
H	2.729853	2.429238	-0.339025
H	5.309058	-1.742184	0.060730
H	6.459021	0.416800	-0.337924
H	-2.064025	-1.803650	2.553829
H	-2.529175	-3.290228	1.735271
H	-0.832677	-2.827881	1.801914
H	-1.911122	-2.088894	-1.751509
H	-2.404595	-3.467598	-0.776770
H	-0.717481	-2.970894	-0.788416
H	-2.274496	2.538232	1.061314
H	-0.613814	1.999383	1.271391
H	-1.210863	2.433278	-0.345871

merocyanine (CCT)

C	1.651934	-2.335491	2.498027
C	0.876853	-3.302254	1.882706
C	1.069738	-4.626413	2.203703
C	2.050428	-4.939223	3.138125
C	2.802974	-3.948965	3.753030
C	2.615410	-2.612016	3.441932
C	0.486599	-1.222682	0.936091
C	0.163886	-0.170769	0.003024
C	1.108236	0.510143	-0.662798
C	2.533271	0.196608	-0.634633
C	2.985767	-1.113091	-0.622443
C	3.488734	1.221755	-0.642227
C	4.331503	-1.386868	-0.576433
C	4.848061	0.930540	-0.617161
C	5.277234	-0.377417	-0.578604
N	1.331393	-1.082686	1.920541
N	4.752904	-2.785715	-0.522372
O	5.938718	-3.012033	-0.520586
O	3.876863	-3.624774	-0.468203
C	-0.057989	-2.626131	0.920943
C	-0.129653	-3.260100	-0.462329
C	-1.475237	-2.529490	1.539387
C	1.923641	0.151292	2.393185
O	3.013519	2.472423	-0.634339
H	3.724028	3.117136	-0.693231
H	0.498900	-5.406594	1.725419
H	2.242743	-5.970370	3.386764
H	3.558141	-4.223283	4.470240
H	3.213866	-1.842745	3.900796
H	-0.879804	0.008330	-0.211169
H	0.801554	1.325501	-1.302025
H	2.297323	-1.936866	-0.681095
H	5.567139	1.736155	-0.620744
H	6.324209	-0.628062	-0.556450
H	0.855962	-3.469678	-0.865081
H	-0.666125	-4.201534	-0.399492
H	-0.668773	-2.616090	-1.151430
H	-1.459874	-2.020322	2.498588
H	-1.852829	-3.535308	1.691034
H	-2.149154	-2.003585	0.869415
H	1.800358	0.192364	3.470520
H	2.981301	0.171052	2.143347
H	1.425244	0.991254	1.930028

merocyanine (TCT)

C	-2.966373	0.155181	0.006378
C	-2.337027	0.958507	0.939998
C	-2.634562	0.794413	2.275381
C	-3.568992	-0.172115	2.628024
C	-4.195534	-0.954857	1.668309
C	-3.900016	-0.806880	0.323135
C	-1.568589	1.439468	-1.203430
C	-0.996729	2.098917	-2.371032
C	0.288641	2.088606	-2.730978
C	1.299779	1.218491	-2.153065
C	0.999431	-0.089522	-1.810262
C	2.607801	1.680953	-1.945749
C	1.947219	-0.877069	-1.200763
C	3.553852	0.866485	-1.339720
C	3.220432	-0.409708	-0.941534
N	-2.469250	0.504210	-1.274683
N	1.590802	-2.240659	-0.827627
O	2.324974	-2.811110	-0.057290
O	0.578764	-2.702616	-1.312885
C	-1.410965	1.900837	0.225115
C	-1.932446	3.352963	0.274053
C	0.024283	1.880800	0.744199
C	-2.921255	-0.147482	-2.489676
O	2.865395	2.941720	-2.322923
H	3.790999	3.161454	-2.188876
H	-2.158477	1.396457	3.033374
H	-3.819039	-0.320695	3.666234
H	-4.918189	-1.693231	1.972831
H	-4.380106	-1.417416	-0.423458
H	-1.701466	2.685318	-2.947244
H	0.599294	2.745167	-3.530179
H	0.040183	-0.518433	-2.043682
H	4.550802	1.240591	-1.163869
H	3.933974	-1.051029	-0.452922
H	-2.960002	3.428472	-0.070144
H	-1.884437	3.699583	1.301413
H	-1.305003	3.993477	-0.338147
H	0.438336	0.879133	0.749487
H	0.030032	2.269318	1.758730
H	0.652906	2.525329	0.139249
H	-2.888708	-1.222017	-2.343694
H	-3.940663	0.156759	-2.706892
H	-2.267076	0.132230	-3.305186

merocyanine (TCC)

C	2.510462	1.558069	0.868959
C	2.249791	1.869073	-0.452114
C	3.285456	1.893556	-1.359062
C	4.565920	1.612646	-0.901579
C	4.804712	1.314840	0.432198
C	3.769592	1.280396	1.353403
C	0.290655	1.906339	0.794765
C	-1.038275	2.209242	1.291513
C	-2.212678	1.661485	0.970156
C	-2.526384	0.465375	0.201124
C	-3.705796	0.450091	-0.537906
C	-1.756855	-0.704323	0.236520
C	-4.068415	-0.673527	-1.240454
C	-2.162400	-1.841798	-0.444589
C	-3.320193	-1.832400	-1.191471
N	1.281970	1.601182	1.576388
N	-5.289575	-0.648621	-2.052306
O	-5.634623	-1.691994	-2.555382
O	-5.853717	0.415151	-2.170954
C	0.788016	2.164651	-0.602472
C	0.562320	3.662597	-0.883193
C	0.109395	1.313239	-1.673829
C	1.181595	1.296200	2.989332
O	-0.615837	-0.699112	0.966568
H	-0.248444	-1.586681	0.993663
H	3.115682	2.136541	-2.396387
H	5.391783	1.631365	-1.593587
H	5.809294	1.107449	0.761835
H	3.956595	1.050644	2.389553
H	-1.054430	3.044772	1.981027
H	-3.082375	2.162726	1.372505
H	-4.341221	1.319724	-0.578497
H	-1.566040	-2.740077	-0.384206
H	-3.651636	-2.701138	-1.734109
H	1.059178	4.281723	-0.141447
H	0.974823	3.903520	-1.857962
H	-0.499333	3.892006	-0.883508
H	0.233530	0.254263	-1.476267
H	0.569221	1.539364	-2.631052
H	-0.948081	1.544373	-1.744187
H	1.822939	0.449514	3.205349
H	1.509903	2.147614	3.577217
H	0.155476	1.043944	3.223446

merocyanine (CCC)

C	-2.579711	-0.782556	0.786434
C	-3.672707	-0.565415	-0.032270
C	-4.835500	-1.266889	0.198329
C	-4.863082	-2.166265	1.256955
C	-3.750118	-2.371287	2.059224
C	-2.572373	-1.677244	1.834804
C	-1.890165	0.788271	-0.666559
C	-1.096032	1.779671	-1.321547
C	0.213470	1.786764	-1.632342
C	1.224923	0.747790	-1.613435
C	2.554138	1.139164	-1.452540
C	0.970626	-0.612576	-1.843875
C	3.559458	0.206463	-1.467158
C	2.008657	-1.531648	-1.910294
C	3.309567	-1.130010	-1.713169
N	-1.533656	0.074876	0.367884
N	4.935135	0.640629	-1.206845
O	5.800187	-0.198279	-1.283924
O	5.098354	1.802408	-0.914653
C	-3.321395	0.493583	-1.037112
C	-3.404541	0.007383	-2.488041
C	-4.190773	1.747470	-0.864646
C	-0.274940	0.126121	1.075784
O	-0.307994	-0.999765	-2.017022
H	-0.337205	-1.913735	-2.313505
H	-5.711403	-1.116588	-0.412831
H	-5.768770	-2.711047	1.467506
H	-3.800957	-3.078378	2.870152
H	-1.703585	-1.844181	2.449591
H	-1.662188	2.651922	-1.617311
H	0.583017	2.727982	-2.016832
H	2.807916	2.174706	-1.294760
H	1.785600	-2.567542	-2.119001
H	4.128945	-1.827645	-1.746122
H	-2.803953	-0.879374	-2.647012
H	-4.438174	-0.225589	-2.726725
H	-3.059567	0.784494	-3.164241
H	-4.135870	2.141671	0.145506
H	-5.222013	1.482383	-1.076586
H	-3.896878	2.522687	-1.566165
H	-0.473494	0.012288	2.134624
H	0.372838	-0.679035	0.742078
H	0.207215	1.076324	0.892653

spiropyran $SP(S)_1$

C	-2.413705	-0.391638	0.765235
C	-2.891976	-0.683699	-0.490209
C	-3.924666	-1.596339	-0.601568
C	-4.442027	-2.176894	0.545695
C	-3.937475	-1.859859	1.798301
C	-2.900211	-0.951406	1.923886
H	-4.321497	-1.863804	-1.568259
H	-5.245400	-2.890557	0.464422
H	-4.348092	-2.325640	2.678787
H	-2.489389	-0.705794	2.891097
C	-2.188350	0.094768	-1.570198
H	-0.514375	0.215617	1.203025
C	-0.875178	0.528628	-0.860249
C	-0.260898	1.814769	-1.241539
C	1.064729	1.953148	-1.275611
H	-0.916639	2.633875	-1.478887
C	1.343545	-0.411907	-0.855206
C	1.935811	0.837893	-1.013503
H	1.507153	2.900407	-1.543428
C	2.089340	-1.566725	-0.723062
C	3.322958	0.924343	-0.981583
C	3.465211	-1.472275	-0.710859
H	1.590317	-2.517390	-0.638051
C	4.057117	-0.226992	-0.820762
H	3.829237	1.869384	-1.089803
H	4.090527	-2.343005	-0.613356
C	-1.671273	1.908601	1.249344
H	-2.490355	2.318648	0.675386
H	-0.805446	2.555169	1.186699
H	-1.983850	1.791404	2.280273
O	-0.013077	-0.553902	-0.881932
N	-1.323665	0.574814	0.702192
C	-1.871564	-0.747971	-2.800862
H	-1.256476	-0.185763	-3.498531
H	-1.360037	-1.666158	-2.542627
H	-2.798603	-0.999395	-3.307827
C	-3.041757	1.284453	-2.011822
H	-2.554558	1.837483	-2.810025
H	-3.984291	0.907494	-2.396944
H	-3.276214	1.970434	-1.204154
N	5.522888	-0.132231	-0.766515
O	6.001581	0.975749	-0.830707
O	6.139626	-1.165738	-0.656261

spiropyran $SP(S)_2$

C	-2.514470	-0.254625	0.648823
C	-3.204562	-0.426811	-0.533003
C	-4.332089	-1.222850	-0.533542
C	-4.728689	-1.821110	0.653213
C	-4.014863	-1.628833	1.825361
C	-2.877106	-0.834530	1.840177
H	-4.894702	-1.382334	-1.439300
H	-5.608617	-2.442884	0.666270
H	-4.346755	-2.098202	2.736773
H	-2.318755	-0.682718	2.749539
C	-2.533370	0.297982	-1.669079
H	-0.569803	0.056973	0.113690
C	-1.782475	1.418881	-0.902071
C	-2.631755	2.565404	-0.507325
C	-2.154149	3.807503	-0.526683
H	-3.645004	2.345160	-0.214408
C	-0.044968	2.999154	-1.402074
C	-0.791732	4.070111	-0.920568
H	-2.781071	4.641156	-0.249240
C	1.264455	3.143976	-1.811695
C	-0.189517	5.320050	-0.844142
C	1.859733	4.384532	-1.711550
H	1.802476	2.294553	-2.198388
C	1.125015	5.450569	-1.228574
H	-0.728415	6.181434	-0.484529
H	2.882269	4.545247	-2.006983
C	-0.930814	1.461152	1.552182
H	-1.790060	1.992772	1.938767
H	-0.185262	2.162023	1.195306
H	-0.500503	0.831928	2.321585
O	-0.600339	1.753318	-1.524415
N	-1.364775	0.617267	0.421917
C	-1.541414	-0.645264	-2.353362
H	-0.977192	-0.123154	-3.118804
H	-0.837445	-1.097364	-1.656299
H	-2.096014	-1.454642	-2.817561
C	-3.493721	0.860060	-2.701782
H	-2.955448	1.453361	-3.435745
H	-3.978311	0.041943	-3.227960
H	-4.266143	1.477198	-2.255045
N	1.782060	6.760701	-1.114733
O	1.113230	7.684176	-0.715030
O	2.948416	6.817029	-1.426687

spiropyran SP(R)$_1$

C	-2.363879	0.048697	1.915181
C	-2.586722	1.205060	1.203593
C	-3.880082	1.520616	0.841124
C	-4.905797	0.667154	1.216939
C	-4.648883	-0.489600	1.936944
C	-3.352967	-0.823132	2.300829
H	-4.093515	2.415843	0.279341
H	-5.919413	0.908954	0.940833
H	-5.461130	-1.137912	2.220174
H	-3.147439	-1.723637	2.855686
C	-1.314006	1.984484	1.014483
C	-0.241659	0.869655	1.178153
C	1.084612	1.260103	1.707643
C	2.196300	1.066897	1.002635
H	1.108484	1.736339	2.675012
C	0.904273	0.060678	-0.781744
C	2.141555	0.495339	-0.318053
H	3.152719	1.374746	1.396808
C	0.735526	-0.431738	-2.059297
C	3.243861	0.390647	-1.153913
C	1.830934	-0.495308	-2.897010
H	-0.239984	-0.747623	-2.390115
C	3.067273	-0.096940	-2.427339
H	4.225453	0.696803	-0.831437
H	1.741905	-0.852025	-3.908931
O	-0.201653	0.104521	0.017407
N	-0.933250	-0.074697	2.221576
C	-1.177518	2.646904	-0.345771
H	-0.180539	3.063056	-0.473448
H	-1.371260	1.947657	-1.150605
H	-1.885209	3.466359	-0.426971
C	-1.211995	3.027135	2.128049
H	-0.282104	3.584987	2.062240
H	-2.034694	3.728445	2.034087
H	-1.288694	2.583551	3.120771
N	4.232278	-0.188308	-3.315472
O	5.312732	0.066045	-2.834489
O	4.026030	-0.512749	-4.461041
C	-0.382331	-1.447240	2.267833
H	-0.625498	-1.945064	1.340315
H	-0.825795	-1.970707	3.105063
H	0.692077	-1.383075	2.399774
H	-0.755996	0.364082	3.124142

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C	-2.235360	0.249785	2.208569
C	-2.870102	1.195132	1.437719
C	-4.166652	0.944988	1.021958
C	-4.775890	-0.242646	1.389320
C	-4.112137	-1.172841	2.176720
C	-2.815709	-0.936946	2.598211
H	-4.696400	1.662299	0.415229
H	-5.781149	-0.450654	1.060381
H	-4.606033	-2.086466	2.463561
H	-2.289341	-1.656798	3.205365
C	-1.996843	2.374483	1.118258
C	-0.848596	2.245020	2.159073
C	-1.064704	2.925503	3.459148
C	-0.029787	3.415530	4.139525
H	-2.071207	2.969654	3.839484
C	1.441392	2.939701	2.277377
C	1.301656	3.376935	3.589683
H	-0.177838	3.883064	5.100699
C	2.652215	2.964208	1.616024
C	2.436587	3.804880	4.266832
C	3.772605	3.393492	2.296196
H	2.706448	2.649284	0.587076
C	3.645509	3.792821	3.613965
H	2.385542	4.153496	5.285281
H	4.740849	3.427379	1.827040
O	0.355829	2.516911	1.564206
N	-0.875127	0.654925	2.537179
C	-1.465894	2.274492	-0.314320
H	-0.814477	3.111458	-0.541030
H	-0.916302	1.356962	-0.499594
H	-2.309760	2.302993	-0.996979
C	-2.721658	3.708696	1.261316
H	-2.025732	4.534124	1.137873
H	-3.471498	3.791798	0.479872
H	-3.227979	3.815740	2.214086
N	4.850540	4.217963	4.339133
O	4.702724	4.609612	5.473594
O	5.900820	4.134585	3.747965
C	0.174555	-0.172626	1.897733
H	0.076413	-0.094242	0.824321
H	0.029561	-1.199982	2.211034
H	1.148199	0.177538	2.217114
H	-0.734736	0.623851	3.544093

TS for rotation from TTT to TTC

C	-0.055157	0.150366	0.081610
C	1.433629	0.023227	-0.060421
C	1.994997	1.282717	-0.097009
N	0.943905	2.229951	-0.046137
C	-0.230472	1.650986	0.016827
C	2.244086	-1.088239	-0.102329
C	3.615587	-0.895708	-0.181858
C	4.160840	0.380506	-0.211657
C	3.354337	1.507174	-0.168579
C	-1.463360	2.376867	-0.041977
C	-2.658438	1.806646	0.145346
C	-3.960554	2.468170	-0.036486
C	-4.612692	2.392238	-1.254488
C	-5.892953	2.890258	-1.371165
C	-6.543633	3.472196	-0.303512
C	-5.891617	3.566503	0.906275
C	-4.608273	3.060328	1.049975
O	-3.931586	3.096229	2.214866
N	-6.592896	2.765500	-2.651271
O	-5.979409	2.285384	-3.578795
C	1.228605	3.652069	-0.062127
C	-0.795930	-0.572842	-1.046198
C	-0.442192	-0.359875	1.483873
O	-7.740071	3.144423	-2.692660
H	-4.471622	3.486846	2.906577
H	1.830925	-2.084057	-0.077204
H	4.270676	-1.750354	-0.224146
H	5.230078	0.498777	-0.273873
H	3.780989	2.496206	-0.198522
H	-1.424651	3.421987	-0.306693
H	-2.706863	0.771000	0.445857
H	-4.150456	1.931740	-2.111633
H	-6.384006	4.020601	1.753028
H	-7.545878	3.842710	-0.433753
H	-0.546690	-0.142687	-2.011857
H	-0.496355	-1.616012	-1.057099
H	-1.871643	-0.533284	-0.920405
H	0.124180	0.162733	2.248745
H	-0.195477	-1.415482	1.546350
H	-1.498371	-0.236886	1.692649
H	1.517021	3.958958	-1.062810
H	0.368240	4.213023	0.270759
H	2.051146	3.841644	0.618064

TS for rotation from TTT to CTT

N	-0.000706	-0.013220	-0.125690
C	1.295972	0.024367	-0.079333
C	2.128340	1.211718	-0.124307
C	2.487563	1.822358	-1.254440
C	3.436946	2.923353	-1.299634
C	3.538567	3.836742	-0.264037
C	4.484561	4.831587	-0.322268
C	5.350482	4.958935	-1.391794
C	5.247716	4.068778	-2.437407
C	4.298547	3.055134	-2.396496
H	2.601290	1.476085	0.813284
H	2.111810	1.460912	-2.201996
H	6.079315	5.751276	-1.395693
C	-0.886301	-4.024499	0.148007
C	-1.969406	-3.158956	0.073609
C	-1.786267	-1.788371	-0.018628
C	-0.480811	-1.349556	-0.029666
C	0.613053	-2.188970	0.065172
C	0.417245	-3.549289	0.149595
C	1.862011	-1.361352	0.040751
O	4.176596	2.135016	-3.368988
N	4.557928	5.783085	0.781415
O	3.632143	5.789519	1.563446
C	-0.902215	1.119747	-0.222223
C	2.689674	-1.480470	1.325281
C	2.717836	-1.638738	-1.202911
O	5.536317	6.490174	0.835841
H	4.792066	2.310710	-4.084959
H	1.249263	-4.232160	0.217094
H	-1.064378	-5.085669	0.211682
H	-2.970069	-3.558503	0.085698
H	-2.626163	-1.115997	-0.080251
H	2.874697	3.798287	0.583358
H	5.906625	4.155944	-3.287884
H	2.098686	-1.225976	2.200419
H	3.037344	-2.503172	1.433818
H	3.557712	-0.829674	1.278542
H	2.143347	-1.488348	-2.113032
H	3.056619	-2.669864	-1.180228
H	3.584127	-0.985652	-1.222543
H	-1.505822	1.017772	-1.117846
H	-1.551833	1.122519	0.646986
H	-0.324591	2.032435	-0.264645

TS for rotation from TTC to CTC

N	-0.094893	-0.005099	-0.163099
C	1.192388	0.064355	-0.017838
C	1.973363	1.292491	-0.042540
C	2.372079	1.921422	1.066510
C	3.231694	3.081021	1.209319
C	3.938849	3.697019	0.162271
C	4.800407	4.754966	0.413838
C	4.965463	5.235887	1.692227
C	4.253329	4.647447	2.718904
C	3.405391	3.590824	2.494026
C	-0.536642	-1.356679	-0.229980
C	0.574470	-2.171838	-0.119637
C	1.787371	-1.311384	0.067280
C	0.418479	-3.539516	-0.165630
C	-0.863388	-4.046792	-0.327089
C	-1.964273	-3.206938	-0.426184
C	-1.821720	-1.828551	-0.378557
O	3.766796	3.227528	-1.088110
N	4.405521	5.170461	4.078042
O	3.689763	4.707614	4.937143
C	-1.007290	1.118851	-0.260385
C	2.409726	-1.507534	1.458987
C	2.835951	-1.473894	-1.035422
O	5.235270	6.033421	4.244970
H	4.327601	3.710483	-1.701404
H	1.263611	-4.203858	-0.078658
H	-1.009204	-5.113800	-0.375229
H	-2.946561	-3.633257	-0.546235
H	-2.674510	-1.175206	-0.462607
H	2.277077	1.623036	-1.024404
H	2.023600	1.528463	2.013744
H	2.878473	3.158232	3.329060
H	5.342342	5.202975	-0.405967
H	5.627405	6.056585	1.907379
H	1.674206	-1.354597	2.243959
H	2.781213	-2.524584	1.538243
H	3.240893	-0.825582	1.607184
H	2.406323	-1.283966	-2.014987
H	3.219417	-2.489499	-1.020219
H	3.663138	-0.789898	-0.871318
H	-1.416711	1.164500	-1.264933
H	-1.815966	0.973192	0.446797
H	-0.470159	2.028401	-0.029425

TS for rotation from CTT to CTC

N	-0.098699	0.028464	-0.055415
C	1.190781	0.115855	0.109891
C	2.001863	1.298427	0.179212
C	1.918362	2.354931	-0.626646
C	2.933712	3.423383	-0.619287
C	4.050908	3.310499	-1.452262
C	5.003600	4.317811	-1.493833
C	4.878138	5.419808	-0.677554
C	3.794119	5.497877	0.173162
C	2.814614	4.527760	0.202785
C	-0.511819	-1.332674	-0.112511
C	0.612767	-2.128058	0.008047
C	1.814206	-1.248357	0.163127
C	0.485828	-3.498530	-0.022210
C	-0.786219	-4.034550	-0.164540
C	-1.903369	-3.216870	-0.265505
C	-1.787972	-1.835206	-0.244012
O	4.161617	2.176932	-2.177571
N	3.689213	6.631058	1.089944
O	2.660691	6.743571	1.718983
C	-1.047461	1.121767	-0.146119
C	2.538985	-1.470808	1.494442
C	2.772354	-1.360822	-1.032528
O	4.644033	7.366827	1.163075
H	4.926362	2.224838	-2.756565
H	1.346328	-4.142591	0.067182
H	-0.911759	-5.104655	-0.193586
H	-2.878851	-3.663488	-0.365713
H	-2.656720	-1.204481	-0.332297
H	2.857578	1.214603	0.832014
H	1.135042	2.413283	-1.371472
H	1.979929	4.645799	0.873053
H	5.850851	4.227512	-2.156492
H	5.609473	6.209537	-0.681669
H	1.867063	-1.330719	2.335684
H	2.918994	-2.486814	1.528147
H	3.382398	-0.794673	1.596541
H	2.253059	-1.148846	-1.962735
H	3.170495	-2.369133	-1.080696
H	3.596113	-0.660883	-0.929955
H	-1.927111	0.859588	0.430037
H	-0.600336	2.021437	0.254629
H	-1.333954	1.280672	-1.181418

TS for rotation from CCT to CCC

C	0.120005	0.295143	-0.212525
C	1.599070	0.397879	0.006903
C	1.901297	1.682680	0.413047
N	0.685090	2.412939	0.507999
C	-0.327387	1.690819	0.137414
C	2.612835	-0.524131	-0.126662
C	3.911140	-0.114485	0.145918
C	4.191759	1.189682	0.528516
C	3.179701	2.124941	0.670956
C	-1.719863	2.112254	0.081555
C	-2.230796	2.928342	-0.836844
C	-1.452511	3.615880	-1.882461
C	-0.701870	4.739209	-1.609834
C	0.056128	5.325687	-2.601758
C	0.036862	4.858081	-3.898895
C	-0.757669	3.769895	-4.196091
C	-1.492931	3.143984	-3.198535
O	-2.261466	2.063693	-3.419995
N	0.915546	6.447786	-2.238430
O	0.985182	6.730961	-1.056752
C	0.661639	3.749122	1.075115
C	-0.230172	-0.035518	-1.667504
C	-0.540008	-0.706929	0.744429
O	1.516333	7.007245	-3.121653
H	-2.292992	1.849028	-4.356153
H	2.412328	-1.537002	-0.438942
H	4.719915	-0.820507	0.052347
H	5.210293	1.483609	0.721190
H	3.395106	3.137862	0.968749
H	-2.386477	1.583153	0.749473
H	-3.305552	3.051258	-0.855459
H	-0.716800	5.194249	-0.638100
H	-0.799846	3.390756	-5.206132
H	0.633305	5.344241	-4.652405
H	0.219328	0.678961	-2.351213
H	0.154714	-1.022685	-1.904957
H	-1.305221	-0.033372	-1.815430
H	-0.334077	-0.461835	1.782289
H	-0.138395	-1.695021	0.543352
H	-1.614340	-0.738239	0.587412
H	1.188149	3.720451	2.023360
H	1.161012	4.445498	0.409693
H	-0.363862	4.052585	1.230756

TS for rotation from TCC to TCT

C	-0.044684	-0.398018	-0.045665
C	1.220293	0.148620	-0.127354
C	1.456770	1.595464	-0.096400
C	1.518743	2.456253	0.931561
C	1.468490	2.279836	2.358086
C	1.066817	1.115360	3.239744
C	-0.459616	0.924161	3.138194
N	1.793450	3.304882	3.119561
C	1.715941	2.993505	4.495564
C	1.347723	1.669128	4.606780
C	1.219977	1.097391	5.852402
C	1.450218	1.891128	6.965385
C	1.790182	3.230315	6.833233
C	1.932114	3.811945	5.585418
C	-0.187996	-1.770692	-0.041069
C	0.892675	-2.620241	-0.161770
C	2.152029	-2.077917	-0.309976
C	2.316443	-0.701131	-0.301729
O	3.515318	-0.101147	-0.408036
N	-1.527384	-2.330740	0.140317
O	-2.439642	-1.545405	0.275544
C	2.218525	4.620898	2.662328
C	1.799006	-0.206629	2.994725
O	-1.628041	-3.534526	0.161064
H	4.207777	-0.745711	-0.576483
H	0.936374	0.063008	5.968743
H	1.357736	1.462525	7.949849
H	1.953697	3.827159	7.714987
H	2.201060	4.850901	5.498116
H	1.716327	3.474132	0.636709
H	1.658228	2.041813	-1.062997
H	-0.922817	0.221429	0.014716
H	3.012062	-2.721023	-0.421564
H	0.733856	-3.684922	-0.145446
H	2.849819	-0.055354	2.768132
H	1.732366	-0.796404	3.903679
H	1.339508	-0.778826	2.199969
H	-0.989173	1.838308	3.388926
H	-0.751657	0.159932	3.851667
H	-0.749406	0.596576	2.148430
H	1.382945	5.156386	2.223816
H	2.594508	5.172079	3.511004
H	3.016716	4.525135	1.936364

TS for rotation from TTT to TCT

C	0.015311	0.059150	0.104532
C	1.504223	0.016017	-0.093971
C	2.007422	1.315149	-0.053725
N	0.950980	2.202086	0.074543
C	-0.247563	1.549603	0.023238
C	2.361900	-1.048413	-0.223984
C	3.725486	-0.797293	-0.304102
C	4.214379	0.503313	-0.258775
C	3.363755	1.585991	-0.138559
C	-1.429654	2.189617	-0.136064
C	-2.729473	1.559044	-0.246063
C	-3.563933	1.268593	0.821659
C	-3.237091	1.636049	2.147536
C	-4.132944	1.432724	3.147760
C	-5.392851	0.885810	2.910385
C	-5.731136	0.486076	1.636370
C	-4.828639	0.640077	0.597699
O	-5.072765	0.232769	-0.641886
N	-3.775316	1.838392	4.512329
O	-2.639155	2.211228	4.695579
C	1.077422	3.632254	0.161081
C	-0.755610	-0.751440	-0.923372
C	-0.297042	-0.399975	1.541302
O	-4.642592	1.768350	5.348576
H	-5.955114	-0.142121	-0.725360
H	1.991264	-2.060753	-0.261371
H	4.414511	-1.619498	-0.405189
H	5.276637	0.671702	-0.326635
H	3.751055	2.590989	-0.118762
H	-2.291996	2.104347	2.361371
H	-6.694821	0.038748	1.446988
H	-6.081136	0.782920	3.732428
H	-0.576509	-0.383715	-1.929491
H	-0.452829	-1.793872	-0.882232
H	-1.824275	-0.716215	-0.721380
H	0.260549	0.190977	2.262129
H	-0.010077	-1.440822	1.661420
H	-1.357062	-0.300683	1.755854
H	2.081589	3.888931	0.471202
H	0.866158	4.097483	-0.800494
H	0.384736	4.015913	0.901985
H	-3.081887	1.273939	-1.229982
H	-1.426841	3.271449	-0.205579

TS for rotation from TTC to TCC

C	0.096228	-0.060127	0.092235
C	1.588469	0.006758	-0.077650
C	2.003446	1.335230	-0.005174
N	0.890268	2.142492	0.144947
C	-0.261755	1.414058	0.087668
C	2.519097	-0.992851	-0.219417
C	3.862210	-0.644881	-0.284648
C	4.261054	0.685822	-0.214970
C	3.337482	1.703344	-0.078107
C	-1.477487	1.995594	-0.043540
C	-2.759079	1.326587	-0.099546
C	-3.607710	0.997071	0.952877
C	-4.888197	0.471632	0.646169
C	-5.815652	0.310633	1.626789
C	-5.553072	0.636200	2.954261
C	-4.309062	1.117167	3.292215
C	-3.333482	1.284463	2.323804
O	-2.115176	1.737902	2.624823
N	-7.147954	-0.192511	1.271965
O	-7.335341	-0.482632	0.114908
C	0.922821	3.573856	0.288334
C	-0.591594	-0.840506	-1.019721
C	-0.215951	-0.665856	1.472300
O	-7.955244	-0.273283	2.166088
H	-2.066462	1.971104	3.557521
H	2.219717	-2.027601	-0.278351
H	4.607577	-1.415071	-0.394722
H	5.308992	0.929414	-0.275038
H	3.653344	2.732538	-0.036506
H	-5.147751	0.230375	-0.371654
H	-4.086096	1.364939	4.319137
H	-6.326337	0.499793	3.691228
H	-0.416581	-0.383893	-1.989210
H	-0.213647	-1.858289	-1.049208
H	-1.663868	-0.893904	-0.843763
H	0.232358	-0.073415	2.263839
H	0.195167	-1.669964	1.521588
H	-1.286718	-0.724141	1.639286
H	1.912187	3.884505	0.595914
H	0.667498	4.060358	-0.651553
H	0.214183	3.879678	1.050039
H	-3.127537	1.061705	-1.084761
H	-1.520698	3.078201	-0.090812

TS for rotation from CCT to CTT

C	-0.048505	-0.134272	0.129045
C	1.443445	-0.016508	0.011096
C	1.791533	1.326275	-0.117140
N	0.635928	2.093133	-0.145341
C	-0.478515	1.305492	-0.089731
C	2.424153	-0.977316	0.042323
C	3.749225	-0.576649	-0.077530
C	4.081982	0.767415	-0.206303
C	3.107954	1.747092	-0.224368
C	-1.763539	1.715279	-0.196139
C	-2.257676	3.073253	-0.373293
C	-2.466808	3.664734	-1.613564
C	-2.311419	2.942096	-2.820157
C	-2.489970	3.569000	-4.016874
C	-2.843278	4.912587	-4.098882
C	-3.005439	5.643473	-2.942305
C	-2.818836	5.047737	-1.707082
O	-2.923301	5.716675	-0.560693
N	-2.304791	2.811725	-5.262458
O	-1.977791	1.651189	-5.162926
C	0.638116	3.521467	-0.287966
C	-0.650123	-1.079107	-0.905930
C	-0.416488	-0.573271	1.554869
O	-2.481319	3.411384	-6.296072
H	-3.209778	6.623442	-0.704730
H	2.176739	-2.022366	0.144721
H	4.532258	-1.316981	-0.077874
H	5.116968	1.051593	-0.302871
H	3.375115	2.784411	-0.338377
H	-2.066863	1.893382	-2.796350
H	-3.275786	6.687056	-2.996936
H	-2.987967	5.358373	-5.068432
H	-0.412782	-0.760862	-1.916791
H	-0.251970	-2.079247	-0.762387
H	-1.730376	-1.135681	-0.799695
H	0.018988	0.094564	2.292213
H	-0.034765	-1.574205	1.735573
H	-1.495235	-0.583659	1.686721
H	1.581687	3.914937	0.068987
H	0.484807	3.821186	-1.323164
H	-0.163452	3.943015	0.312158
H	-2.460137	3.672365	0.505344
H	-2.510076	0.931265	-0.122080

TS for rotation from CTC to CCC

C	0.046422	0.055195	-0.116362
C	1.541850	-0.029923	-0.013750
C	2.071063	1.259357	0.025800
N	1.024151	2.170826	0.047914
C	-0.177140	1.531822	0.142278
C	2.379801	-1.117365	0.012255
C	3.750181	-0.897935	0.072127
C	4.266210	0.393123	0.098356
C	3.436710	1.498531	0.072392
C	-1.372062	2.076329	0.478351
C	-1.708621	3.415529	0.919256
C	-2.066748	4.537942	0.174609
C	-2.358629	5.737473	0.867825
C	-2.792314	6.837845	0.194872
C	-2.973330	6.829059	-1.185355
C	-2.695373	5.677931	-1.890536
C	-2.228569	4.547274	-1.241108
O	-1.919800	3.423252	-1.897587
N	-3.086590	8.061976	0.954938
O	-2.853046	8.041052	2.141161
C	1.169570	3.598784	-0.017727
C	-0.374802	-0.222455	-1.573179
C	-0.683022	-0.861000	0.852606
O	-3.537716	8.997944	0.339592
H	-2.166319	3.491115	-2.825439
H	1.989040	-2.122166	-0.010490
H	4.424797	-1.737699	0.103596
H	5.333272	0.534488	0.152482
H	3.847158	2.493916	0.111291
H	-2.254883	5.780458	1.939542
H	-2.832039	5.657800	-2.961546
H	-3.328847	7.717807	-1.679104
H	0.163573	0.427338	-2.257664
H	-0.148532	-1.252986	-1.831662
H	-1.440885	-0.050977	-1.695833
H	-0.432678	-0.624842	1.882330
H	-0.406846	-1.894124	0.662402
H	-1.759472	-0.783133	0.726574
H	2.189821	3.850217	-0.274718
H	0.506608	3.998280	-0.778260
H	0.914129	4.050473	0.940022
H	-1.636653	3.583543	1.988592
H	-2.207645	1.384644	0.445982

TS for inversion between $SP(S)_1$ and $SP(S)_2$

N	0.132303	-0.248294	-0.249278
C	1.550135	-0.040615	0.029111
C	1.860780	1.294801	0.060407
C	0.704372	2.187518	-0.273071
C	-0.500014	1.196308	-0.500052
C	3.166740	1.664910	0.332039
C	4.115897	0.682163	0.545170
C	3.772795	-0.662157	0.496571
C	2.469320	-1.045996	0.239759
O	-1.419716	1.260862	0.550065
C	-2.735043	1.590688	0.382135
C	-3.268116	1.764698	-0.889115
C	-2.393995	1.567095	-2.013662
C	-1.109192	1.273419	-1.844453
C	-4.604119	2.113893	-1.009405
C	-5.358140	2.271111	0.129191
C	-4.830888	2.083688	1.393655
C	-3.499512	1.739143	1.522580
C	0.392603	3.153274	0.864353
C	1.033284	2.987405	-1.534725
N	-6.768328	2.653452	-0.016148
O	-7.408308	2.807645	0.996907
C	-0.142598	-1.281138	-1.274744
O	-7.182178	2.786197	-1.145331
H	3.445429	2.706985	0.364227
H	5.136334	0.963014	0.749050
H	4.525499	-1.414972	0.661255
H	2.199016	-2.089113	0.209034
H	-0.341124	-0.528431	0.608908
H	-0.451799	1.155958	-2.687676
H	-2.799156	1.677793	-3.007498
H	-3.052033	1.594471	2.491660
H	-5.057968	2.268084	-1.974070
H	-5.462291	2.219867	2.255039
H	0.443899	-1.060763	-2.156689
H	-1.199533	-1.279804	-1.511408
H	0.147647	-2.242463	-0.868800
H	-0.488952	3.747868	0.642389
H	0.235862	2.635777	1.803739
H	1.230892	3.832639	0.983161
H	0.181348	3.572265	-1.868306
H	1.842095	3.674925	-1.307687
H	1.366854	2.351809	-2.349458

TS for inversion between $SP(R)_1$ and $SP(R)_2$

N	0.074796	-0.043595	-0.182807
C	1.509254	0.033629	0.063281
C	1.961817	1.326406	0.006355
C	0.908004	2.330753	-0.351349
C	-0.408329	1.491506	-0.522406
C	3.301950	1.573692	0.248413
C	4.145327	0.514822	0.527638
C	3.662669	-0.786231	0.564986
C	2.324998	-1.045343	0.333858
O	-1.307966	1.844635	0.452726
C	-2.661899	1.806196	0.275295
C	-3.209277	1.676444	-0.995798
C	-2.293615	1.515049	-2.094472
C	-0.981094	1.432666	-1.886415
C	-4.590153	1.734302	-1.132917
C	-5.363215	1.890006	-0.006305
C	-4.816378	1.983317	1.259746
C	-3.444371	1.952888	1.402567
C	0.753468	3.365671	0.760016
C	1.293961	3.039199	-1.651185
N	-6.821860	1.986687	-0.154321
O	-7.473894	2.084619	0.858365
C	-0.686458	-0.680760	0.918305
O	-7.258188	1.970062	-1.280688
H	3.685541	2.581773	0.215694
H	5.189534	0.699255	0.721357
H	4.331582	-1.602999	0.779622
H	1.947587	-2.054980	0.365748
H	-0.292546	1.316253	-2.705523
H	-2.688651	1.469732	-3.097475
H	-2.980081	2.056603	2.368935
H	-5.061315	1.666627	-2.099555
H	-5.471072	2.093911	2.107081
H	-0.035636	4.074318	0.530042
H	0.534825	2.901684	1.715323
H	1.685039	3.915266	0.850992
H	0.485825	3.667673	-2.013517
H	2.151695	3.676193	-1.460009
H	1.577805	2.338983	-2.430885
H	-0.574367	-0.077999	1.808213
H	-0.278703	-1.670009	1.089442
H	-1.729121	-0.751667	0.630564
H	-0.112701	-0.568144	-1.033965

TS between SP(S) and merocyanine CCC

H	-1.450140	4.728830	-1.343208
H	-5.408705	4.473206	-2.868215
H	-1.719685	2.484302	-0.236966
H	-6.808699	2.405801	-2.365000
H	-6.967005	0.148857	-1.522675
H	-2.466197	-0.300283	-1.850284
H	-3.744187	-0.211533	-3.075975
H	-2.920768	-1.729264	-2.764059
H	-5.029151	-2.993703	-2.194854
H	-5.880254	-1.557481	-2.756406
H	-6.249114	-2.259038	-1.172514
H	-6.574105	-0.520654	2.351670
H	-7.153399	-1.075039	0.784216
H	-7.093803	0.663840	1.146786
H	-4.514144	-1.341657	3.260662
H	-2.940681	-3.240906	3.459302
H	-1.946811	-4.248632	1.459477
H	-2.480608	-3.379575	-0.784522
H	-4.337645	0.942508	0.747361
C	-4.379128	-1.345265	1.114704
C	-3.813863	-1.881987	-0.022965
C	-3.718625	2.288245	-0.950654
C	-2.631116	-3.423399	1.352978
C	-3.199807	-2.857829	2.485353
C	-4.087588	-1.799307	2.381840
C	-2.929654	-2.936387	0.090152
C	-6.601070	-0.289679	1.293883
C	-5.454181	-2.044915	-1.883535
C	-4.985955	0.054133	-0.630544
C	-4.348533	-1.193577	-1.254093
C	-3.303662	-0.827649	-2.295082
C	-6.078219	0.734530	-1.354541
C	-5.981074	1.975608	-1.823183
C	-4.782687	2.777948	-1.690073
C	-2.515297	2.931730	-0.809479
C	-2.365762	4.167867	-1.416625
C	-3.428093	4.688379	-2.126021
C	-4.622154	4.020104	-2.287784
N	-5.221750	-0.219764	0.803566
N	-3.283588	6.023184	-2.734496
O	-3.893238	1.071123	-0.278313
O	-4.250866	6.474767	-3.300845
O	-2.212382	6.564291	-2.609412