

Scope of negative solvatochromism and solvatofluorochromism of merocyanines

Andrii V. Kulinich,* Elena K. Mikitenko and Alexander A. Ishchenko

Institute of organic chemistry, National Academy of Sciences of Ukraine, Murmans'ka str. 5, 02660, Kyiv, Ukraine

SUPPORTING INFORMATION

Additional experimental details

Dye 1 1,3-Dibutyl-5-[2-(1,3-dibutyl-1,3-dihydro-2H-benzimidazol-2-ylidene)ethylidene]-2-thioxodihydropyrimidine-4,6(1H,5H)-dione

Yellow microcrystalline powder.

Yield 42%. M.p. = 161-163 °C.

Calcd for C₂₉H₄₂N₄O₂S (510.73): C, 68.20; H, 8.29; N, 10.97. Found: C, 68.11; H, 8.23; N, 10.90.

Dye 2 1,3-Dibutyl-5-[(E)-4-(1,3-dibutyl-1,3-dihydro-2H-benzimidazol-2-ylidene)but-2-enylidene]-2-thioxodihydropyrimidine-4,6(1H,5H)-dione

Garnet-coloured needles.

Yield 36%. M.p. = 212-214 °C.

Calcd for C₃₁H₄₄N₄O₂S (536.77): C, 69.37; H, 8.26; N, 10.44. Found: C, 69.30; H, 8.24; N, 10.38.

Dye 3 1,3-Dibutyl-5-[(2E,4E)-6-(1,3-dibutyl-1,3-dihydro-2H-benzimidazol-2-ylidene)hexa-2,4-dienylidene]-2-thioxodihydropyrimidine-4,6(1H,5H)-dione

Pure **3** was obtained only after third chromatography.

Indigo-coloured thin needles (filaments).

Yield 14%. M.p. = 224-226 °C (decomp.).

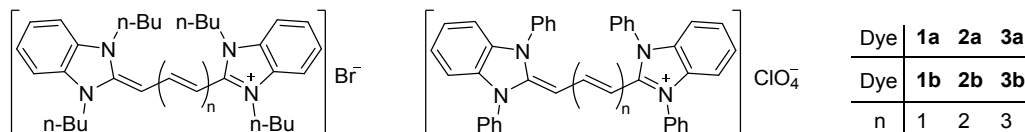
Calcd for C₃₃H₄₆N₄O₂S (562.81): C, 70.42; H, 8.24; N, 9.95. Found: C, 70.32; H, 8.18; N, 9.83.

Table S1 ¹H NMR characteristics of dyes **1–3** (top down in lines are given: chemical shifts (ppm), integral intensity, multiplicity, SSCC in Hz, attribution of a signal).

1 CDCl ₃													
0.97	1.01	1.35-1.57	1.77	1.97	4.35	4.54	7.46	7.68	8.18				
6H	6H	8H	4H	4H	4H	4H	4H	1H	1H				
t	t	m	quint	quint	t	t	s	d	d				
7.3	7.3	-	7.4	7.5	7.4	7.7		15.6	15.6				
CH ₃	CH ₃	CH ₃ CH ₂	NCH ₂ CH ₂		NCH ₂	NCH ₂	Ar-H	H ₂ or H ₁	H ₁ or H ₂				
2 (CD ₃) ₂ SO													
0.87-0.97		1.22-1.46	1.60	1.80	4.37	4.49	6.49	7.43	7.48-7.59	7.69	7.87-7.95		
12H		8H	4H	4H	4H	4H	1H	1H	3H	1H	2H		
m		m	quint	quint	t	t	d	d	m	dd	m		
-		-	7.5	7.5	7.3	7.4	15	14.5		14.5; 11.2	-		
CH ₃		CH ₃ CH ₂	NCH ₂ CH ₂		NCH ₂	NCH ₂	H1	H4	H2+AA'	H3	BB'		
3 CDCl ₃													
0.98	1.07	1.40-1.61	1.82	2.04	4.26	4.56	5.94	6.28	6.87	7.18	7.20	7.33-7.41	7.41-7.53
6H	6H	8H	4H	4H	4H	4H	1H	1H	1H	1H	1H	2H	2H
t	t	m	quint	quint	t	t	d	dd	dd	dd	d	m	m
7.3	7.3	-	7.4	7.6	7.7	7.7	15.2	13.7; 11.2	13.6; 11.8	15.2; 11.2	14.6	-	11.8; 14.6
CH ₃	CH ₃	CH ₃ CH ₂	NCH ₂ CH ₂		NCH ₂		H ₁	H ₃	H ₄	H ₂	H ₆	AA'	BB'+H ₅
3 (CD ₃) ₂ SO													
0.85-0.98		1.20-1.46	1.58	1.80	4.35	4.49	6.43	6.62	7.04	7.16	7.36-7.54	7.54-7.63	7.90-8.00
12H		8H	4H	4H	4H	4H	1H	1H	1H	1H	2H	2H	2H
m		m	quint	quint	t	t	dd	d	dd	d	m	m	m
-		-	7.5	7.6	7.3	7.4	14.3; 10.5	14.8	14.3; 11.3	14.7	-	-	-
CH ₃		CH ₃ CH ₂	NCH ₂ CH ₂		NCH ₂		H ₃	H ₁	H ₄	H ₆	H ₂ +H ₅	AA'	BB'

About evaluation of deviations of merocyanines **2** and **3**

Spectral data of cationic symmetrical dyes **1a–3a** with a 1,3-dibutylbenzimidazole terminus (or any other 1,3-dialkylbenzimidazole) have not been found in the literature, so we tried to synthesize them. But only carbocyanine **1a** ($n = 1$) was obtained in a pure state. However, the values of deviations of merocyanine **1** cannot be used to evaluate its electronic asymmetry because of strong steric hindrances in the correspondent anionic monomethine dye. Dicarbo-cyanine **2a** ($n = 2$) was synthesized but could not be cleared out from some minor impurities. Still its absorption maxima in DCM and ethanol could be registered. Dye **3a** ($n = 3$) was found even more elusive and was not obtained at all.



Therefore, we compared the absorption maxima of dyes **1a** and **2a** with the corresponding parameters of the analogous dyes **1b** and **2b** and, knowing the difference, estimated the positions of maxima of dye **3a** from the relative data of dye **3b**.

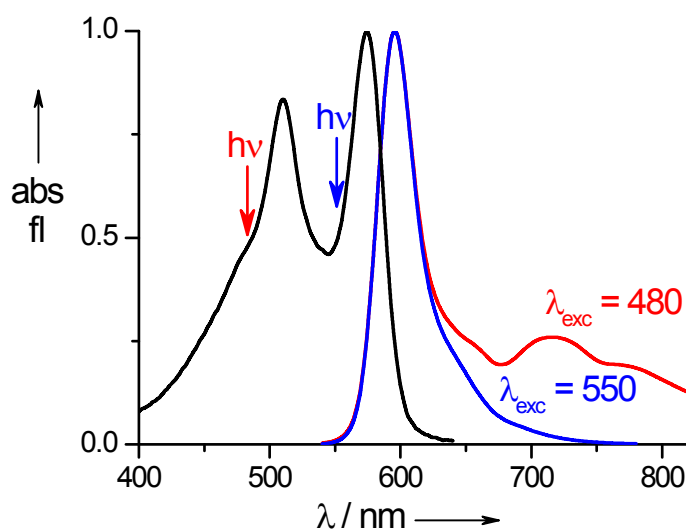


Figure S1. Normalized absorption and fluorescence spectra of dye **2** in n-hexane. The maximum at 510 nm corresponds to a short-wavelength aggregate (dimer or H-aggregate). This suggestion was sustained by registering the correspondent broad and of very low intensity fluorescence band with its maximum at 714 nm, when excited at 480 nm. The "normal" fluorescence band (not "spoiled" with the long-wavelength H-aggregate shoulder) can be registered under excitation at 530-560 nm.

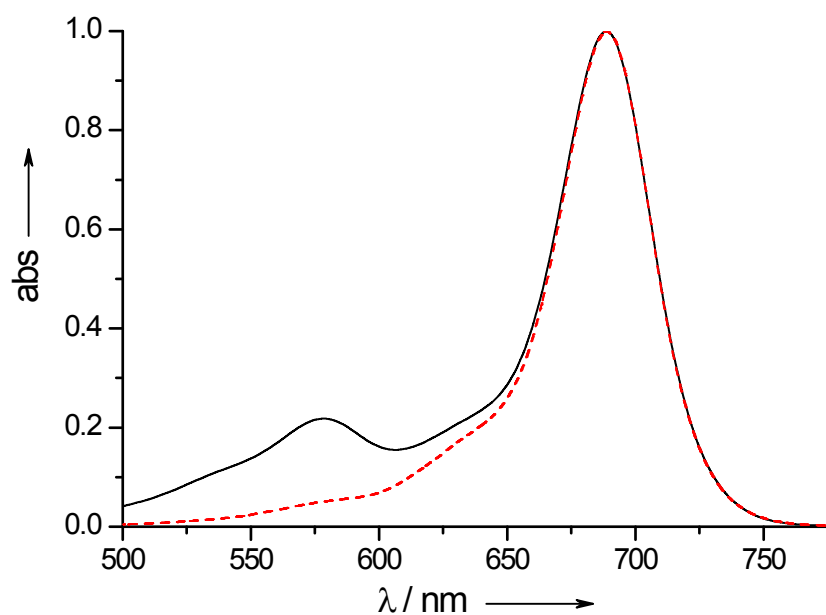


Figure S2 Normalized Vis absorption spectra of dye **3** in toluene before (solid) and after (dash) 15-fold dilution of the initial 1.19×10^{-5} M solution. The absorption maximum of the aggregate, defined more precisely from the difference spectrum, is 577 nm.

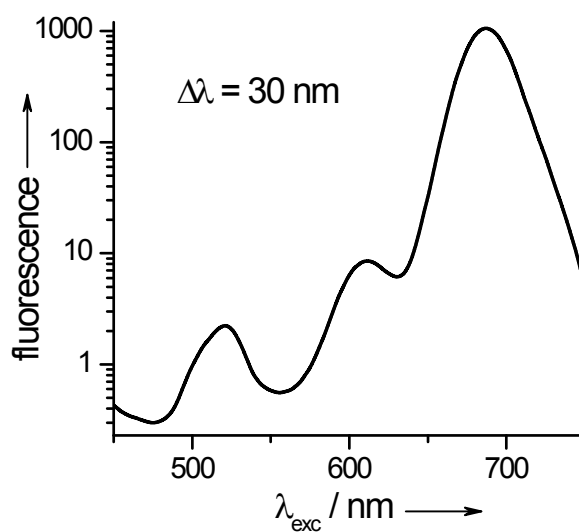


Figure S3 Synchronous fluorescence spectrum of a sample of dye **3** in toluene after the first chromatography. The short-wavelength bands correspond to impurities (i.e. vinyllogues **1** and **2**).

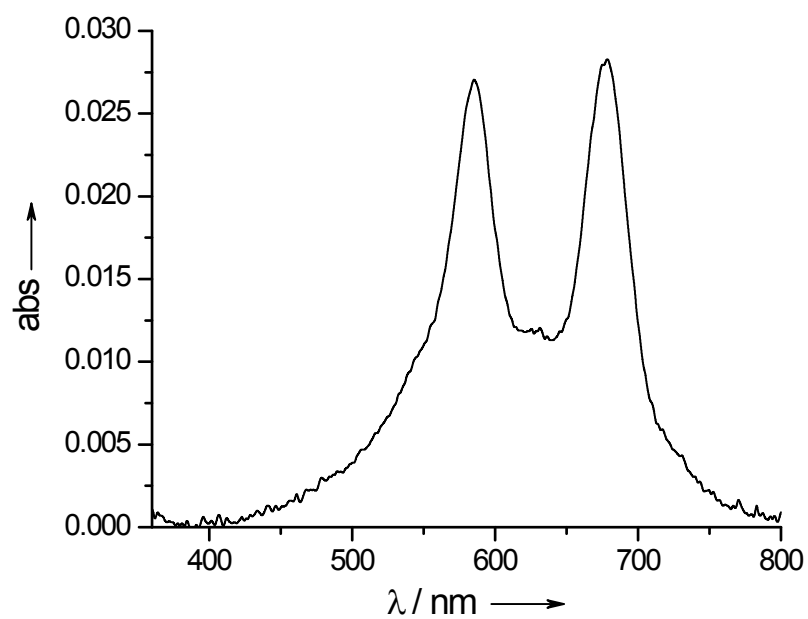


Figure S4 Vis absorption spectrum of dye **3** (with a didodecylbenzimidazole terminus) in n-hexane.

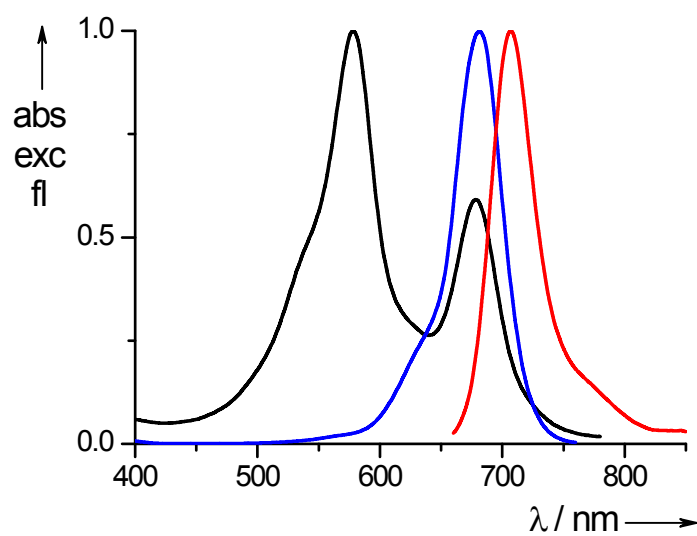


Figure S5 Normalized Vis absorption (black), fluorescence (red), and excitation (blue) spectra of dye **3** in an n-hexane–acetone (98 : 2) mixture.

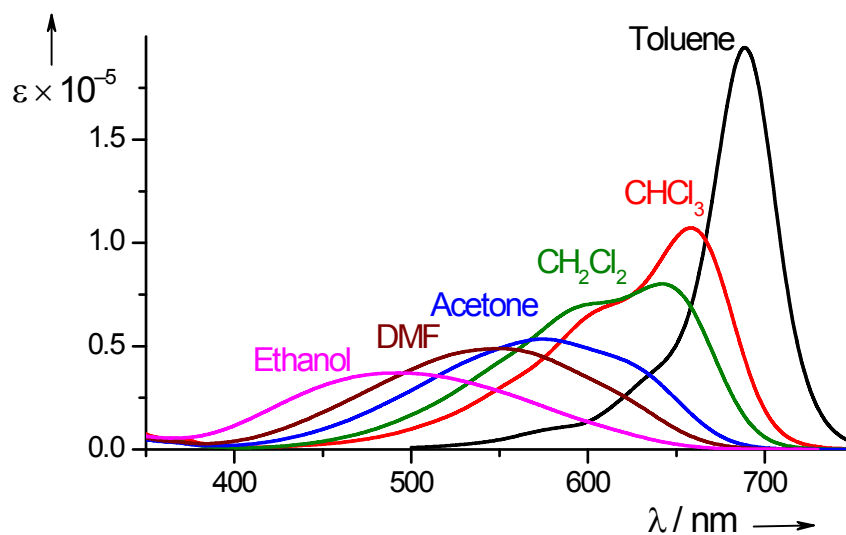


Figure S6 Vis absorption spectra of dye **3** in solvents of various polarity.

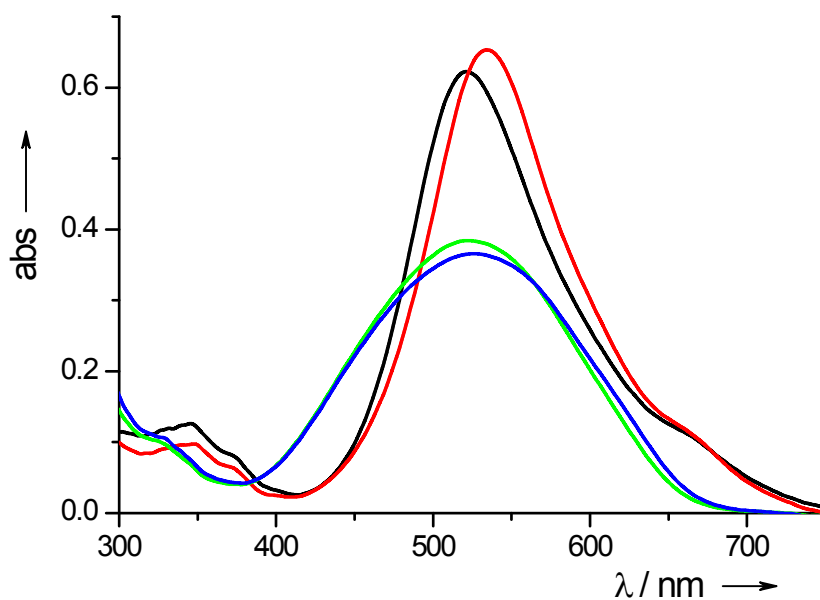


Figure S7 UV/Vis absorption spectra of dye **3** in four DMF-water mixtures: 1:9 - black, 5:5 - red, 8:2 - green, 9:1 - blue.

Optimized atomic coordinates of dyes 1–3 (from B3LYP calculations)

(given in angstroms)

Merocyanine 1 in vacuum, ground state

N	3.799674087	0.782767581	-0.194730695
C	5.013503200	0.106582968	-0.147703696
C	6.329581046	0.549467397	-0.255697945
C	7.338383440	-0.414101775	-0.175727300
C	7.038165099	-1.770265626	0.008917644
C	5.717272009	-2.213543326	0.118020142
C	4.712445362	-1.252852188	0.039094868
N	3.324569868	-1.358266678	0.125530416
C	2.760342855	-0.108807617	-0.024857592
C	1.414785321	0.295314400	0.005589716
C	0.299294994	-0.524648662	-0.113734531
C	-1.052201680	-0.162560289	-0.070067387
C	-2.008008136	-1.240633195	-0.237317743
N	-3.377891672	-0.881001399	-0.233529728
C	-3.852265066	0.400905375	-0.012865027
N	-2.907335197	1.392749465	0.181157262
C	-1.500788107	1.193167747	0.129694295
O	-1.696692002	-2.425550232	-0.386631314
O	-0.755998980	2.169697906	0.262225210
S	-5.505499719	0.736060851	0.018666131
C	3.649170103	2.221069295	-0.417322593
C	3.588508689	3.036470327	0.880272606
C	3.433377420	4.538151384	0.610298962
C	3.374103409	5.368108160	1.895866846
C	2.631527756	-2.604027287	0.463833755
C	2.260780005	-3.458916599	-0.755604484
C	1.362769129	-4.643424868	-0.375331391
C	1.051055736	-5.552279570	-1.567419090
C	-4.321881966	-1.999348516	-0.452361200
C	-4.715358065	-2.704287119	0.848402832
C	-5.696877465	-3.855511261	0.598285406
C	-6.096316222	-4.587856156	1.882762317
C	-3.333252508	2.787575824	0.429986520
C	-3.471963639	3.602480090	-0.858704235
C	-3.918878189	5.042197169	-0.578331412
C	-4.051294567	5.883703229	-1.851183728
H	6.567941900	1.598646485	-0.390425158
H	8.374647328	-0.102816541	-0.257522703
H	7.845193213	-2.493293127	0.066040188
H	5.489877084	-3.265204028	0.251712750
H	1.231407836	1.356059929	0.103206261
H	0.425704496	-1.585016239	-0.293324465
H	2.746295903	2.374516076	-1.014321627
H	4.496339068	2.538946016	-1.033139218
H	4.499475041	2.851195143	1.464078627
H	2.747441069	2.681284441	1.487341629
H	2.520546888	4.706172193	0.024423369
H	4.268435831	4.886052140	-0.013433192
H	4.285875931	5.245244438	2.491088041
H	2.525920249	5.067521296	2.520029295
H	3.262502361	6.433656505	1.673581603
H	1.745365460	-2.342446882	1.045694202
H	3.293958372	-3.162946071	1.132835635
H	3.180572139	-3.814434131	-1.237977238
H	1.746643953	-2.834239230	-1.495497118
H	0.423931795	-4.256452728	0.039114267
H	1.845278078	-5.230042953	0.419001920
H	1.965226447	-5.974300173	-2.000591341

H	0.530406485	-4.998340081	-2.355596693
H	0.407329617	-6.385097137	-1.268981336
H	-3.812461338	-2.697850197	-1.116341455
H	-5.199666221	-1.588829464	-0.949249701
H	-5.168924097	-1.973753434	1.528184328
H	-3.808211531	-3.088065421	1.330042030
H	-5.249106024	-4.570264045	-0.105703243
H	-6.597056862	-3.463500052	0.106341505
H	-6.577657806	-3.905907716	2.592580120
H	-5.220511111	-5.018809837	2.381125839
H	-6.797331241	-5.403550071	1.677246664
H	-2.568141429	3.227744984	1.069631059
H	-4.281907287	2.745526331	0.963092650
H	-4.199605571	3.111570786	-1.515170208
H	-2.506588727	3.608087459	-1.378574521
H	-3.202264914	5.520730711	0.103299891
H	-4.881140814	5.026187091	-0.049435112
H	-4.786779610	5.448783984	-2.537054350
H	-3.096795364	5.944663336	-2.386368393
H	-4.371643233	6.905896664	-1.624164100

Merocyanine 1 in vacuum, excited state

N	3.796030019	0.869853513	-0.123680377
C	5.027957406	0.239032044	-0.098522655
C	6.328637259	0.738343748	-0.140556220
C	7.380936805	-0.192627649	-0.103891629
C	7.135031312	-1.562753927	-0.020442867
C	5.823809360	-2.067879377	0.025605480
C	4.778934361	-1.147392550	-0.013569278
N	3.402011788	-1.317597538	0.032786507
C	2.769834220	-0.074706162	-0.036030545
C	1.400208859	0.253870923	-0.028838172
C	0.315111168	-0.580263274	-0.196281218
C	-1.096798077	-0.206933349	-0.128109974
C	-2.024006837	-1.273187406	-0.240507531
N	-3.459686346	-0.910405900	-0.182211021
C	-3.869682681	0.343083754	-0.020257182
N	-3.000309058	1.338189402	0.092836760
C	-1.523979808	1.125525649	0.042459999
O	-1.792773889	-2.474504340	-0.383798229
O	-0.852889398	2.154163633	0.158559556
S	-5.616673033	0.689102710	0.045534589
C	3.601909955	2.306270902	-0.248953788
C	3.500075794	3.031252507	1.100140821
C	3.297377391	4.541877734	0.936692526
C	3.200382403	5.278833413	2.275636995
C	2.760855977	-2.597454456	0.314315592
C	2.451918139	-3.425845434	-0.941032303
C	1.627414064	-4.678271275	-0.619202999
C	1.379411018	-5.558118724	-1.847752897
C	-4.407063585	-2.036745593	-0.286575584
C	-4.696544644	-2.702540231	1.062404620
C	-5.672695653	-3.877466958	0.923557474
C	-5.960077370	-4.569440777	2.259164787
C	-3.435356311	2.738735431	0.250589695
C	-3.551138197	3.484372671	-1.082806678
C	-3.994296203	4.939822962	-0.888179191
C	-4.097380163	5.709306198	-2.208244410
H	6.526807206	1.803225653	-0.190281527
H	8.404464825	0.167395775	-0.137648523
H	7.969018361	-2.256932029	0.007620355

H	5.637883939	-3.134626362	0.080651638
H	1.185390281	1.304667034	0.120346256
H	0.454761268	-1.628139528	-0.417876128
H	2.699055811	2.475893568	-0.843651392
H	4.443380263	2.699960286	-0.829636720
H	4.410828221	2.834856637	1.680582862
H	2.666588548	2.604023689	1.670619370
H	2.385006634	4.722202978	0.353071689
H	4.125510120	4.960371671	0.347873350
H	4.111108429	5.143655228	2.869869422
H	2.359032858	4.906576015	2.870269945
H	3.055100520	6.353870600	2.129172507
H	1.847647458	-2.395790626	0.877572399
H	3.429211742	-3.156341859	0.979369809
H	3.394329717	-3.704927319	-1.429972899
H	1.905416575	-2.800348210	-1.656706559
H	0.664543864	-4.369440765	-0.192686757
H	2.139505708	-5.266636677	0.155210858
H	2.321600347	-5.908317644	-2.284836747
H	0.838161172	-5.005435120	-2.623285910
H	0.782889937	-6.439331032	-1.591271734
H	-3.937665516	-2.752817494	-0.961077358
H	-5.324712133	-1.675264943	-0.763755406
H	-5.102000062	-1.964264784	1.765360158
H	-3.745268797	-3.055491338	1.473548529
H	-5.260514408	-4.606887931	0.214135806
H	-6.615759097	-3.522901273	0.485178380
H	-6.404093542	-3.873145527	2.979292280
H	-5.040744075	-4.964847500	2.704380371
H	-6.655333671	-5.405004832	2.131965880
H	-2.678706199	3.212294072	0.875934368
H	-4.382175146	2.748399684	0.801903434
H	-4.258433026	2.966319797	-1.742217565
H	-2.571277370	3.455365979	-1.570267233
H	-3.283816848	5.447325624	-0.222602886
H	-4.965318394	4.963469866	-0.374567522
H	-4.825754033	5.244889000	-2.882259832
H	-3.133368539	5.732380337	-2.727780107
H	-4.411269269	6.744350333	-2.041191185

Merocyanine 1 in n-hexane, ground state

N	3.788222046	0.778059464	-0.209944071
C	5.001063761	0.099519885	-0.160381300
C	6.317897871	0.538628656	-0.282995904
C	7.323257384	-0.426455722	-0.193617326
C	7.020303568	-1.780088823	0.014042401
C	5.700080099	-2.218923132	0.137207084
C	4.697668759	-1.255504351	0.048039158
N	3.309671120	-1.354929908	0.142879651
C	2.751865996	-0.107976790	-0.022075118
C	1.401265779	0.300476469	0.013597693
C	0.289822095	-0.514695196	-0.121608139
C	-1.068346285	-0.153343767	-0.076700401
C	-2.021451683	-1.226132426	-0.261634217
N	-3.395283771	-0.868311163	-0.249084304
C	-3.868054085	0.407715792	-0.010394221
N	-2.926576267	1.396371313	0.194286546
C	-1.517044306	1.195854454	0.141496510
O	-1.713497015	-2.410014546	-0.432655790
O	-0.775360988	2.173858377	0.289331014
S	-5.527282983	0.742394812	0.029885954

C	3.644947432	2.216143052	-0.449394606
C	3.627282967	3.047109589	0.839235233
C	3.495704875	4.547991636	0.552974308
C	3.479302253	5.394653120	1.828848246
C	2.616585367	-2.596788296	0.499289636
C	2.270923476	-3.478084473	-0.708128945
C	1.402355133	-4.678633005	-0.311138636
C	1.114179962	-5.612658165	-1.489666691
C	-4.336951690	-1.985831566	-0.482975380
C	-4.724095977	-2.714168250	0.806771600
C	-5.696852435	-3.869099427	0.539625203
C	-6.090488023	-4.622936808	1.813466043
C	-3.350788505	2.788710317	0.460410323
C	-3.480438137	3.622007900	-0.817408963
C	-3.923423097	5.059543160	-0.519765016
C	-4.047027345	5.918146846	-1.782079349
H	6.558262454	1.584726822	-0.435572198
H	8.359987107	-0.119888500	-0.285795388
H	7.826219245	-2.503682057	0.078188830
H	5.471178553	-3.267554210	0.289638380
H	1.224426628	1.360623649	0.127243741
H	0.419259854	-1.572185776	-0.316947564
H	2.729561233	2.370010741	-1.025979148
H	4.479259613	2.516434340	-1.090451474
H	4.547184746	2.852021220	1.405102441
H	2.793605857	2.715659646	1.469684233
H	2.575010017	4.727122109	-0.017017341
H	4.324792784	4.870468584	-0.091575447
H	4.400842159	5.260824236	2.406378003
H	2.638700484	5.118544968	2.474354244
H	3.384002670	6.459359438	1.594992374
H	1.721229236	-2.326662483	1.062356581
H	3.272043935	-3.137420894	1.189350548
H	3.200686791	-3.819580454	-1.180820057
H	1.744899594	-2.878443400	-1.460417577
H	0.454849947	-4.309222569	0.099768521
H	1.898597327	-5.241024979	0.491762861
H	2.039629789	-6.019306327	-1.913228204
H	0.584013691	-5.083477741	-2.288532044
H	0.489580389	-6.455902905	-1.179773847
H	-3.828630047	-2.671398473	-1.160842267
H	-5.217497044	-1.571008627	-0.970864200
H	-5.182143406	-1.998289812	1.499015448
H	-3.814084959	-3.098343657	1.282546615
H	-5.243243862	-4.569822721	-0.174521852
H	-6.599994166	-3.477112158	0.053154541
H	-6.577187050	-3.955033209	2.532967684
H	-5.211230369	-5.054312783	2.305327469
H	-6.785121482	-5.440842674	1.595628191
H	-2.588966776	3.218203113	1.110860634
H	-4.301791291	2.741924110	0.988460635
H	-4.205767893	3.142943308	-1.485215368
H	-2.512824070	3.630956203	-1.332834975
H	-3.207864085	5.525970783	0.171138504
H	-4.887987235	5.040198483	0.004813184
H	-4.781416430	5.495282841	-2.476663288
H	-3.089862734	5.982405157	-2.312060202
H	-4.364322828	6.938356714	-1.542398405

Merocyanine 1 in n-hexane, excited state

N	3.788756287	0.886018068	-0.125687009
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C	5.026598384	0.267068020	-0.093518007
C	6.321879506	0.778170057	-0.139776011
C	7.384297557	-0.140418011	-0.094738007
C	7.152456537	-1.512800113	0.000526000
C	5.846125452	-2.029427157	0.050771004
C	4.792011368	-1.121002083	0.003801000
N	3.416518262	-1.306578099	0.050552004
C	2.769804211	-0.069590006	-0.031206002
C	1.404632109	0.247184019	-0.030984002
C	0.312700024	-0.598850043	-0.162982013
C	-1.090209085	-0.224470017	-0.109337008
C	-2.024902157	-1.290089100	-0.231856018
N	-3.447883264	-0.928594072	-0.189787015
C	-3.860365293	0.326413025	-0.022738002
N	-2.988240229	1.321333101	0.102350008
C	-1.525550115	1.111849084	0.055136004
O	-1.783473139	-2.492795193	-0.374227029
O	-0.846388063	2.139885166	0.169187013
S	-5.600865450	0.671348051	0.034256003
C	3.581455275	2.319486178	-0.267455020
C	3.451234263	3.057405235	1.072085081
C	3.236637246	4.564087350	0.888195066
C	3.111016240	5.314984427	2.217002171
C	2.793790212	-2.594383196	0.337693026
C	2.497222189	-3.430486261	-0.915143069
C	1.740922134	-4.722673363	-0.584183044
C	1.501891114	-5.603434447	-1.813935137
C	-4.403219335	-2.048297157	-0.313713024
C	-4.732495364	-2.706123206	1.029863076
C	-5.721062453	-3.868222295	0.871226067
C	-6.046995474	-4.552481350	2.201999166
C	-3.431040261	2.720728207	0.265050020
C	-3.558109271	3.467252263	-1.066612081
C	-4.005945304	4.920507373	-0.866085067
C	-4.126496316	5.689512429	-2.184961166
H	6.509083473	1.844587142	-0.199552015
H	8.403853625	0.230530017	-0.131660010
H	7.993006601	-2.198782170	0.034759003
H	5.671118440	-3.097582234	0.115666009
H	1.185119088	1.301464098	0.078055006
H	0.454112035	-1.653886129	-0.345920026
H	2.687029205	2.474562190	-0.878726069
H	4.427303340	2.716373205	-0.838960066
H	4.355068333	2.876980220	1.668312125
H	2.613259197	2.628795201	1.634877124
H	2.332120179	4.728904362	0.288031022
H	4.070172309	4.983612379	0.307976024
H	4.013577305	5.195391395	2.826894218
H	2.263878174	4.940950379	2.802320216
H	2.957620228	6.386816487	2.055678158
H	1.879731142	-2.406504185	0.904169070
H	3.471822264	-3.141624239	1.002432078
H	3.442065262	-3.663890279	-1.422897111
H	1.908244143	-2.828286218	-1.617113126
H	0.776522061	-4.464178342	-0.128497010
H	2.300083174	-5.292084387	0.171354013
H	2.448165188	-5.905198461	-2.277417174
H	0.916062070	-5.070545385	-2.570746198
H	0.954278070	-6.513836490	-1.550164118
H	-3.925992300	-2.769143210	-0.977341075
H	-5.305372398	-1.677205129	-0.813146064
H	-5.145647395	-1.960026148	1.719938134

H	-3.796812291	-3.069797233	1.466963114
H	-5.303244418	-4.604829352	0.172740013
H	-6.649007515	-3.501115267	0.411569032
H	-6.497201485	-3.848050296	2.910329224
H	-5.143068391	-4.959273380	2.668114203
H	-6.750685537	-5.378726419	2.060992156
H	-2.676214203	3.196968246	0.890368069
H	-4.376261336	2.722221206	0.819681065
H	-4.268666325	2.947436223	-1.721248133
H	-2.582438200	3.443057263	-1.562835119
H	-3.290847254	5.430822438	-0.207811016
H	-4.971490378	4.938390379	-0.342291026
H	-4.859852373	5.221530396	-2.851124217
H	-3.167990241	5.717274444	-2.714440205
H	-4.443521342	6.722940509	-2.013855153

Merocyanine 1 in DCM, ground state

N	3.775818305	0.758347829	-0.239270562
C	4.984391180	0.071370598	-0.191570098
C	6.302563002	0.498333306	-0.348780767
C	7.299768582	-0.472121446	-0.246717986
C	6.989329024	-1.818444759	0.006225727
C	5.669710193	-2.244268971	0.162780853
C	4.673810575	-1.273912845	0.059305942
N	3.286298716	-1.357792217	0.176721308
C	2.742253375	-0.113460545	-0.012477671
C	1.385588157	0.306191909	0.038264478
C	0.278992367	-0.498744462	-0.123548749
C	-1.088948029	-0.136682126	-0.076490621
C	-2.038819259	-1.197425385	-0.300598860
N	-3.417443851	-0.839689246	-0.282119026
C	-3.886421071	0.426591131	-0.012037453
N	-2.949985312	1.405726061	0.226043914
C	-1.535987502	1.201073163	0.179071107
O	-1.736977123	-2.378332789	-0.511043386
O	-0.797335084	2.176809884	0.364892134
S	-5.554662773	0.765015488	0.025813420
C	3.645437694	2.193421007	-0.514615618
C	3.713861984	3.057066133	0.750258222
C	3.599272557	4.552430777	0.429787870
C	3.669069464	5.431809353	1.681554378
C	2.589208382	-2.586023884	0.576097337
C	2.261630578	-3.513864359	-0.600586962
C	1.424992261	-4.721287220	-0.159284131
C	1.142667436	-5.694024565	-1.307710443
C	-4.356395297	-1.951282118	-0.553519164
C	-4.741511883	-2.724862213	0.710343832
C	-5.710970196	-3.873052699	0.404129781
C	-6.101949208	-4.670722583	1.651839472
C	-3.370582015	2.791868267	0.529382178
C	-3.482751759	3.664574828	-0.723626059
C	-3.916356083	5.096436699	-0.386675454
C	-4.022464604	5.992941288	-1.624009983
H	6.547931697	1.537308460	-0.536098729
H	8.337410500	-0.177789532	-0.364015671
H	7.791256663	-2.545446011	0.079786936
H	5.436352975	-3.285679441	0.351686785
H	1.221107597	1.364705108	0.181651146
H	0.412455188	-1.550273843	-0.347637953
H	2.704383662	2.347626845	-1.046853476
H	4.449563064	2.457830198	-1.207042610

H	4.658907018	2.857733863	1.270586071
H	2.909441587	2.760538613	1.434371388
H	2.654360484	4.738231603	-0.097066212
H	4.400319046	4.837632300	-0.264991586
H	4.617407959	5.291247028	2.212034255
H	2.858983288	5.191486633	2.378754829
H	3.584386091	6.492114769	1.424200178
H	1.687406465	-2.293409048	1.116625486
H	3.237437971	-3.096814298	1.294241850
H	3.197174297	-3.851453869	-1.063289351
H	1.721104525	-2.953127032	-1.372663685
H	0.475514129	-4.362913338	0.257958689
H	1.944216036	-5.249474051	0.651439869
H	2.072624075	-6.091373548	-1.729563037
H	0.593776567	-5.199475400	-2.116475428
H	0.540917861	-6.542180811	-0.966906018
H	-3.847748295	-2.611648138	-1.255317122
H	-5.237561742	-1.523982735	-1.028622283
H	-5.200173019	-2.035427281	1.428842423
H	-3.830957268	-3.122216906	1.173846380
H	-5.255038704	-4.547404731	-0.333305345
H	-6.615272783	-3.468072731	-0.069486536
H	-6.591369688	-4.029398519	2.393444821
H	-5.221109145	-5.115380620	2.128660316
H	-6.793442477	-5.482989154	1.405375380
H	-2.614535679	3.197645847	1.200974117
H	-4.325849282	2.735190568	1.048208297
H	-4.204754942	3.212215298	-1.413675790
H	-2.511199554	3.680882822	-1.231186396
H	-3.202372802	5.535517511	0.323201308
H	-4.884940640	5.070159588	0.130299451
H	-4.754712119	5.597361821	-2.336828390
H	-3.060285007	6.064816841	-2.143666433
H	-4.333167940	7.007903992	-1.355678996

Merocyanine 1 in DCM, excited state

N	3.760636115	0.862543379	-0.164138470
C	4.986857172	0.246727794	-0.095925956
C	6.288504668	0.756274237	-0.167343991
C	7.337242428	-0.160015423	-0.066669293
C	7.100510540	-1.536336224	0.103045360
C	5.804153759	-2.051863097	0.177579571
C	4.748215056	-1.140528454	0.076568231
N	3.382197159	-1.321015600	0.125694617
C	2.745225483	-0.089070835	-0.030122614
C	1.385544532	0.236461084	-0.068147944
C	0.270856642	-0.622305618	-0.130859407
C	-1.085440679	-0.228700743	-0.086186156
C	-2.067055882	-1.300315143	-0.193877682
N	-3.424386821	-0.937290586	-0.196770779
C	-3.892356122	0.352668210	-0.017983730
N	-2.936690829	1.342236734	0.125677290
C	-1.541517684	1.141640583	0.054677865
O	-1.746443685	-2.494805384	-0.297211366
O	-0.785298895	2.126214845	0.126795313
S	-5.562305257	0.701603946	0.023164245
C	3.557900971	2.300098870	-0.345726054
C	3.396396302	3.063061351	0.976406818
C	3.201361778	4.567077339	0.749026186
C	3.043496822	5.346842538	2.057635088
C	2.752322120	-2.617589841	0.391353869

C	2.467558232	-3.429431446	-0.880022522
C	1.752588523	-4.750128693	-0.567702946
C	1.511011759	-5.600118040	-1.818467948
C	-4.371227829	-2.062727799	-0.372246632
C	-4.739483245	-2.740474858	0.950170390
C	-5.704899052	-3.913522079	0.740332296
C	-6.082098817	-4.614554048	2.048858889
C	-3.348279268	2.749734026	0.335626440
C	-3.470345553	3.534654442	-0.973249530
C	-3.897357535	4.987246483	-0.729157374
C	-4.017010617	5.797243551	-2.023607408
H	6.478566085	1.816118808	-0.288683424
H	8.359639014	0.200140737	-0.118006166
H	7.943936365	-2.215155121	0.176136957
H	5.629863464	-3.114279343	0.300715857
H	1.159124012	1.294882462	-0.059171126
H	0.399287188	-1.688891416	-0.244821065
H	2.684312033	2.441280962	-0.987572511
H	4.420470619	2.676003199	-0.902619094
H	4.282429442	2.889885033	1.599752048
H	2.538651317	2.656072875	1.525329729
H	2.316967156	4.725792069	0.118411473
H	4.056517049	4.963939405	0.185943272
H	3.926975765	5.232951359	2.695604104
H	2.175395060	4.994337744	2.625260943
H	2.905469414	6.415507895	1.866050063
H	1.840864814	-2.439096180	0.962953476
H	3.429338359	-3.169300267	1.049872385
H	3.414407353	-3.626314953	-1.397770553
H	1.855960595	-2.830450199	-1.565439269
H	0.792584258	-4.532478641	-0.082172406
H	2.344830820	-5.323524130	0.157766283
H	2.455357590	-5.861262515	-2.308982110
H	0.894225967	-5.063062887	-2.547259951
H	0.995355820	-6.532385316	-1.568097829
H	-3.875455619	-2.774504987	-1.032438286
H	-5.257780943	-1.666274724	-0.863693345
H	-5.196003738	-2.000354370	1.617984347
H	-3.822776579	-3.097024921	1.434108763
H	-5.250460987	-4.640325133	0.053625131
H	-6.614796100	-3.550622038	0.243926441
H	-6.569722740	-3.920558210	2.742657894
H	-5.195276706	-5.016738658	2.551583520
H	-6.770726379	-5.446879104	1.870895792
H	-2.583828116	3.197687224	0.970486219
H	-4.298911350	2.732173258	0.865043043
H	-4.201630944	3.038084921	-1.621886765
H	-2.504839373	3.513786724	-1.491529411
H	-3.173778366	5.471813989	-0.059814631
H	-4.859563204	4.998778943	-0.199952023
H	-4.758860932	5.355939782	-2.698623420
H	-3.061215004	5.830785186	-2.558659969
H	-4.322414180	6.828975088	-1.821355403

Merocyanine 1 in ethanol, ground state

N	3.773936726	0.755774376	-0.243319047
C	4.982489201	0.068495965	-0.197229440
C	6.300321672	0.494179898	-0.362823479
C	7.296849058	-0.476402563	-0.259175146
C	6.986609635	-1.821487301	0.003129389
C	5.667825476	-2.245934011	0.167556393

C	4.672225208	-1.275108373	0.062257691
N	3.285112428	-1.357419645	0.185081521
C	2.742427665	-0.114422824	-0.008456630
C	1.383845195	0.306166415	0.045675284
C	0.278908365	-0.497173285	-0.121352001
C	-1.091527297	-0.135383303	-0.074157188
C	-2.040229829	-1.193592539	-0.306475254
N	-3.419984754	-0.836120993	-0.288247387
C	-3.888478724	0.428314760	-0.014131070
N	-2.953752033	1.405570562	0.231505738
C	-1.538659953	1.199656333	0.188819064
O	-1.739400283	-2.373963880	-0.524101799
O	-0.800976337	2.174648269	0.384520151
S	-5.559112095	0.767442766	0.019506269
C	3.643165200	2.190123370	-0.524633981
C	3.717357020	3.058696311	0.736486093
C	3.602427395	4.552702478	0.409848432
C	3.677329148	5.437352485	1.657621417
C	2.588323270	-2.583959352	0.591156552
C	2.262710793	-3.518132676	-0.581008626
C	1.428328481	-4.724778372	-0.133421268
C	1.144889795	-5.702372812	-1.277498079
C	-4.357917973	-1.946970948	-0.566455553
C	-4.742224002	-2.728604999	0.692773666
C	-5.711749833	-3.875082829	0.380232080
C	-6.101479511	-4.680487999	1.623355766
C	-3.373689518	2.790875922	0.540203890
C	-3.477314224	3.671027579	-0.708408154
C	-3.910501604	5.101722799	-0.365796099
C	-4.008366824	6.005183274	-1.598746225
H	6.545610408	1.531704627	-0.557847580
H	8.334205750	-0.183632156	-0.382633548
H	7.788561616	-2.548337420	0.077706264
H	5.434640981	-3.285980871	0.363748301
H	1.221109655	1.364066635	0.195306750
H	0.413838964	-1.547329098	-0.350924881
H	2.700208057	2.342258945	-1.053969989
H	4.444550798	2.450836083	-1.221283776
H	4.664484308	2.861341164	1.253501573
H	2.915831995	2.765542820	1.425575616
H	2.655886033	4.736967817	-0.114781665
H	4.401335517	4.834008129	-0.288743340
H	4.627627086	5.298222631	2.184898993
H	2.869848255	5.200470121	2.359143382
H	3.592429607	6.496654316	1.396056257
H	1.685990429	-2.288489313	1.129146555
H	3.236285656	-3.090217881	1.312476642
H	3.198692369	-3.857143831	-1.041397426
H	1.721949388	-2.962216874	-1.356520313
H	0.479367683	-4.366264675	0.285269812
H	1.949926615	-5.248998426	0.678115345
H	2.074708357	-6.100353210	-1.698828761
H	0.594853480	-5.211705633	-2.088037718
H	0.544551266	-6.549868751	-0.932414424
H	-3.848935853	-2.602415361	-1.272491935
H	-5.239290617	-1.518017373	-1.039525334
H	-5.200112873	-2.043973795	1.416476455
H	-3.831419277	-3.128533177	1.153495127
H	-5.256308105	-4.544695253	-0.361745774
H	-6.616486663	-3.467508083	-0.090398030
H	-6.590555390	-4.043962705	2.369340151
H	-5.220111053	-5.127789134	2.096657687

H	-6.792851703	-5.491364548	1.372199438
H	-2.620959853	3.191559055	1.218440903
H	-4.331507970	2.733469049	1.054110147
H	-4.195689718	3.224002886	-1.405779301
H	-2.503097253	3.688754757	-1.210726674
H	-3.199689911	5.535568947	0.350360116
H	-4.881823569	5.074310312	0.146022442
H	-4.737364112	5.614863617	-2.317813242
H	-3.043210304	6.078317317	-2.112609666
H	-4.318820374	7.019068733	-1.326252661

Merocyanine 1 in ethanol, excited state

N	3.757080615	0.866548971	-0.161087341
C	4.985404216	0.256680057	-0.092021569
C	6.284795929	0.772675768	-0.161363339
C	7.337322704	-0.138470752	-0.060704021
C	7.106889296	-1.516858157	0.107049206
C	5.813494425	-2.038806913	0.179650725
C	4.753105156	-1.132452929	0.078954117
N	3.388483467	-1.319653667	0.126937599
C	2.745649931	-0.090344681	-0.028654987
C	1.386320930	0.230630199	-0.067013571
C	0.270380513	-0.629692478	-0.118765148
C	-1.084594821	-0.236314689	-0.077442704
C	-2.067656546	-1.307413083	-0.184835256
N	-3.424307682	-0.943752126	-0.195024629
C	-3.892255827	0.347502752	-0.026822245
N	-2.936966229	1.336625799	0.120940018
C	-1.541926961	1.134540247	0.062410864
O	-1.747845375	-2.502954364	-0.281433652
O	-0.785566436	2.118529281	0.142747755
S	-5.563784254	0.698803344	-0.003054608
C	3.547710901	2.303893129	-0.338601994
C	3.367741831	3.059688820	0.985269923
C	3.165922031	4.563473510	0.762468405
C	2.990647424	5.336331119	2.072988885
C	2.765053591	-2.621062551	0.384900408
C	2.477668920	-3.423283269	-0.891879463
C	1.785676675	-4.757586134	-0.585775545
C	1.532163318	-5.592724746	-1.844193497
C	-4.371108970	-2.069838291	-0.366939405
C	-4.743608467	-2.738983372	0.958675861
C	-5.712790090	-3.909944836	0.754391181
C	-6.093848140	-4.602258641	2.066430733
C	-3.348517102	2.745096793	0.325684184
C	-3.455075386	3.530177555	-0.984405877
C	-3.880759192	4.983936881	-0.744563613
C	-3.985924513	5.794191362	-2.040093566
H	6.469780896	1.833528306	-0.281294630
H	8.358057674	0.226442872	-0.110531594
H	7.953590833	-2.191516101	0.180111553
H	5.644537655	-3.102125105	0.301592017
H	1.159161758	1.288687283	-0.068705331
H	0.400184914	-1.696974159	-0.223909010
H	2.680722555	2.442854688	-0.989848180
H	4.413983747	2.687148005	-0.884088392
H	4.248520488	2.889339991	1.616549758
H	2.507118095	2.644978251	1.523954725
H	2.287009395	4.719969209	0.123541870
H	4.024285963	4.967637714	0.209817257
H	3.868803284	5.224756351	2.718616430

H	2.119477572	4.975910527	2.631036103
H	2.847971194	6.405040875	1.884895859
H	1.856336332	-2.451414453	0.963572989
H	3.447847624	-3.175302640	1.034871062
H	3.421474420	-3.601999544	-1.421338573
H	1.850670749	-2.825918346	-1.564825974
H	0.832281309	-4.560768917	-0.078517905
H	2.398996583	-5.332999208	0.120068114
H	2.470813884	-5.833225011	-2.355595889
H	0.894842438	-5.053902628	-2.553923796
H	1.034403867	-6.535847247	-1.598091744
H	-3.874381383	-2.785746961	-1.021764860
H	-5.255806334	-1.676125194	-0.863656160
H	-5.198034577	-1.993603736	1.622209272
H	-3.828913426	-3.095590861	1.446314707
H	-5.260066703	-4.642077858	0.072293396
H	-6.620844702	-3.546929836	0.254630033
H	-6.580101970	-3.902802451	2.755730318
H	-5.208942825	-5.004453258	2.572465802
H	-6.784902932	-5.433292849	1.892104126
H	-2.590809620	3.192152935	0.969115476
H	-4.304500932	2.729610569	0.845277463
H	-4.180449159	3.035638719	-1.641297918
H	-2.484493444	3.506879971	-1.492969821
H	-3.162396409	5.466552909	-0.068317462
H	-4.847823587	4.998149646	-0.224272527
H	-4.722492729	5.354940696	-2.722245723
H	-3.024950762	5.825204695	-2.565885779
H	-4.290441259	6.826660520	-1.840477895

Merocyanine 2 in vacuum, ground state

N	5.057139436	0.871081950	-0.212963970
C	6.239485868	0.139470736	-0.188146301
C	7.571185816	0.522803614	-0.320438467
C	8.539062593	-0.484919977	-0.256883649
C	8.182909159	-1.824635196	-0.062780057
C	6.844212218	-2.208154656	0.070954340
C	5.881901697	-1.204892103	0.006176800
N	4.491993216	-1.250191374	0.118433502
C	3.976124462	0.026163969	-0.020795383
C	2.653671638	0.474248074	0.028193605
C	1.466647867	-0.268006932	-0.062595906
C	0.192107794	0.276871915	0.020302960
C	-0.939303804	-0.538913243	-0.117693752
C	-2.288890303	-0.201075614	-0.070178651
C	-3.240156894	-1.287860766	-0.256323310
N	-4.614048488	-0.939302857	-0.250413606
C	-5.101930348	0.332122635	-0.004584253
N	-4.167962423	1.330248594	0.209167488
C	-2.758242815	1.151834844	0.150693291
O	-2.917975671	-2.462875336	-0.426962171
O	-2.029390384	2.133221035	0.298597627
S	-6.758556519	0.648758385	0.032619827
C	4.976408065	2.308714351	-0.457305288
C	4.994857184	3.150920174	0.824998449
C	4.921217725	4.654724401	0.532962978
C	4.941646369	5.508626522	1.804029267
C	3.767429814	-2.458605596	0.511938250
C	3.373051775	-3.356495623	-0.667658045
C	2.615664721	-4.610508456	-0.212524275
C	2.229145948	-5.526645695	-1.377097471

C	-5.545246381	-2.062878435	-0.495707974
C	-5.932957724	-2.801024578	0.788253424
C	-6.899600777	-3.958417689	0.510240129
C	-7.293364108	-4.723327839	1.777384531
C	-4.609572881	2.715326254	0.485370238
C	-4.753972430	3.554579114	-0.786925464
C	-5.214800331	4.984080881	-0.478216240
C	-5.354179474	5.849420375	-1.734239498
H	7.853982688	1.560244473	-0.460432829
H	9.586196469	-0.219177407	-0.358376812
H	8.957412187	-2.583143810	-0.017030304
H	6.573575204	-3.248451742	0.212991455
H	2.537513120	1.549037494	0.112874732
H	1.520277362	-1.337864582	-0.245416579
H	0.058918357	1.338641118	0.191236922
H	-0.767673149	-1.601549001	-0.286815659
H	4.069738622	2.500944983	-1.038311518
H	5.822287023	2.572785128	-1.100025312
H	5.908390406	2.922956457	1.388889779
H	4.154168476	2.853613800	1.463912957
H	4.008048440	4.869598246	-0.037792888
H	5.760429854	4.941454913	-0.115409402
H	5.858663990	5.341503404	2.379763610
H	4.093176983	5.270457029	2.454436774
H	4.888129986	6.574883330	1.564791080
H	2.891987856	-2.151597816	1.088188575
H	4.418774876	-3.008714382	1.199885705
H	4.278946011	-3.644606600	-1.216042185
H	2.758379660	-2.784824256	-1.373739540
H	1.710647543	-4.311296055	0.332581284
H	3.233012890	-5.168150059	0.504993411
H	3.114860623	-5.870636943	-1.922750066
H	1.579224050	-5.007835971	-2.089669229
H	1.691716349	-6.410620838	-1.021577404
H	-5.026676093	-2.740899814	-1.173748450
H	-6.426700365	-1.651495285	-0.985282486
H	-6.397093109	-2.091205542	1.482750815
H	-5.022331559	-3.184271194	1.263506019
H	-6.440933169	-4.652184080	-0.207540857
H	-7.803305923	-3.567061246	0.024156773
H	-7.785056611	-4.062925650	2.500400348
H	-6.413476754	-5.153913974	2.268759675
H	-7.983586028	-5.543097657	1.552251796
H	-3.850556231	3.150612208	1.135507297
H	-5.558799616	2.652257216	1.015246497
H	-5.476058149	3.070156438	-1.454363186
H	-3.787881351	3.579902505	-1.304623043
H	-4.502938533	5.455548033	0.213148741
H	-6.177263355	4.948651136	0.049504556
H	-6.085027549	5.421328151	-2.429364494
H	-4.399806178	5.929762022	-2.267000992
H	-5.684253677	6.863927193	-1.487308434

Merocyanine 2 in vacuum, excited state

N	5.024980244	0.944317880	-0.139374307
C	6.250380146	0.297046259	-0.115278838
C	7.555434696	0.777949803	-0.185393858
C	8.595852837	-0.163468687	-0.141099853
C	8.333545813	-1.529036827	-0.023253031
C	7.017901738	-2.014241130	0.050500118
C	5.985231863	-1.082025782	0.003530250

N	4.605070916	-1.234326968	0.070385416
C	3.988338270	0.014047816	-0.019176639
C	2.631878579	0.353729273	0.000753109
C	1.496166067	-0.444920195	-0.116868895
C	0.168937001	0.072735476	-0.030217148
C	-0.940937300	-0.706439007	-0.167092114
C	-2.350029690	-0.313055853	-0.107355699
C	-3.299894624	-1.350714657	-0.272768379
N	-4.732566898	-0.951085063	-0.208054739
C	-5.111455745	0.307447729	-0.016237830
N	-4.218811303	1.277046050	0.132350706
C	-2.742751564	1.024603060	0.102515350
O	-3.105070145	-2.548542391	-0.462771482
O	-2.051879338	2.028350678	0.265541316
S	-6.847088667	0.696444425	0.042232466
C	4.851955466	2.378085038	-0.315636964
C	4.769160135	3.155791631	1.005258821
C	4.595052475	4.663111522	0.785734773
C	4.513429726	5.451512845	2.096098103
C	3.961553069	-2.503094707	0.392785861
C	3.660320905	-3.371698960	-0.836030477
C	3.000562497	-4.703718372	-0.459415340
C	2.706817200	-5.588188956	-1.674571059
C	-5.707273152	-2.048688970	-0.350146467
C	-6.023800048	-2.744000168	0.977725798
C	-7.031280715	-3.886763094	0.800196393
C	-7.345139816	-4.609165113	2.113549596
C	-4.619448763	2.683249725	0.321420461
C	-4.700448268	3.465679548	-0.993327478
C	-5.111157601	4.925910612	-0.766448236
C	-5.178185832	5.731707753	-2.067019369
H	7.766543398	1.838825555	-0.262319361
H	9.623098433	0.182650947	-0.196239735
H	9.158677028	-2.233270678	0.010382479
H	6.819539170	-3.077025947	0.133179852
H	2.444189580	1.418224185	0.111443436
H	1.589264797	-1.508493431	-0.314064370
H	0.049299741	1.136097325	0.152643284
H	-0.801875716	-1.770057437	-0.346087207
H	3.951112455	2.539888354	-0.916310836
H	5.696291719	2.736795118	-0.914249346
H	5.679090389	2.964573697	1.588415664
H	3.933161276	2.765628304	1.598760523
H	3.686866118	4.841468385	0.194439900
H	5.430651831	5.042363214	0.181423573
H	5.421782767	5.320615931	2.694683081
H	3.665315269	5.119566550	2.704773460
H	4.389605096	6.522617763	1.908527168
H	3.049088373	-2.285129339	0.951472420
H	4.630932036	-3.040126873	1.075015056
H	4.595111287	-3.557873068	-1.380180447
H	3.011080847	-2.813680376	-1.521573105
H	2.066270244	-4.505910397	0.082728182
H	3.649660740	-5.246875738	0.241283918
H	3.625865666	-5.831580381	-2.219485664
H	2.029638986	-5.086136931	-2.373931706
H	2.236911883	-6.530209181	-1.375568329
H	-5.251617261	-2.757799534	-1.041413433
H	-6.612123596	-1.650868252	-0.823216498
H	-6.412963029	-2.014799835	1.698992621
H	-5.085305906	-3.135086402	1.383979273
H	-6.635726860	-4.606510538	0.071635613

H	-7.961723017	-3.493296028	0.368026282
H	-7.773107841	-3.921854282	2.851825054
H	-6.439574453	-5.043120964	2.551055724
H	-8.062954043	-5.420774526	1.958963555
H	-3.858368438	3.120968704	0.967447842
H	-5.572225002	2.703774098	0.862449805
H	-5.411394277	2.981923265	-1.674391472
H	-3.715321577	3.425762343	-1.469544567
H	-4.397771386	5.398720641	-0.078769157
H	-6.088193775	4.959655139	-0.264898057
H	-5.908177835	5.302469491	-2.762309203
H	-4.206951340	5.744899348	-2.573312930
H	-5.469662037	6.769425714	-1.877095754

Merocyanine 2 in n-hexane, ground state

N	5.048363640	0.865614306	-0.222459148
C	6.231668015	0.135414640	-0.192775277
C	7.563026961	0.519418473	-0.335516884
C	8.529898989	-0.486757844	-0.261525218
C	8.174710457	-1.825659366	-0.047901682
C	6.838414076	-2.209216545	0.095933661
C	5.875565170	-1.205799700	0.020495220
N	4.485971676	-1.248597148	0.138165983
C	3.974797630	0.022946713	-0.015304990
C	2.645811742	0.474903499	0.038818490
C	1.467129540	-0.264696700	-0.062765940
C	0.184918753	0.281301124	0.022095146
C	-0.940690730	-0.529022295	-0.123982769
C	-2.298824161	-0.193215770	-0.074873239
C	-3.244365219	-1.276201097	-0.270715774
N	-4.622689233	-0.932584042	-0.257225072
C	-5.110736328	0.333689192	-0.001271529
N	-4.181569274	1.330906626	0.216230140
C	-2.768425222	1.152377738	0.156821097
O	-2.924083271	-2.451874334	-0.455769014
O	-2.043345000	2.137491850	0.314047115
S	-6.774102054	0.647255992	0.043740875
C	4.968626831	2.303845915	-0.479032148
C	5.019664558	3.154416786	0.796323795
C	4.950811391	4.656132335	0.492399187
C	5.005064262	5.519779144	1.755823617
C	3.759691544	-2.457589030	0.533495558
C	3.380380816	-3.361649005	-0.646055025
C	2.630442059	-4.620008214	-0.190658369
C	2.260844977	-5.543475490	-1.354921314
C	-5.550238745	-2.057420776	-0.510875632
C	-5.931272506	-2.811419043	0.765841137
C	-6.889813591	-3.973090964	0.477396450
C	-7.277187954	-4.752570364	1.737657401
C	-4.623366553	2.713784004	0.502843880
C	-4.763158884	3.564635757	-0.762279695
C	-5.222345308	4.992330855	-0.442597331
C	-5.357249919	5.868284538	-1.691776522
H	7.844243657	1.554934190	-0.490668405
H	9.576718217	-0.222812826	-0.369909609
H	8.950461973	-2.582307350	0.005295588
H	6.569604628	-3.247503234	0.254075723
H	2.533520764	1.548867835	0.138025220
H	1.521108027	-1.332836509	-0.254833961
H	0.056566561	1.341936135	0.202382992
H	-0.767579791	-1.589609625	-0.302437373

H	4.051505449	2.494761113	-1.042532707
H	5.802002971	2.556139096	-1.141729311
H	5.943443636	2.925009807	1.342308491
H	4.190180406	2.869246903	1.455128599
H	4.027085231	4.872736633	-0.060172960
H	5.778180417	4.930483507	-0.175884839
H	5.933248242	5.350182651	2.312650959
H	4.169103562	5.292912602	2.426255530
H	4.954156865	6.584415294	1.508690211
H	2.879044313	-2.148731935	1.100224621
H	4.406895450	-3.000145362	1.230366770
H	4.292177696	-3.645253778	-1.186609240
H	2.765804827	-2.798033367	-1.358755341
H	1.719230920	-4.326261823	0.346794441
H	3.247903181	-5.169372834	0.532797620
H	3.153973394	-5.881515769	-1.892136967
H	1.612349303	-5.032628650	-2.074620074
H	1.728441308	-6.430829694	-1.000022327
H	-5.032168789	-2.725906174	-1.198409004
H	-6.434752908	-1.645613305	-0.994053853
H	-6.399122451	-2.112447928	1.468750949
H	-5.017804971	-3.192670740	1.237152335
H	-6.426359839	-4.656529118	-0.247097561
H	-7.796545578	-3.583854639	-0.004684708
H	-7.773318719	-4.102480750	2.466996537
H	-6.393827239	-5.181433456	2.224277983
H	-7.961563735	-5.575007892	1.504736114
H	-3.866926832	3.142996485	1.159708827
H	-5.573770570	2.647247548	1.029839581
H	-5.483426678	3.087544546	-1.437013200
H	-3.795950637	3.592563721	-1.277588812
H	-4.511180045	5.456487534	0.254295192
H	-6.186011237	4.954212011	0.082724053
H	-6.087536748	5.447457442	-2.391949413
H	-4.401440669	5.951266728	-2.221541062
H	-5.685897672	6.881160009	-1.436581582

Merocyanine 2 in n-hexane, excited state

N	4.992671380	0.924924069	-0.178737014
C	6.217248464	0.287530022	-0.125705010
C	7.523276595	0.773946058	-0.223294017
C	8.560992651	-0.159895012	-0.133102010
C	8.304186636	-1.525777117	0.052275004
C	6.997384531	-2.016265153	0.152986012
C	5.958650444	-1.087604083	0.061404004
N	4.583679349	-1.241862092	0.135889010
C	3.969838302	-0.004896000	-0.016501001
C	2.605632197	0.334306026	-0.016616001
C	1.471095115	-0.478437037	-0.104515008
C	0.161824013	0.052789004	-0.033862003
C	-0.978677073	-0.737981056	-0.133475010
C	-2.337110177	-0.325712025	-0.089805007
C	-3.332994253	-1.369713104	-0.226232017
N	-4.693034357	-0.966430076	-0.222567017
C	-5.122422393	0.326099025	-0.014203001
N	-4.149331314	1.286387098	0.153553012
C	-2.747324211	1.047242077	0.077808006
O	-3.057715232	-2.567833193	-0.360517027
O	-1.974898151	2.010525152	0.177069014
S	-6.779314502	0.716597056	0.032486003
C	4.813692369	2.359774183	-0.390300030

C	4.726684363	3.163448244	0.914581072
C	4.550884346	4.664966357	0.656347051
C	4.462610342	5.482405419	1.948351148
C	3.940469303	-2.517253194	0.455870035
C	3.657882281	-3.386827259	-0.776926062
C	3.009459231	-4.725539361	-0.402018030
C	2.732235208	-5.611134452	-1.620239124
C	-5.667669421	-2.061524159	-0.424121032
C	-6.066728441	-2.746269211	0.885973067
C	-7.066924560	-3.884893299	0.652421048
C	-7.475667576	-4.592794348	1.947712151
C	-4.523215345	2.697772207	0.393689030
C	-4.635603354	3.507726268	-0.900969067
C	-5.013035380	4.968852377	-0.629117050
C	-5.122155391	5.803076460	-1.909055144
H	7.729872579	1.829740137	-0.355487027
H	9.587847714	0.183866014	-0.205538016
H	9.135450697	-2.220375168	0.117589009
H	6.805426542	-3.074421236	0.288335022
H	2.412416185	1.401144106	0.044665003
H	1.564476119	-1.548806117	-0.255633020
H	0.037041003	1.121574087	0.104511008
H	-0.850941067	-1.809969139	-0.263334020
H	3.916357300	2.503911191	-0.999040079
H	5.659140407	2.702418208	-0.994602075
H	5.635918416	2.987954229	1.503167114
H	3.889202299	2.787823214	1.515337116
H	3.644758278	4.826794369	0.057725004
H	5.388974413	5.029719387	0.047343004
H	5.368755397	5.367136432	2.553271193
H	3.611621278	5.164379396	2.560262196
H	4.338286333	6.548040496	1.733388131
H	3.025221230	-2.303947173	1.010511075
H	4.608543351	-3.045005231	1.144359089
H	4.599181354	-3.563962273	-1.312083098
H	3.008065230	-2.837549217	-1.469140112
H	2.070338157	-4.537900347	0.135057010
H	3.661439278	-5.260889404	0.301292023
H	3.656911278	-5.844553426	-2.159648163
H	2.052962156	-5.116256393	-2.322582177
H	2.270915173	-6.557567486	-1.322743099
H	-5.181332394	-2.777939210	-1.086253082
H	-6.539153494	-1.633900126	-0.917598070
H	-6.505431515	-2.001037152	1.560162118
H	-5.164088396	-3.138445238	1.368864103
H	-6.630569498	-4.615865354	-0.041703003
H	-7.961535583	-3.486001267	0.155762012
H	-7.945446584	-3.893672297	2.648593204
H	-6.605742513	-5.030428384	2.450350187
H	-8.189522605	-5.400102428	1.753745136
H	-3.739218285	3.113550237	1.026505076
H	-5.470404420	2.695159203	0.930724074
H	-5.390455421	3.044816235	-1.547671116
H	-3.676048280	3.463941264	-1.428858108
H	-4.266185325	5.419618432	0.038510003
H	-5.968238447	5.002501382	-0.088276007
H	-5.885684468	5.396420413	-2.581557199
H	-4.172389319	5.814306448	-2.455711187
H	-5.391814401	6.841036520	-1.687898129

Merocyanine 2 in DCM, ground state

N	5.030619395	0.856656864	-0.244475645
C	6.215159061	0.127884844	-0.224172114
C	7.543365962	0.510197751	-0.408580637
C	8.509169476	-0.493852432	-0.328828800
C	8.158718562	-1.829043190	-0.070733888
C	6.828704996	-2.210329723	0.112739642
C	5.864342115	-1.206725480	0.030579842
N	4.477569452	-1.244435751	0.177368512
C	3.971669202	0.019086989	0.003927235
C	2.632205362	0.475535591	0.080415540
C	1.468434644	-0.261750233	-0.043731616
C	0.172302264	0.282906429	0.050503828
C	-0.943799371	-0.517391159	-0.120776380
C	-2.316075281	-0.183319400	-0.072421870
C	-3.253453028	-1.256471353	-0.300416520
N	-4.638100245	-0.917377472	-0.285262765
C	-5.125998599	0.339443050	-0.008471573
N	-4.204542097	1.330146426	0.236715402
C	-2.785841430	1.148890624	0.187456642
O	-2.936987163	-2.431615275	-0.515053248
O	-2.065936069	2.135656124	0.377953080
S	-6.800019726	0.653008461	0.028751117
C	4.947214753	2.293572558	-0.526294153
C	5.064935318	3.163233403	0.730985274
C	5.008124568	4.659735275	0.400224794
C	5.128052463	5.544578136	1.644323023
C	3.755039563	-2.448898845	0.601963045
C	3.392950840	-3.384816417	-0.557597570
C	2.665488214	-4.644531457	-0.071032105
C	2.312971122	-5.601255401	-1.213558137
C	-5.559767270	-2.040026413	-0.568574781
C	-5.937870976	-2.829826727	0.687358648
C	-6.890854060	-3.988318632	0.368557085
C	-7.274902702	-4.801694026	1.608263155
C	-4.646201065	2.706934477	0.551764386
C	-4.771202764	3.589927276	-0.692849306
C	-5.223690159	5.012510516	-0.341693134
C	-5.343932116	5.919371786	-1.570169431
H	7.820121165	1.540651146	-0.599309734
H	9.553462941	-0.234532108	-0.467582517
H	8.936817085	-2.582920624	-0.014228124
H	6.564827692	-3.243666842	0.305877708
H	2.524585532	1.546266383	0.215109670
H	1.526018136	-1.324436434	-0.262604093
H	0.050512511	1.339548313	0.256810084
H	-0.767689156	-1.572458646	-0.325119298
H	4.006552905	2.479257981	-1.049617173
H	5.750557840	2.524984823	-1.231137114
H	6.007262306	2.929442614	1.241638869
H	4.258579857	2.905019793	1.428589778
H	4.066384114	4.881265451	-0.118675495
H	5.812713889	4.906164855	-0.305118768
H	6.075420124	5.368189442	2.165626644
H	4.316456803	5.343691763	2.352209107
H	5.084989929	6.605493958	1.379508773
H	2.868747762	-2.129432851	1.152990382
H	4.401916082	-2.965884093	1.317135450
H	4.309555395	-3.666983712	-1.089904511
H	2.768990870	-2.849705837	-1.284054061
H	1.749721298	-4.353556722	0.459865663
H	3.293834317	-5.164950188	0.663752458
H	3.212891079	-5.935951650	-1.741317821

H	1.657484667	-5.118083631	-1.946283531
H	1.795751585	-6.489468724	-0.838158929
H	-5.039441907	-2.687319130	-1.274027793
H	-6.445658351	-1.621770468	-1.042928494
H	-6.407920129	-2.152884627	1.410405263
H	-5.023246771	-3.218695883	1.149972442
H	-6.423710460	-4.650299823	-0.373081831
H	-7.799117115	-3.591591697	-0.104528278
H	-7.775259106	-4.173272605	2.353622915
H	-6.389590911	-5.238308009	2.084224011
H	-7.954558963	-5.621186809	1.352857639
H	-3.896502151	3.118120096	1.227189235
H	-5.600865662	2.631392239	1.069405603
H	-5.487830121	3.134705643	-1.386612597
H	-3.800430805	3.624261894	-1.200931386
H	-4.514576045	5.454465971	0.371287581
H	-6.191009528	4.968288644	0.176497193
H	-6.071900143	5.520769394	-2.285701152
H	-4.383652863	6.009172742	-2.090547695
H	-5.667877176	6.927468521	-1.291701953

Merocyanine 2 in DCM, excited state

N	4.979521395	0.929344360	-0.142854429
C	6.209207933	0.307672033	-0.100088130
C	7.509394106	0.813903359	-0.183924025
C	8.557787847	-0.106503627	-0.112363357
C	8.318790446	-1.482473987	0.041032858
C	7.020727068	-1.992961431	0.127723328
C	5.968685655	-1.076737534	0.056375176
N	4.598394980	-1.251953502	0.123906522
C	3.968076745	-0.019256843	-0.004484416
C	2.605044350	0.306121880	-0.007089304
C	1.466735038	-0.514506304	-0.057734068
C	0.166450930	0.024395313	-0.012021854
C	-0.988208910	-0.763343532	-0.078082100
C	-2.337839108	-0.343965995	-0.053093073
C	-3.345351579	-1.385597952	-0.155909521
N	-4.698528185	-0.978082241	-0.179211670
C	-5.125427135	0.325988717	-0.034154711
N	-4.146362265	1.286602912	0.109578715
C	-2.749859557	1.037537887	0.069135304
O	-3.073203203	-2.591412824	-0.235985019
O	-1.970551626	1.998626109	0.151152646
S	-6.782099298	0.727701438	-0.033289957
C	4.785290637	2.370155756	-0.307828607
C	4.667881933	3.124389692	1.023775712
C	4.485025502	4.632655932	0.815169236
C	4.367381022	5.401802728	2.134246147
C	3.971438100	-2.551406865	0.377994782
C	3.669171156	-3.343623747	-0.901222156
C	3.052776834	-4.714812266	-0.596305531
C	2.755973152	-5.523373369	-1.862571892
C	-5.677192865	-2.077662430	-0.341092816
C	-6.079722282	-2.712666779	0.992595684
C	-7.082530473	-3.856917598	0.799976319
C	-7.494416008	-4.515436810	2.120069049
C	-4.514640584	2.709179448	0.294315106
C	-4.582850187	3.482010577	-1.025574740
C	-4.958142004	4.952678487	-0.805615348
C	-5.024609947	5.751532638	-2.110741771
H	7.701714157	1.874777170	-0.293483564

H	9.580086854	0.252132998	-0.174705455
H	9.159666430	-2.166474311	0.091532685
H	6.844172900	-3.056460188	0.238166651
H	2.406593489	1.372975651	0.018116473
H	1.557778603	-1.590164002	-0.158090051
H	0.050111286	1.099223497	0.076374303
H	-0.861748666	-1.839440951	-0.164830320
H	3.898067484	2.525833342	-0.927720284
H	5.636454684	2.742010938	-0.884770237
H	5.568522031	2.935906938	1.621016247
H	3.822445986	2.721771437	1.595128859
H	3.588689768	4.809032995	0.206204321
H	5.331605196	5.024279698	0.235871719
H	5.263970581	5.270769143	2.750157558
H	3.508477732	5.054869038	2.719122545
H	4.238516625	6.473818095	1.955793936
H	3.069832608	-2.383632689	0.969000242
H	4.659788257	-3.113442047	1.015852802
H	4.599287305	-3.471145293	-1.468590815
H	2.992463624	-2.763268268	-1.540237785
H	2.126552857	-4.579159303	-0.022570071
H	3.733564232	-5.282604817	0.051539999
H	3.669450927	-5.703989078	-2.439928856
H	2.050353640	-4.994944324	-2.512900489
H	2.318534907	-6.495732489	-1.616134386
H	-5.195396327	-2.819234176	-0.978178731
H	-6.545953474	-1.666789375	-0.851963184
H	-6.516394480	-1.943060313	1.640247734
H	-5.179315699	-3.088710699	1.492099858
H	-6.647189791	-4.613795652	0.133697375
H	-7.975377219	-3.474789694	0.287245064
H	-7.964051133	-3.790054179	2.793906329
H	-6.626059797	-4.935996434	2.639677546
H	-8.209394904	-5.327800041	1.954113952
H	-3.748376623	3.138563176	0.939499134
H	-5.475499709	2.731060996	0.804798489
H	-5.320197458	3.006265387	-1.682970213
H	-3.609368634	3.418117965	-1.525049911
H	-4.228076170	5.417160245	-0.129103479
H	-5.928044789	5.007248991	-0.293376709
H	-5.771234648	5.331071309	-2.793759890
H	-4.059260827	5.742360673	-2.629349271
H	-5.293603073	6.796464185	-1.925153372

Merocyanine 2 in ethanol, ground state

N	5.026553144	0.856095508	-0.250226373
C	6.212059511	0.128936434	-0.230639113
C	7.539308231	0.512039531	-0.422856291
C	8.505778297	-0.490558971	-0.340570459
C	8.157605543	-1.825105227	-0.072801873
C	6.829304237	-2.207065995	0.118063904
C	5.863654978	-1.204440080	0.033203970
N	4.477521218	-1.242506927	0.184753566
C	3.971618825	0.018602821	0.006029495
C	2.629051238	0.474538567	0.085689252
C	1.469603676	-0.263288852	-0.044820807
C	0.169792257	0.280516530	0.051597897
C	-0.944257438	-0.517349877	-0.124870268
C	-2.319916632	-0.183139468	-0.075363535
C	-3.256210476	-1.253300613	-0.310248688
N	-4.642226462	-0.914633386	-0.292549017

C	-5.129164222	0.340185850	-0.010747836
N	-4.208828538	1.328860801	0.239749227
C	-2.788981165	1.145932915	0.192237401
O	-2.941455816	-2.428238050	-0.532866091
O	-2.069644083	2.132381967	0.390881655
S	-6.805751245	0.654485617	0.026099537
C	4.940785250	2.292950024	-0.535499605
C	5.066776823	3.164560432	0.719542118
C	5.008898225	4.660275851	0.385588617
C	5.136280079	5.547559415	1.627225121
C	3.756600599	-2.446215625	0.616164262
C	3.397907262	-3.389520057	-0.538332116
C	2.676858873	-4.649660714	-0.043463975
C	2.324698806	-5.612983398	-1.180566015
C	-5.563298681	-2.036663052	-0.580344921
C	-5.937030325	-2.834584470	0.671845409
C	-6.890133796	-3.991946169	0.349127003
C	-7.269336551	-4.813173013	1.585141829
C	-4.649000460	2.704835829	0.560711789
C	-4.768292580	3.595007520	-0.679408908
C	-5.220796083	5.016099116	-0.322103954
C	-5.335309913	5.929903154	-1.545968721
H	7.814317202	1.541418273	-0.621422078
H	9.549316678	-0.231310622	-0.484947605
H	8.936946998	-2.577560985	-0.014660555
H	6.567311597	-3.239342866	0.318851556
H	2.521040563	1.544200073	0.228705300
H	1.528942882	-1.324452664	-0.270237095
H	0.049516448	1.336114244	0.264227278
H	-0.767646484	-1.571028180	-0.335501707
H	3.996696371	2.476881351	-1.052899755
H	5.739457713	2.522320119	-1.245998454
H	6.012089937	2.931447397	1.224739747
H	4.264329368	2.908463710	1.422406712
H	4.064362260	4.880966598	-0.128544972
H	5.809857443	4.904412405	-0.324489244
H	6.086559464	5.371533895	2.143326162
H	4.328636971	5.348375934	2.340186554
H	5.092339857	6.608032474	1.360513104
H	2.869123636	-2.124748791	1.163950056
H	4.403980461	-2.957254260	1.334895607
H	4.315146994	-3.670919298	-1.069699693
H	2.770732509	-2.861430590	-1.267130825
H	1.761729933	-4.359661872	0.489098165
H	3.309869869	-5.163987578	0.691408732
H	3.224498524	-5.946548213	-1.709193661
H	1.665513799	-5.135517117	-1.913839394
H	1.812057944	-6.501601435	-0.799629893
H	-5.044359578	-2.678906921	-1.291292571
H	-6.450824656	-1.617063378	-1.050310157
H	-6.404954302	-2.162700018	1.401108741
H	-5.020768681	-3.225395728	1.129496918
H	-6.424912063	-4.648896937	-0.398109100
H	-7.800251565	-3.593262839	-0.118790646
H	-7.767850201	-4.189859164	2.336033016
H	-6.382055162	-5.251879780	2.055434567
H	-7.949020118	-5.631640600	1.326740821
H	-3.901020325	3.111060776	1.240922946
H	-5.605085216	2.628813294	1.075521833
H	-5.482157923	3.144507858	-1.379181837
H	-3.795699616	3.631300295	-1.183826086
H	-4.514075750	5.453242619	0.396118320

H	-6.190069286	4.970064521	0.192314173
H	-6.060873306	5.536155645	-2.266650740
H	-4.372881206	6.021699161	-2.061958265
H	-5.659312337	6.936635512	-1.262860824

Merocyanine 2 in ethanol, excited state

N	4.979304405	0.931100255	-0.142041345
C	6.209121148	0.311131992	-0.098702596
C	7.508828680	0.819270359	-0.181544384
C	8.558012377	-0.099580535	-0.109350239
C	8.320686330	-1.476527802	0.043673110
C	7.023714962	-1.988941451	0.129304311
C	5.970293560	-1.074111079	0.057341819
N	4.600751751	-1.251380726	0.123762914
C	3.968879221	-0.019221518	-0.004861883
C	2.606684937	0.305083105	-0.009005875
C	1.467217124	-0.516663990	-0.053237090
C	0.168825220	0.022903713	-0.011315926
C	-0.988172392	-0.764715387	-0.073567690
C	-2.336657858	-0.345573470	-0.050036814
C	-3.345235192	-1.386844683	-0.151252701
N	-4.697997135	-0.979522572	-0.176105330
C	-5.124682212	0.324790680	-0.034599191
N	-4.146056570	1.285778560	0.107061166
C	-2.749913179	1.036382006	0.069303178
O	-3.073519195	-2.593313380	-0.228703381
O	-1.970558775	1.997683391	0.150841038
S	-6.782903541	0.726594632	-0.035254638
C	4.783424001	2.372394991	-0.303634183
C	4.657833772	3.121688179	1.029950174
C	4.474318531	4.630341125	0.824989480
C	4.348865095	5.395012590	2.145963385
C	3.975421852	-2.552847698	0.373022901
C	3.671612796	-3.339011274	-0.909496784
C	3.061342785	-4.713991141	-0.609526750
C	2.762057183	-5.516361929	-1.879163684
C	-5.676606696	-2.079607167	-0.336414012
C	-6.078609052	-2.713520569	0.997919085
C	-7.083020068	-3.856726184	0.807143660
C	-7.494137502	-4.513822835	2.128182173
C	-4.514379673	2.709093949	0.287946943
C	-4.579968314	3.479482142	-1.033510081
C	-4.957421910	4.950194058	-0.817168076
C	-5.021395407	5.746551334	-2.123934509
H	7.699704395	1.880378659	-0.290905008
H	9.579894921	0.260297146	-0.170902626
H	9.162559231	-2.159219614	0.094659992
H	6.848730069	-3.052638179	0.239730718
H	2.408008308	1.371978374	0.008564309
H	1.558210433	-1.592927418	-0.145425355
H	0.053740836	1.098356133	0.070744925
H	-0.860705859	-1.840975084	-0.156222903
H	3.899501777	2.528623673	-0.927947189
H	5.637111076	2.747216888	-0.874513649
H	5.555611429	2.932567697	1.631150055
H	3.809688507	2.716289097	1.595287332
H	3.581002548	4.807460386	0.211815681
H	5.323650498	5.024555045	0.251656693
H	5.242545353	5.262964377	2.765881319
H	3.487464262	5.044909996	2.725378436
H	4.219592030	6.467523003	1.970415136

H	3.075276371	-2.389052909	0.967261519
H	4.665731214	-3.117045040	1.006497932
H	4.600420962	-3.460491050	-1.480169123
H	2.990650414	-2.757836978	-1.543266843
H	2.137193797	-4.584768740	-0.030961494
H	3.747242718	-5.282804206	0.031846859
H	3.673895645	-5.690418540	-2.461091327
H	2.052097602	-4.986537740	-2.523736255
H	2.329095190	-6.491766518	-1.636547202
H	-5.195509761	-2.821516681	-0.973505043
H	-6.545443506	-1.669574096	-0.847661767
H	-6.513329591	-1.943217595	1.646067181
H	-5.178332043	-3.090134303	1.497164275
H	-6.649384237	-4.614476645	0.140806370
H	-7.975973232	-3.474018191	0.294986061
H	-7.962368825	-3.787513768	2.802026887
H	-6.625647938	-4.934887744	2.647126726
H	-8.210048067	-5.325533734	1.963348079
H	-3.749892737	3.139826470	0.934214516
H	-5.475924426	2.732423580	0.796929703
H	-5.314650410	3.001917651	-1.692644695
H	-3.605300907	3.415801936	-1.530687358
H	-4.229641418	5.416602387	-0.139608977
H	-5.928588572	5.004754434	-0.307260754
H	-5.765832489	5.324127022	-2.808172313
H	-4.054679322	5.737526427	-2.639941637
H	-5.291943679	6.791442610	-1.940664547

Merocyanine 3 in vacuum, ground state

N	6.326340471	0.899100071	-0.221515017
C	7.480627554	0.123974010	-0.203750016
C	8.824726654	0.458027035	-0.341483026
C	9.755941767	-0.584835043	-0.284274022
C	9.352030721	-1.910355148	-0.090567007
C	8.000089585	-2.244437170	0.048923004
C	7.074880528	-1.206922090	-0.009838001
N	5.684734435	-1.202125093	0.109189008
C	5.213076398	0.094211007	-0.024832002
C	3.910808300	0.588560043	0.029717002
C	2.691139208	-0.110381008	-0.045346003
C	1.441019109	0.474729036	0.049281004
C	0.242927018	-0.255376020	-0.070226005
C	-1.033642079	0.272568021	0.013304001
C	-2.161803163	-0.555915041	-0.118892009
C	-3.511157268	-0.227536017	-0.069054005
C	-4.457341340	-1.321819102	-0.255512020
N	-5.833014451	-0.982877074	-0.247160019
C	-6.329998461	0.284300022	0.003314000
N	-5.403102387	1.289212100	0.217708017
C	-3.992685302	1.123274085	0.154334012
O	-4.126663314	-2.493173189	-0.428356033
O	-3.271941248	2.109631160	0.300709023
S	-7.988318619	0.588037047	0.045031003
C	6.298796477	2.337516178	-0.466361036
C	6.354619491	3.180037242	0.814870060
C	6.337776467	4.685404357	0.522369040
C	6.398001495	5.538940441	1.792441137
C	4.921891378	-2.381823183	0.513545039
C	4.487556345	-3.270872252	-0.658914053
C	3.698152284	-4.500698345	-0.192772015
C	3.271118251	-5.407781425	-1.350348101

C	-6.756322492	-2.113012164	-0.493835038
C	-7.135227531	-2.858116220	0.788709061
C	-8.093098625	-4.022389307	0.508969039
C	-8.478264625	-4.794093368	1.774632137
C	-5.854933449	2.670428205	0.498548038
C	-6.007931451	3.512042270	-0.771146060
C	-6.478364469	4.937289378	-0.457179035
C	-6.627009511	5.805036427	-1.710468131
H	9.144943714	1.484677116	-0.480682037
H	10.811556820	-0.357099027	-0.390337030
H	10.098128784	-2.697086208	-0.049456004
H	7.692334597	-3.274430249	0.190798015
H	3.836382292	1.667831130	0.106555008
H	2.703823206	-1.181650088	-0.226215017
H	1.371947105	1.547656119	0.222565017
H	0.334197025	-1.330050100	-0.242065018
H	-1.177129088	1.333416101	0.180946014
H	-1.979567150	-1.616629124	-0.286761022
H	7.151150527	2.570091198	-1.112837085
H	5.397611432	2.563962198	-1.044048080
H	5.506291422	2.915111224	1.458086112
H	7.261110544	2.917571221	1.375009105
H	7.184123562	4.938984375	-0.130448010
H	5.431049402	4.935577378	-0.044529003
H	6.384436512	6.606359480	1.552756118
H	5.544877439	5.334087408	2.448208189
H	7.311032543	5.336848390	2.363168183
H	5.558318435	-2.952404224	1.198987093
H	4.061978311	-2.042753158	1.095379083
H	3.883600297	-2.682421203	-1.360649102
H	5.378336416	-3.587721273	-1.215966094
H	4.306312327	-5.075295386	0.519016040
H	2.809346213	-4.173527320	0.363368028
H	2.710082208	-6.273908478	-0.987308076
H	2.631785201	-4.871126373	-2.059527156
H	4.140185316	-5.780765447	-1.903418147
H	-7.641916599	-1.706785132	-0.980157076
H	-6.234205473	-2.784785213	-1.175361091
H	-6.220632500	-3.235548247	1.260885099
H	-7.603610569	-2.154220165	1.486395116
H	-9.000822713	-3.636911278	0.025650002
H	-7.630093562	-4.710328362	-0.211588016
H	-9.162246699	-5.618749419	1.548312119
H	-7.593986582	-5.218965400	2.263024172
H	-8.973935694	-4.139805314	2.500494193
H	-6.802592533	2.598407197	1.030002081
H	-5.098228388	3.109635236	1.148727087
H	-5.043181386	3.545953271	-1.290744100
H	-6.727917527	3.024356232	-1.438508110
H	-7.439240549	4.893454372	0.072843006
H	-5.768096415	5.411867415	0.233628018
H	-6.963770557	6.816420517	-1.459805113
H	-5.674501417	5.893757437	-2.245160169
H	-7.356449551	5.373650392	-2.405057182

Merocyanine 3 in vacuum, excited state

N	6.292965632	0.977862786	-0.144443792
C	7.499512091	0.293810192	-0.127375426
C	8.817380774	0.735347166	-0.205962704
C	9.828947378	-0.235751200	-0.167948597
C	9.526404573	-1.593567908	-0.048362336

C	8.198145336	-2.038328987	0.033514867
C	7.194123318	-1.075734806	-0.006744355
N	5.809212958	-1.186727871	0.068895946
C	5.230787902	0.079040069	-0.018202789
C	3.890445194	0.460043565	0.009982670
C	2.725558076	-0.312166422	-0.095228807
C	1.424468625	0.224210127	-0.003619293
C	0.263067166	-0.504756266	-0.130772195
C	-1.060371515	0.036625301	-0.040466222
C	-2.171647802	-0.734507060	-0.172534664
C	-3.579177569	-0.341031726	-0.107058291
C	-4.531224813	-1.377026948	-0.273247441
N	-5.962857032	-0.974953661	-0.199534444
C	-6.339039137	0.284427477	-0.003179374
N	-5.443625934	1.252593685	0.144067681
C	-3.968236520	0.997306145	0.109437552
O	-4.339812047	-2.573599834	-0.469605337
O	-3.274983933	1.997572189	0.274081301
S	-8.071708593	0.675983041	0.063224633
C	6.161192295	2.416157796	-0.323247190
C	6.102746626	3.198699910	0.996052196
C	5.970963922	4.709942586	0.773403075
C	5.914276179	5.503174197	2.082173539
C	5.131605941	-2.436611137	0.396970457
C	4.792189166	-3.295181438	-0.828901608
C	4.097495868	-4.607567056	-0.445829994
C	3.765042029	-5.482183270	-1.658155954
C	-6.941074674	-2.069602293	-0.339518831
C	-7.253962841	-2.766635148	0.988323938
C	-8.267314042	-3.904570385	0.813309702
C	-8.577137425	-4.629096405	2.126451520
C	-5.841825834	2.658891596	0.337289243
C	-5.927090207	3.443974327	-0.975607591
C	-6.337250518	4.903682982	-0.744460286
C	-6.407626065	5.712297373	-2.043101817
H	9.059677595	1.789409142	-0.285162066
H	10.865672549	0.079381350	-0.229708845
H	10.330185603	-2.322194882	-0.019916293
H	7.968621478	-3.094767292	0.117556257
H	3.734546026	1.530198318	0.111225001
H	2.793820894	-1.377856745	-0.290554629
H	1.334897522	1.295571244	0.181545445
H	0.348756282	-1.577635635	-0.312434365
H	-1.164545761	1.101389330	0.140412119
H	-2.035602422	-1.798514584	-0.353645902
H	7.014729903	2.748675930	-0.923672210
H	5.265089336	2.602477057	-0.924012349
H	5.257568483	2.833599978	1.592577373
H	7.008047188	2.983263592	1.577894890
H	6.815784393	5.063909227	0.166701381
H	5.067266402	4.912923120	0.183065499
H	5.820144966	6.576785351	1.892181582
H	5.058589641	5.196748687	2.693643867
H	6.819905202	5.348273380	2.679052053
H	5.792465821	-2.993480195	1.071340449
H	4.232836876	-2.193169018	0.967402867
H	4.153422347	-2.718414644	-1.508869205
H	5.715624469	-3.508614048	-1.382255436
H	4.737639829	-5.169987262	0.247722222
H	3.175483042	-4.382953190	0.107037284
H	3.270192069	-6.409755263	-1.354518706
H	3.096635838	-4.959936598	-2.351201855

H	4.670852877	-5.752906276	-2.212072578
H	-7.846833821	-1.667683272	-0.807605901
H	-6.491066046	-2.778627088	-1.034616633
H	-6.315214307	-3.162859227	1.389104492
H	-7.636336584	-2.037376314	1.713067333
H	-9.198363892	-3.505839751	0.387312522
H	-7.878953557	-4.624144983	0.080692055
H	-9.299402086	-5.437130866	1.973746650
H	-7.671088765	-5.068190065	2.557797045
H	-8.997926368	-3.941819049	2.868878204
H	-6.792777724	2.678828217	0.881758398
H	-5.078309558	3.094814277	0.981746698
H	-4.943477116	3.405379922	-1.455150285
H	-6.640184755	2.961461436	-1.655233912
H	-7.313016217	4.936191240	-0.240343453
H	-5.622095301	5.375068482	-0.057638746
H	-6.698782880	6.749580668	-1.850231468
H	-5.437622260	5.726716765	-2.551703860
H	-7.139262190	5.284403332	-2.737510550

Merocyanine 3 in n-hexane, ground state

N	6.321255077	0.888190330	-0.228925659
C	7.474215884	0.110808972	-0.213521964
C	8.818320805	0.441671375	-0.367457508
C	9.745537454	-0.602692203	-0.306973959
C	9.339435879	-1.926836363	-0.095312476
C	7.989717499	-2.257198772	0.059698599
C	7.066895667	-1.216330830	-0.002474511
N	5.677875980	-1.204889621	0.127992782
C	5.214282536	0.088088957	-0.015194347
C	3.907259875	0.590705180	0.050136751
C	2.694142892	-0.102493356	-0.030038321
C	1.438274436	0.487853256	0.067468144
C	0.247838953	-0.239300979	-0.056574852
C	-1.037308664	0.287938250	0.028151630
C	-2.157683000	-0.537140128	-0.110682622
C	-3.516720625	-0.213997040	-0.063322842
C	-4.453761615	-1.307020290	-0.258269317
N	-5.834663738	-0.976060191	-0.248210724
C	-6.335331457	0.285955151	0.005280895
N	-5.416145336	1.292757984	0.222124036
C	-4.001581486	1.129031835	0.164199155
O	-4.121949493	-2.479285218	-0.439927378
O	-3.287068616	2.121149137	0.319190478
S	-8.001333310	0.582912039	0.048120568
C	6.298299421	2.328672266	-0.478749334
C	6.390184965	3.171877985	0.799369390
C	6.386234815	4.676245558	0.500931525
C	6.482467445	5.532671331	1.766772426
C	4.909349094	-2.384580276	0.528650756
C	4.472724591	-3.265370179	-0.648875973
C	3.674721622	-4.491638598	-0.187967165
C	3.244536291	-5.391046089	-1.350314588
C	-6.751110996	-2.110107452	-0.502302941
C	-7.126968662	-2.866565117	0.774456005
C	-8.074017552	-4.037466139	0.485332836
C	-8.456122738	-4.819428248	1.745666779
C	-5.871909561	2.672076952	0.505373982
C	-6.016875499	3.519412629	-0.761548345
C	-6.490562533	4.943119673	-0.445164106
C	-6.631290979	5.815462806	-1.696229252

H	9.139229340	1.465817244	-0.521151782
H	10.800909139	-0.379868575	-0.424533843
H	10.084592748	-2.714280801	-0.052485526
H	7.681300775	-3.284699431	0.216148559
H	3.839862448	1.669386482	0.140208373
H	2.702864024	-1.172721931	-0.216065499
H	1.373421107	1.560072941	0.246136185
H	0.338436085	-1.313022716	-0.234300521
H	-1.178296575	1.348016202	0.201778747
H	-1.971689373	-1.596150245	-0.283865021
H	7.137888340	2.550854764	-1.144426289
H	5.387084880	2.559615171	-1.037284893
H	5.551522953	2.920322197	1.460429822
H	7.304918429	2.900673607	1.341356506
H	7.222860395	4.916072042	-0.169076096
H	5.471564747	4.935443295	-0.048579527
H	6.478121629	6.599346294	1.523268795
H	5.639592494	5.340889981	2.439593622
H	7.403919872	5.320173221	2.319935936
H	5.544446583	-2.958607192	1.211407862
H	4.051804196	-2.043638254	1.112417516
H	3.873786890	-2.671322631	-1.350208996
H	5.362772201	-3.586435299	-1.204381473
H	4.278462433	-5.072454783	0.522166690
H	2.787116387	-4.160612061	0.367594707
H	2.677885567	-6.255338695	-0.991501573
H	2.609662676	-4.847365176	-2.058229777
H	4.112637333	-5.766556827	-1.903192120
H	-7.638590508	-1.707106988	-0.987408228
H	-6.225545805	-2.774106072	-1.188484274
H	-6.210742812	-3.238781515	1.247552928
H	-7.602581637	-2.171463463	1.475993587
H	-8.983557988	-3.657232727	0.001326151
H	-7.602824477	-4.717134068	-0.237688779
H	-9.132248593	-5.648543897	1.512301438
H	-7.569544731	-5.239408078	2.234133422
H	-8.959655793	-4.173421886	2.473568654
H	-6.822748630	2.597209738	1.030398937
H	-5.121208709	3.109564056	1.163344143
H	-5.048857526	3.556068113	-1.274700605
H	-6.730949554	3.034427602	-1.437252886
H	-7.454897316	4.896623397	0.078290288
H	-5.785248584	5.415296536	0.252231766
H	-6.970158838	6.825592270	-1.443509660
H	-5.675202736	5.906639993	-2.224082716
H	-7.356058648	5.386393880	-2.397158142

Merocyanine 3 in n-hexane, excited state

N	6.246642302	0.965294683	-0.181221848
C	7.459438450	0.302005046	-0.128382648
C	8.774367184	0.760783547	-0.225649478
C	9.792681538	-0.193782858	-0.137101350
C	9.507236768	-1.554013565	0.046448228
C	8.190460201	-2.015953219	0.146572560
C	7.172283750	-1.066072723	0.057110605
N	5.792411422	-1.191003232	0.132612658
C	5.205728957	0.057748015	-0.018878677
C	3.852101026	0.427376232	-0.015052632
C	2.699246214	-0.363608355	-0.095585763
C	1.401772408	0.174903116	-0.028492924
C	0.227346481	-0.572140631	-0.121546348

C	-1.064455012	-0.014674084	-0.055516841
C	-2.219364969	-0.789609758	-0.150506825
C	-3.567452594	-0.369122368	-0.095488005
C	-4.575199930	-1.404734197	-0.227661320
N	-5.931213714	-0.988360192	-0.215100665
C	-6.349303059	0.308731793	-0.003259191
N	-5.364828478	1.259732546	0.162920730
C	-3.965744772	1.007738747	0.083223539
O	-4.314305089	-2.604781328	-0.362566565
O	-3.185460562	1.962494384	0.183496614
S	-7.998593125	0.713569956	0.049865402
C	6.098275819	2.403196922	-0.395487605
C	6.027731888	3.211125034	0.907570272
C	5.883338678	4.715501371	0.646669902
C	5.812784746	5.537350845	1.936954216
C	5.124505414	-2.452307767	0.457110980
C	4.815123999	-3.316278174	-0.773038810
C	4.146398895	-4.643557523	-0.393080999
C	3.840307163	-5.522554573	-1.609198264
C	-6.917172796	-2.074221455	-0.412208215
C	-7.311744022	-2.759357045	0.898953113
C	-8.326457484	-3.886145713	0.670547057
C	-8.730534056	-4.594882672	1.966858990
C	-5.724447071	2.674382276	0.406479859
C	-5.826354226	3.488595966	-0.886189019
C	-6.190698583	4.952549262	-0.611562791
C	-6.288405394	5.791240776	-1.889509824
H	9.003153263	1.812218677	-0.356726105
H	10.826290014	0.128854450	-0.209666402
H	10.323269150	-2.266453436	0.110665920
H	7.976485211	-3.070117321	0.280475872
H	3.683874102	1.498581576	0.041221167
H	2.775467698	-1.435766390	-0.242728116
H	1.305867922	1.252180419	0.107217463
H	0.313616461	-1.651511689	-0.252351133
H	-1.168682530	1.056897964	0.075588872
H	-2.100551622	-1.862680892	-0.282663215
H	6.951138514	2.726740089	-0.999811481
H	5.205041196	2.565080408	-1.005878446
H	5.183064005	2.853809024	1.509560882
H	6.933013558	3.017929517	1.496566268
H	6.728605034	5.061308405	0.036654292
H	4.980848836	4.895348323	0.047490772
H	5.710130868	6.604820263	1.719877903
H	4.956230817	5.238118680	2.550662006
H	6.716902015	5.404889895	2.541277693
H	5.786216238	-2.994097295	1.140749322
H	4.218476821	-2.219913112	1.019541760
H	4.170037793	-2.755262028	-1.460398728
H	5.748400332	-3.510426353	-1.316187588
H	4.795969138	-5.191674988	0.302460203
H	3.216910550	-4.440043345	0.155219706
H	3.364838304	-6.460777263	-1.308066960
H	3.163772651	-5.014619197	-2.304953753
H	4.755023482	-5.772395133	-2.157939005
H	-7.788530448	-1.637564313	-0.897513862
H	-6.442786612	-2.793055042	-1.080500211
H	-6.409066115	-3.163256221	1.371948614
H	-7.736238475	-2.012002736	1.579652599
H	-9.221414060	-3.475505401	0.184158959
H	-7.904864615	-4.619091076	-0.030631247
H	-9.455116460	-5.393575874	1.776765293

H	-7.860639791	-5.044004590	2.459334887
H	-9.185733119	-3.893444158	2.675037228
H	-6.671944227	2.680407155	0.942518090
H	-4.937179981	3.080574911	1.041629581
H	-4.865873230	3.437246574	-1.411663271
H	-6.583973378	3.034548874	-1.535770343
H	-7.147066496	4.993802629	-0.073274142
H	-5.441464986	5.394562154	0.059269938
H	-6.548921153	6.831188425	-1.666478230
H	-5.337034026	5.794898555	-2.433475667
H	-7.053801811	5.393486707	-2.565241045

Merocyanine 3 in DCM, ground state

N	6.305861999	0.881156226	-0.244807411
C	7.461679622	0.107870869	-0.236617695
C	8.802431041	0.440801695	-0.426138703
C	9.730020125	-0.599715523	-0.359691436
C	9.330714721	-1.922532765	-0.109465734
C	7.988139175	-2.254428724	0.079240680
C	7.061980563	-1.214585476	0.010557870
N	5.675857010	-1.201300852	0.165280322
C	5.216184156	0.082331847	0.003710171
C	3.896906443	0.588629292	0.089393905
C	2.701746788	-0.104402419	-0.012389466
C	1.430903351	0.486370959	0.094498707
C	0.256310426	-0.237407595	-0.048090891
C	-1.044956270	0.288306998	0.043289338
C	-2.154816854	-0.526119261	-0.114977837
C	-3.530048769	-0.205582336	-0.066554514
C	-4.457487435	-1.290213573	-0.283606813
N	-5.845611833	-0.965517192	-0.268315534
C	-6.346311673	0.288184001	-0.000940356
N	-5.434869638	1.290668031	0.232839166
C	-4.014207560	1.124227609	0.182146946
O	-4.129539164	-2.463845250	-0.488894510
O	-3.305048466	2.120481987	0.362256373
S	-8.023825196	0.583612485	0.038819779
C	6.276064134	2.322514066	-0.512700495
C	6.416633720	3.175951416	0.753379659
C	6.417421771	4.676291734	0.435276027
C	6.560489232	5.545906371	1.687607600
C	4.909482066	-2.381194881	0.580662099
C	4.484793262	-3.277446607	-0.589103265
C	3.689502569	-4.500208126	-0.114663426
C	3.273711066	-5.418324488	-1.267586933
C	-6.755824324	-2.100212107	-0.540364760
C	-7.122309574	-2.884076608	0.722674202
C	-8.063086390	-4.055579590	0.415401752
C	-8.435329829	-4.863106713	1.662524948
C	-5.890266032	2.665716543	0.535875723
C	-6.025199192	3.536130746	-0.716573227
C	-6.494841143	4.956276400	-0.378283868
C	-6.625779280	5.850408878	-1.614972810
H	9.117173233	1.461383723	-0.611076308
H	10.782552351	-0.378983125	-0.502883745
H	10.079864126	-2.705868645	-0.063406034
H	7.686262605	-3.278419717	0.266225479
H	3.832095872	1.663972872	0.214975326
H	2.713352132	-1.169845805	-0.222388824
H	1.368942199	1.554800404	0.295450064
H	0.347920157	-1.306900865	-0.247803611

H	-1.179974866	1.345463705	0.238892507
H	-1.966932117	-1.580958588	-0.309131905
H	7.092062808	2.531656668	-1.209773594
H	5.346672037	2.547586136	-1.040958844
H	5.596532812	2.941663307	1.443428987
H	7.346038676	2.902997621	1.268210690
H	7.235874186	4.898609278	-0.262066001
H	5.488553876	4.936738118	-0.088820733
H	6.558729930	6.609807546	1.431454246
H	5.736750283	5.369477565	2.387963211
H	7.496700731	5.330239284	2.214207920
H	5.545586642	-2.940194363	1.273455958
H	4.048528356	-2.034732307	1.155247514
H	3.887062926	-2.696396420	-1.302216795
H	5.379432712	-3.603399795	-1.133612023
H	4.291722752	-5.066707580	0.607639122
H	2.796091657	-4.164556469	0.428213916
H	2.708691276	-6.280513509	-0.900541232
H	2.642220692	-4.887590733	-1.988470785
H	4.148772863	-5.796852648	-1.807284591
H	-7.647346222	-1.695337710	-1.015739833
H	-6.230289244	-2.747412562	-1.242017247
H	-6.202370434	-3.258999372	1.186214003
H	-7.598267043	-2.206558218	1.441297874
H	-8.976736470	-3.672778965	-0.058812969
H	-7.590255988	-4.718344672	-0.321920932
H	-9.106393945	-5.692162549	1.415358177
H	-7.544142794	-5.285955223	2.139939163
H	-8.940962500	-4.234256410	2.403957594
H	-6.843841953	2.585214729	1.054767190
H	-5.144382301	3.090643773	1.207013855
H	-5.054807526	3.577658677	-1.224813012
H	-6.736081250	3.066279230	-1.406450796
H	-7.461653428	4.905142352	0.140241606
H	-5.791189393	5.413176864	0.330663015
H	-6.961751957	6.857084772	-1.345733009
H	-5.666590905	5.946866989	-2.136151942
H	-7.348875754	5.436629523	-2.326834169

Merocyanine 3 in DCM, excited state

N	6.227386336	0.975302383	-0.152735418
C	7.449798905	0.333514270	-0.109672530
C	8.756811781	0.817834331	-0.199690148
C	9.790604358	-0.118910543	-0.125854309
C	9.529273772	-1.489153347	0.035611880
C	8.222777955	-1.976655114	0.127861983
C	7.187134898	-1.043509870	0.054061519
N	5.811447515	-1.194769386	0.125613354
C	5.204209023	0.045517262	-0.007039251
C	3.845786730	0.395360215	-0.002495348
C	2.700151451	-0.408983166	-0.060922723
C	1.402253764	0.128117057	-0.009193788
C	0.226041073	-0.622909378	-0.080433653
C	-1.061262237	-0.057273379	-0.030878703
C	-2.226751103	-0.823086050	-0.104913798
C	-3.571264993	-0.391857711	-0.067105262
C	-4.588666856	-1.420857710	-0.174508958
N	-5.940461087	-0.996691950	-0.183655597
C	-6.349991095	0.309627207	-0.022284582
N	-5.360937809	1.257591283	0.124281700
C	-3.964713480	0.991355245	0.072227604

O	-4.336409469	-2.628809875	-0.270234946
O	-3.177218621	1.943555374	0.159246970
S	-8.000988287	0.729720837	-0.005180951
C	6.055784632	2.417564027	-0.331396727
C	5.959095164	3.187179150	0.992793390
C	5.798546121	4.695893200	0.769653838
C	5.701619105	5.480713163	2.081142374
C	5.164826493	-2.480787489	0.398156098
C	4.852653245	-3.287788461	-0.869170324
C	4.220464024	-4.647175978	-0.544498867
C	3.911450869	-5.469589275	-1.798878250
C	-6.933036472	-2.082897623	-0.349982551
C	-7.335486459	-2.725713586	0.980029698
C	-8.355970440	-3.853456202	0.783011949
C	-8.767711086	-4.519807200	2.099218455
C	-5.711326809	2.682466765	0.324139152
C	-5.781315845	3.467054806	-0.988701633
C	-6.135231441	4.940697274	-0.753772636
C	-6.202740594	5.750783852	-2.051912755
H	8.966413598	1.874831865	-0.315636649
H	10.818325685	0.222886986	-0.192991912
H	10.358310685	-2.187287885	0.087995370
H	8.028550061	-3.036469983	0.244500937
H	3.665646312	1.465118381	0.035311030
H	2.781125460	-1.484116653	-0.175051797
H	1.305271481	1.209031322	0.093927342
H	0.310899436	-1.705244866	-0.179829745
H	-1.154388813	1.018633850	0.069217754
H	-2.112923648	-1.899744451	-0.206452550
H	6.909409078	2.769503236	-0.917180121
H	5.167485085	2.580941067	-0.947708282
H	5.111510282	2.803873018	1.574236126
H	6.860524424	2.990773892	1.586257753
H	6.647321345	5.067947050	0.180820384
H	4.901232505	4.880065616	0.164349892
H	5.588309133	6.552664712	1.892155917
H	4.841403042	5.153458517	2.675407366
H	6.600119316	5.342162441	2.692567277
H	5.844106853	-3.043536510	1.045131396
H	4.265286792	-2.290381503	0.985710400
H	4.183325142	-2.709019520	-1.517440675
H	5.781095284	-3.434814205	-1.434526771
H	4.895912167	-5.214057233	0.109647651
H	3.297307862	-4.492882551	0.029566199
H	3.463029158	-6.433195275	-1.538243284
H	3.211084108	-4.941881562	-2.455502077
H	4.821575474	-5.669088569	-2.375251257
H	-7.799760330	-1.657087614	-0.852085307
H	-6.463703296	-2.824020409	-0.996667269
H	-6.437053347	-3.119727524	1.469114193
H	-7.756439764	-1.956793695	1.638755898
H	-9.246955646	-3.453289434	0.280887053
H	-7.936403474	-4.609479476	0.105724861
H	-9.495527345	-5.320060242	1.930202046
H	-7.901742576	-4.958164409	2.607979749
H	-9.221904289	-3.794840344	2.784011710
H	-6.667456328	2.711336157	0.843169094
H	-4.934824592	3.097462714	0.966367828
H	-4.813074327	3.394493328	-1.497085486
H	-6.530402860	3.006490922	-1.643617608
H	-7.099716721	5.003972130	-0.232365457
H	-5.393062360	5.390099338	-0.080257748

H	-6.456158710	6.797683303	-1.855737510
H	-5.242252686	5.732960633	-2.579235561
H	-6.960922419	5.345675278	-2.731484274

Merocyanine 3 in ethanol, ground state

N	6.299756193	0.882890530	-0.249086040
C	7.457620303	0.112754492	-0.244909659
C	8.796544843	0.448606730	-0.444886058
C	9.726235555	-0.589314253	-0.379036968
C	9.331539232	-1.912578803	-0.119796617
C	7.991705407	-2.247339215	0.078854666
C	7.062710457	-1.209412838	0.010802475
N	5.677614408	-1.198439966	0.173214784
C	5.216227379	0.082135483	0.008570521
C	3.892871048	0.586415685	0.100716734
C	2.703709628	-0.108712418	-0.008707644
C	1.428070665	0.480305142	0.101686047
C	0.257945702	-0.243011486	-0.047128547
C	-1.047573020	0.282412130	0.046658413
C	-2.155599444	-0.528183112	-0.117521704
C	-3.534785414	-0.206714684	-0.068310875
C	-4.461242810	-1.287868694	-0.292023679
N	-5.850798352	-0.963145848	-0.274754146
C	-6.350071054	0.288956291	-0.003633459
N	-5.439330814	1.289041721	0.235211590
C	-4.017388677	1.120059682	0.187081746
O	-4.135571198	-2.461873705	-0.504629662
O	-3.308373340	2.116143200	0.375033506
S	-8.030225065	0.586164289	0.034508788
C	6.264672006	2.324638120	-0.519577894
C	6.415176472	3.179132983	0.744533794
C	6.409782727	4.679041826	0.424581100
C	6.562143599	5.549906528	1.674978711
C	4.915017715	-2.379461169	0.594979228
C	4.496475813	-3.284041765	-0.570448317
C	3.708894412	-4.508937635	-0.088850088
C	3.299717979	-5.436277938	-1.236752939
C	-6.760713128	-2.097115774	-0.550630497
C	-7.123144562	-2.888120830	0.709217933
C	-8.064502522	-4.058361755	0.398727580
C	-8.432252452	-4.872806786	1.642675901
C	-5.892748667	2.663744845	0.542717651
C	-6.022523249	3.539821646	-0.706374839
C	-6.491022653	4.959309051	-0.363615539
C	-6.616468195	5.858915984	-1.596891607
H	9.107573587	1.468858764	-0.637337628
H	10.777370224	-0.367112062	-0.529880377
H	10.083188364	-2.693555812	-0.074725484
H	7.693580650	-3.271066587	0.272729296
H	3.826371090	1.660208458	0.238102917
H	2.718093169	-1.172275527	-0.227460839
H	1.365949675	1.547278811	0.310345973
H	0.350239941	-1.310927746	-0.254193405
H	-1.180490650	1.338602340	0.249340725
H	-1.968301385	-1.581834445	-0.318419474
H	7.073962511	2.533505275	-1.224186376
H	5.330143079	2.546611715	-1.039585004
H	5.601774048	2.944088108	1.442154644
H	7.349926753	2.908870669	1.250842410
H	7.221609102	4.902262416	-0.280009096
H	5.475559029	4.936651682	-0.091255857

H	6.555609001	6.613671546	1.418042693
H	5.745187168	5.371902679	2.382914569
H	7.503663487	5.336668152	2.193062394
H	5.552614540	-2.931026542	1.292027587
H	4.051808959	-2.032701198	1.165727504
H	3.895096583	-2.710848007	-1.286824124
H	5.393179679	-3.607790913	-1.112640755
H	4.314846639	-5.067139171	0.636659430
H	2.813149098	-4.175587163	0.451464097
H	2.739921312	-6.299999879	-0.865073180
H	2.665507582	-4.913471401	-1.961108850
H	4.177675217	-5.812293669	-1.773504281
H	-7.653733974	-1.690947788	-1.021952654
H	-6.236773782	-2.740024655	-1.257285985
H	-6.201725473	-3.265084275	1.168094546
H	-7.596671204	-2.214932522	1.433650570
H	-8.979830887	-3.673528132	-0.070640307
H	-7.593870321	-4.716810116	-0.343792110
H	-9.103642964	-5.700764325	1.392948663
H	-7.539298917	-5.297823896	2.114800920
H	-8.935826729	-4.248350702	2.389232940
H	-6.847489519	2.583601040	1.059409450
H	-5.148005948	3.084438895	1.217665256
H	-5.050631461	3.581994702	-1.211691327
H	-6.731497094	3.074073419	-1.401093707
H	-7.459496660	4.907629903	0.151789119
H	-5.789015003	5.411934514	0.349619590
H	-6.951732304	6.864835790	-1.324174322
H	-5.655389599	5.956175693	-2.114388305
H	-7.337860454	5.449437253	-2.312989897

Merocyanine 3 in ethanol, excited state

N	6.225764302	0.976841728	-0.152881765
C	7.449033503	0.337900427	-0.108371960
C	8.755140957	0.825241754	-0.198032628
C	9.790662780	-0.108943238	-0.122203400
C	9.532237483	-1.480113983	0.040817896
C	8.227172666	-1.970639628	0.132615315
C	7.189298757	-1.039879539	0.056748987
N	5.814337087	-1.194313114	0.127135721
C	5.204670851	0.044648830	-0.007239621
C	3.846374191	0.392281668	-0.004585953
C	2.700933152	-0.414455810	-0.056806354
C	1.404212826	0.122377187	-0.009158354
C	0.226613140	-0.629986340	-0.076269337
C	-1.058736395	-0.063364571	-0.029624978
C	-2.227012713	-0.827709276	-0.101138176
C	-3.570369366	-0.395107955	-0.064877882
C	-4.589631477	-1.422431959	-0.172316724
N	-5.940705302	-0.997026617	-0.182310242
C	-6.348474156	0.309696165	-0.022533269
N	-5.358992765	1.256819626	0.122928625
C	-3.963299613	0.988661203	0.072889536
O	-4.339037257	-2.631201767	-0.267340413
O	-3.174647682	1.940203332	0.160183707
S	-8.000556214	0.731632204	-0.005802958
C	6.051085644	2.419190299	-0.330876613
C	5.945830913	3.186532543	0.993909700
C	5.783644383	4.695145822	0.771421512
C	5.678401506	5.478112416	2.083394907
C	5.170181962	-2.482594396	0.396399522

C	4.857739665	-3.285615220	-0.873339701
C	4.231124506	-4.648324367	-0.551934617
C	3.922250345	-5.467124473	-1.808724180
C	-6.934384709	-2.082464963	-0.348803030
C	-7.337141619	-2.725876588	0.980789104
C	-8.359893390	-3.851581618	0.783543693
C	-8.771684202	-4.518350185	2.099516271
C	-5.707939757	2.682560372	0.321067629
C	-5.775872304	3.466544832	-0.992262540
C	-6.131465181	4.940047709	-0.758599664
C	-6.196800843	5.749548752	-2.057204141
H	8.962283846	1.882542068	-0.315261455
H	10.817681412	0.234982152	-0.188971667
H	10.362905373	-2.176158049	0.094763001
H	8.035458258	-3.030685530	0.250817371
H	3.664836221	1.461960960	0.025464026
H	2.782837005	-1.490254744	-0.162441255
H	1.306766581	1.203943320	0.086861171
H	0.311785007	-1.712736370	-0.169775336
H	-1.149987598	1.013128137	0.065949810
H	-2.113584437	-1.904636938	-0.199876431
H	6.906818596	2.773748640	-0.911631390
H	5.165647458	2.580948894	-0.951556078
H	5.095658729	2.801115332	1.570123922
H	6.844607725	2.991333576	1.591675813
H	6.634961881	5.069263305	0.187689977
H	4.889100561	4.878109591	0.161713645
H	5.564032227	6.550169323	1.895228034
H	4.815750958	5.148265489	2.672779557
H	6.574083267	5.340380490	2.699160905
H	5.851590001	-3.046121229	1.040120870
H	4.271573053	-2.295995873	0.986495546
H	4.184751942	-2.707025188	-1.517972541
H	5.785503118	-3.427573198	-1.440973351
H	4.910407131	-5.214986442	0.098303511
H	3.308734858	-4.499209844	0.024675680
H	3.477793463	-6.433373343	-1.550764374
H	3.218681273	-4.939232384	-2.461860877
H	4.831941872	-5.661201817	-2.387652732
H	-7.800691206	-1.655823526	-0.850754787
H	-6.466405962	-2.823402082	-0.996548522
H	-6.439294519	-3.121829729	1.469335500
H	-7.755842217	-1.956996412	1.641009543
H	-9.250539605	-3.449442802	0.282362921
H	-7.942340260	-4.607646300	0.105120577
H	-9.500893785	-5.317182946	1.930109525
H	-7.906052195	-4.958614311	2.607174061
H	-9.224198114	-3.793278736	2.785332266
H	-6.664269411	2.713055137	0.839492942
H	-4.932258135	3.097332166	0.964306286
H	-4.806793665	3.394625903	-1.499159829
H	-6.522894628	3.005295580	-1.649115908
H	-7.097030776	5.002797870	-0.239081977
H	-5.391198968	5.390214857	-0.083588167
H	-6.451508512	6.796202189	-1.861679784
H	-5.235110556	5.732426005	-2.582313520
H	-6.953161982	5.343632231	-2.738357593

Optimized atomic coordinates of dyes 1–3 (from CAM-B3LYP calculations)
(given in angstroms)

Merocyanine 1 in vacuum, ground state

N	3.800510166	0.752301243	-0.210558958
C	4.999734135	0.054759807	-0.172161794
C	6.317227509	0.470276799	-0.298383608
C	7.302572533	-0.508381665	-0.222591735
C	6.978438239	-1.852363909	-0.025045157
C	5.656538866	-2.266155398	0.102244783
C	4.675749539	-1.288439776	0.027705465
N	3.289637862	-1.363969420	0.131495370
C	2.756114792	-0.112587556	-0.022157724
C	1.419831365	0.314680366	0.021916673
C	0.308631699	-0.497761155	-0.112237485
C	-1.037797856	-0.140767402	-0.068356462
C	-1.987762185	-1.212381189	-0.249148282
N	-3.350438862	-0.855169606	-0.251373674
C	-3.822546482	0.417140359	-0.013716193
N	-2.885690229	1.402192474	0.199204384
C	-1.485699994	1.206220549	0.144937282
O	-1.676944821	-2.390785975	-0.405888539
O	-0.745818028	2.177099513	0.287168560
S	-5.466702296	0.748368488	0.015666629
C	3.671964826	2.184564051	-0.443013518
C	3.640458369	3.002580128	0.845119615
C	3.502115979	4.497957006	0.569752671
C	3.473223562	5.328944546	1.848342443
C	2.578241311	-2.583596040	0.498219628
C	2.175638873	-3.444900927	-0.697728569
C	1.216684685	-4.564108152	-0.296180842
C	0.867214591	-5.478055053	-1.465642753
C	-4.287574008	-1.965656255	-0.486988848
C	-4.682327218	-2.678079172	0.800649956
C	-5.662931644	-3.818358611	0.539222785
C	-6.060537437	-4.557642903	1.812913084
C	-3.310797506	2.785886674	0.464998396
C	-3.447312192	3.608916923	-0.809996507
C	-3.900823164	5.036752221	-0.517235054
C	-4.029012294	5.884983044	-1.778595061
H	6.573517576	1.513102586	-0.444256900
H	8.343328819	-0.219847579	-0.318323489
H	7.771436118	-2.589792964	0.028095683
H	5.408035907	-3.311036138	0.246659091
H	1.247809674	1.374871471	0.133987808
H	0.434930402	-1.554846977	-0.307561844
H	2.764869141	2.348654078	-1.028945711
H	4.515635559	2.485056637	-1.070452315
H	4.555808383	2.808446966	1.417060567
H	2.803834763	2.662210516	1.464961120
H	2.584009697	4.674587799	-0.002699088
H	4.331532545	4.830745317	-0.067100958
H	4.390961049	5.194159380	2.429186336
H	2.631526290	5.040471945	2.484619500
H	3.372730940	6.394190890	1.626521770
H	1.705618894	-2.293544459	1.085523575
H	3.234944959	-3.145557285	1.168520375
H	3.077435366	-3.860147849	-1.163534705
H	1.700963145	-2.814893949	-1.457641677
H	0.297273883	-4.116307754	0.097046685
H	1.660928806	-5.154512691	0.515564539
H	1.760191636	-5.953243998	-1.884506448

H	0.379239979	-4.914140297	-2.265792414
H	0.181300054	-6.269865458	-1.155225743
H	-3.775664828	-2.657547036	-1.154345028
H	-5.163098994	-1.553759369	-0.984368962
H	-5.133728836	-1.953214271	1.486194145
H	-3.776963980	-3.068676684	1.277911583
H	-5.217719611	-4.525860702	-0.171466100
H	-6.560603323	-3.418102793	0.052517916
H	-6.536971378	-3.879836423	2.527895610
H	-5.185135421	-4.993516635	2.304660753
H	-6.763431036	-5.368702373	1.603547423
H	-2.547328237	3.219854311	1.109121969
H	-4.258454511	2.739509363	0.997390781
H	-4.168966235	3.121574496	-1.473912640
H	-2.480041989	3.624187084	-1.324026131
H	-3.190958095	5.510370320	0.172532989
H	-4.864700351	5.009404261	0.005309502
H	-4.756724718	5.451066431	-2.471201157
H	-3.072259277	5.953481017	-2.305976923
H	-4.355458844	6.902558085	-1.546826697

Merocyanine 1 in vacuum, excited state

N	3.800510166	0.752301243	-0.210558958
C	4.999734135	0.054759807	-0.172161794
C	6.317227509	0.470276799	-0.298383608
C	7.302572533	-0.508381665	-0.222591735
C	6.978438239	-1.852363909	-0.025045157
C	5.656538866	-2.266155398	0.102244783
C	4.675749539	-1.288439776	0.027705465
N	3.289637862	-1.363969420	0.131495370
C	2.756114792	-0.112587556	-0.022157724
C	1.419831365	0.314680366	0.021916673
C	0.308631699	-0.497761155	-0.112237485
C	-1.037797856	-0.140767402	-0.068356462
C	-1.987762185	-1.212381189	-0.249148282
N	-3.350438862	-0.855169606	-0.251373674
C	-3.822546482	0.417140359	-0.013716193
N	-2.885690229	1.402192474	0.199204384
C	-1.485699994	1.206220549	0.144937282
O	-1.676944821	-2.390785975	-0.405888539
O	-0.745818028	2.177099513	0.287168560
S	-5.466702296	0.748368488	0.015666629
C	3.671964826	2.184564051	-0.443013518
C	3.640458369	3.002580128	0.845119615
C	3.502115979	4.497957006	0.569752671
C	3.473223562	5.328944546	1.848342443
C	2.578241311	-2.583596040	0.498219628
C	2.175638873	-3.444900927	-0.697728569
C	1.216684685	-4.564108152	-0.296180842
C	0.867214591	-5.478055053	-1.465642753
C	-4.287574008	-1.965656255	-0.486988848
C	-4.682327218	-2.678079172	0.800649956
C	-5.662931644	-3.818358611	0.539222785
C	-6.060537437	-4.557642903	1.812913084
C	-3.310797506	2.785886674	0.464998396
C	-3.447312192	3.608916923	-0.809996507
C	-3.900823164	5.036752221	-0.517235054
C	-4.029012294	5.884983044	-1.778595061
H	6.573517576	1.513102586	-0.444256900
H	8.343328819	-0.219847579	-0.318323489
H	7.771436118	-2.589792964	0.028095683
H	5.408035907	-3.311036138	0.246659091

H	1.247809674	1.374871471	0.133987808
H	0.434930402	-1.554846977	-0.307561844
H	2.764869141	2.348654078	-1.028945711
H	4.515635559	2.485056637	-1.070452315
H	4.555808383	2.808446966	1.417060567
H	2.803834763	2.662210516	1.464961120
H	2.584009697	4.674587799	-0.002699088
H	4.331532545	4.830745317	-0.067100958
H	4.390961049	5.194159380	2.429186336
H	2.631526290	5.040471945	2.484619500
H	3.372730940	6.394190890	1.626521770
H	1.705618894	-2.293544459	1.085523575
H	3.234944959	-3.145557285	1.168520375
H	3.077435366	-3.860147849	-1.163534705
H	1.700963145	-2.814893949	-1.457641677
H	0.297273883	-4.116307754	0.097046685
H	1.660928806	-5.154512691	0.515564539
H	1.760191636	-5.953243998	-1.884506448
H	0.379239979	-4.914140297	-2.265792414
H	0.181300054	-6.269865458	-1.155225743
H	-3.775664828	-2.657547036	-1.154345028
H	-5.163098994	-1.553759369	-0.984368962
H	-5.133728836	-1.953214271	1.486194145
H	-3.776963980	-3.068676684	1.277911583
H	-5.217719611	-4.525860702	-0.171466100
H	-6.560603323	-3.418102793	0.052517916
H	-6.536971378	-3.879836423	2.527895610
H	-5.185135421	-4.993516635	2.304660753
H	-6.763431036	-5.368702373	1.603547423
H	-2.547328237	3.219854311	1.109121969
H	-4.258454511	2.739509363	0.997390781
H	-4.168966235	3.121574496	-1.473912640
H	-2.480041989	3.624187084	-1.324026131
H	-3.190958095	5.510370320	0.172532989
H	-4.864700351	5.009404261	0.005309502
H	-4.756724718	5.451066431	-2.471201157
H	-3.072259277	5.953481017	-2.305976923
H	-4.355458844	6.902558085	-1.546826697

Merocyanine 1 in n-hexane, ground state

N	3.787396889	0.740918614	-0.225172412
C	4.984962030	0.040072429	-0.181761195
C	6.303522454	0.450663986	-0.322461231
C	7.284465781	-0.529851564	-0.234189882
C	6.956588775	-1.870530903	-0.010722843
C	5.635447131	-2.278565578	0.130657943
C	4.657706918	-1.297459460	0.042717822
N	3.271593171	-1.364939581	0.154578815
C	2.746082750	-0.116554135	-0.016488753
C	1.403744758	0.316642302	0.033632074
C	0.297290531	-0.488656199	-0.119766535
C	-1.056842961	-0.130724236	-0.074006534
C	-2.004729634	-1.195477764	-0.272096229
N	-3.371281053	-0.838190240	-0.266256249
C	-3.839861717	0.428359674	-0.011576571
N	-2.905597718	1.408222290	0.213790576
C	-1.502654828	1.209261826	0.158973714
O	-1.699205826	-2.373385992	-0.449899150
O	-0.764831282	2.180741920	0.318103234
S	-5.490149663	0.762308858	0.023308925
C	3.668486506	2.172123972	-0.479249596
C	3.697017262	3.009751797	0.795884932

C	3.585584249	4.503417009	0.499883315
C	3.616787540	5.354750933	1.764942780
C	2.557608843	-2.580029803	0.534800244
C	2.183092504	-3.464726246	-0.652680313
C	1.242371124	-4.596064425	-0.243066693
C	0.930187027	-5.540962744	-1.398504781
C	-4.307382393	-1.946461647	-0.517097525
C	-4.697622737	-2.680918827	0.759520115
C	-5.671027792	-3.823431775	0.481064591
C	-6.064915003	-4.582888431	1.744043031
C	-3.327246960	2.789402031	0.498343325
C	-3.453940338	3.632081541	-0.764732585
C	-3.900857836	5.058106502	-0.453319290
C	-4.019299288	5.924723726	-1.703122553
H	6.562256473	1.489811246	-0.487990254
H	8.325838929	-0.247324650	-0.339953177
H	7.748012298	-2.608835006	0.051907837
H	5.385032889	-3.319665458	0.296612993
H	1.239751474	1.375607541	0.167278368
H	0.425700792	-1.542212648	-0.333840653
H	2.743814612	2.338122324	-1.035357497
H	4.492813186	2.449032483	-1.141791087
H	4.625851093	2.803505038	1.340803167
H	2.873851041	2.699116015	1.448723496
H	2.655080324	4.693680006	-0.047547404
H	4.402793077	4.804739526	-0.167266967
H	4.549045842	5.206389868	2.318700265
H	2.789054213	5.096868270	2.432064282
H	3.534956348	6.418495101	1.528488256
H	1.674011444	-2.281410478	1.100452914
H	3.204786264	-3.125475950	1.227133153
H	3.096953238	-3.870793482	-1.102202162
H	1.705162473	-2.855418290	-1.427458069
H	0.309242646	-4.160069342	0.130595250
H	1.686812172	-5.160306716	0.586601093
H	1.839769782	-6.008423533	-1.789069781
H	0.449214140	-5.003929933	-2.221200928
H	0.252799689	-6.338457571	-1.083612160
H	-3.796937404	-2.626286668	-1.197525395
H	-5.184822064	-1.529290404	-1.006142907
H	-5.152851979	-1.969749738	1.456779082
H	-3.790278995	-3.073002464	1.231629704
H	-5.220464988	-4.517849620	-0.238976830
H	-6.570781359	-3.422242404	-0.000990440
H	-6.546314426	-3.918150978	2.467973541
H	-5.187054938	-5.020155545	2.230140722
H	-6.762465605	-5.395223679	1.522244250
H	-2.566253282	3.210787266	1.153335506
H	-4.277223285	2.738937370	1.025777368
H	-4.174499566	3.158456070	-1.439801324
H	-2.484630237	3.649318606	-1.274613110
H	-3.190910548	5.517598669	0.245716583
H	-4.866845625	5.028853356	0.065234721
H	-4.746963176	5.504930854	-2.404492190
H	-3.059999389	5.995200028	-2.225582537
H	-4.340782986	6.940634187	-1.457662903

Merocyanine 1 in n-hexane, excited state

N	3.784054896	0.844733310	-0.179948008
C	4.992656913	0.198748693	-0.107683003
C	6.301242652	0.672824498	-0.165369741
C	7.322727942	-0.265809513	-0.060837370

C	7.051381619	-1.628928532	0.099104733
C	5.746160695	-2.107686032	0.160435946
C	4.719622535	-1.173329569	0.055067308
N	3.351708067	-1.319205634	0.093885596
C	2.752897728	-0.076848002	-0.057487753
C	1.398747679	0.267901912	-0.114724720
C	0.296709956	-0.589473747	-0.242968354
C	-1.058290457	-0.200760249	-0.156914876
C	-2.030152124	-1.271739778	-0.242365536
N	-3.383564564	-0.915384913	-0.213381351
C	-3.848613267	0.361950373	0.002304007
N	-2.899392310	1.349283063	0.129179463
C	-1.511480652	1.159196949	0.002740061
O	-1.707398141	-2.456961569	-0.356901140
O	-0.763390205	2.142963760	0.047235674
S	-5.498503150	0.695753627	0.106169823
C	3.609545400	2.278407756	-0.353595932
C	3.447340021	3.028526969	0.967279733
C	3.264419533	4.529043005	0.752870421
C	3.106018251	5.292714955	2.063638207
C	2.682695206	-2.580961171	0.390109714
C	2.379593389	-3.417206473	-0.853036202
C	1.484275116	-4.611458419	-0.527168240
C	1.246453663	-5.509763512	-1.736461116
C	-4.324896927	-2.036477713	-0.378640108
C	-4.660258230	-2.716035325	0.942859669
C	-5.632852733	-3.877004129	0.751113139
C	-5.975101770	-4.580329832	2.060778025
C	-3.309881278	2.745297155	0.360266867
C	-3.493232839	3.520009001	-0.938916468
C	-3.923724564	4.961989657	-0.682239223
C	-4.100780127	5.761084605	-1.969565499
H	6.518253638	1.728129612	-0.278333768
H	8.353480714	0.068847680	-0.101483116
H	7.875756533	-2.329276407	0.175763904
H	5.540670533	-3.165112273	0.276069830
H	1.168939303	1.324694445	-0.058608756
H	0.425606133	-1.647171171	-0.414715119
H	2.742578110	2.440061267	-0.999028087
H	4.481883268	2.646345883	-0.899999709
H	4.326654282	2.842398841	1.595184047
H	2.583277792	2.623842520	1.505776556
H	2.384181271	4.697690069	0.121512204
H	4.123392263	4.925504389	0.197227814
H	3.984049918	5.165084292	2.704350689
H	2.233473760	4.939173550	2.620810266
H	2.975953765	6.363046798	1.885273628
H	1.769552994	-2.355452625	0.940676638
H	3.330971293	-3.135481602	1.074240706
H	3.321555044	-3.754898024	-1.300915294
H	1.889387716	-2.785988404	-1.602165641
H	0.522614105	-4.241038536	-0.153014618
H	1.934861362	-5.196953981	0.284173182
H	2.186850112	-5.917752186	-2.120423021
H	0.767469326	-4.954047961	-2.547990819
H	0.596151626	-6.350328605	-1.482077797
H	-3.838732093	-2.743225241	-1.050022989
H	-5.222432538	-1.641296584	-0.849145236
H	-5.096282407	-1.976740746	1.622959211
H	-3.732830269	-3.079984403	1.397877272
H	-5.201578795	-4.600431127	0.048114725
H	-6.552485479	-3.504794065	0.283588999

H	-6.436707477	-3.886631265	2.770256557
H	-5.076837832	-4.988545703	2.534636767
H	-6.672731854	-5.406982791	1.900980143
H	-2.520623973	3.199247969	0.957868019
H	-4.235793887	2.721684573	0.930181217
H	-4.245678177	3.013664565	-1.552871743
H	-2.548858046	3.507091721	-1.493316051
H	-3.180562286	5.455431561	-0.043541962
H	-4.863890683	4.963627133	-0.117505464
H	-4.861556133	5.307204833	-2.612067585
H	-3.167422063	5.800339820	-2.540009837
H	-4.409186036	6.789664680	-1.763391169

Merocyanine 1 in DCM, ground state

N	3.776336190	0.718466073	-0.252152105
C	4.968682331	0.007718884	-0.211407610
C	6.288559279	0.403354836	-0.390701183
C	7.259735582	-0.583533484	-0.289694470
C	6.923499798	-1.915511504	-0.017462702
C	5.603635217	-2.307932995	0.160516165
C	4.633627348	-1.318428574	0.058445472
N	3.248937696	-1.367716360	0.195051421
C	2.738578149	-0.122760360	-0.002225610
C	1.388609648	0.322451672	0.063379408
C	0.289051863	-0.470964189	-0.121601790
C	-1.076877676	-0.112236879	-0.073350674
C	-2.020737812	-1.164743700	-0.308200153
N	-3.392424113	-0.807271461	-0.296701615
C	-3.856907014	0.449038482	-0.012657207
N	-2.928120989	1.419029222	0.243999768
C	-1.520566710	1.215327309	0.195977233
O	-1.721993432	-2.340140992	-0.523076889
O	-0.785851430	2.184622075	0.392876312
S	-5.516945612	0.787275012	0.020044175
C	3.670699780	2.146557487	-0.539844563
C	3.780578874	3.012472303	0.711463126
C	3.696505759	4.500900602	0.381987068
C	3.806931996	5.380968914	1.622780688
C	2.528363900	-2.567992037	0.613172892
C	2.173861367	-3.495505835	-0.547169270
C	1.238636730	-4.619339022	-0.106593475
C	0.939765845	-5.603714858	-1.232439123
C	-4.325315395	-1.909811677	-0.583781954
C	-4.709485324	-2.691115654	0.666716438
C	-5.678849137	-3.827387449	0.350353677
C	-6.066331029	-4.632366921	1.586855765
C	-3.345908697	2.794259703	0.562856497
C	-3.454943452	3.673222759	-0.677025732
C	-3.891250739	5.094411612	-0.329857867
C	-3.991651047	5.995759527	-1.556496777
H	6.553281097	1.433878232	-0.594855131
H	8.301659815	-0.315577443	-0.423583594
H	7.710087964	-2.658056438	0.054335943
H	5.348067107	-3.340733259	0.365055159
H	1.237461999	1.378196080	0.233690630
H	0.422245028	-1.517217442	-0.367865673
H	2.723349269	2.315339105	-1.054271816
H	4.465726164	2.388738308	-1.249140375
H	4.728285468	2.795147435	1.217408589
H	2.981625047	2.740679623	1.410546384
H	2.749026812	4.704680411	-0.130579889
H	4.492154377	4.761178290	-0.326482649

H	4.758712572	5.218569401	2.137915303
H	3.003371724	5.162506574	2.332554533
H	3.744136146	6.440751820	1.363236255
H	1.636750073	-2.246329227	1.152244359
H	3.165153756	-3.085116147	1.335304386
H	3.094374140	-3.912034890	-0.971536890
H	1.700814144	-2.917851166	-1.349038255
H	0.301317263	-4.177828737	0.250479800
H	1.681972624	-5.152713795	0.743077287
H	1.855683010	-6.078229949	-1.598190536
H	0.465460354	-5.097498763	-2.078638736
H	0.264242760	-6.394634287	-0.896909504
H	-3.815341485	-2.562944538	-1.289811234
H	-5.204907404	-1.480544231	-1.057447007
H	-5.164484152	-2.008347582	1.392264882
H	-3.799890732	-3.095687298	1.123345809
H	-5.226725446	-4.493775770	-0.394539430
H	-6.581400994	-3.414072997	-0.116121769
H	-6.549714231	-3.995961941	2.334656208
H	-5.185261990	-5.082140891	2.055287906
H	-6.760210357	-5.439599054	1.337152849
H	-2.590408525	3.192757927	1.237701521
H	-4.300065845	2.735466936	1.081257967
H	-4.172695093	3.225566890	-1.372853967
H	-2.481881812	3.695725344	-1.179281607
H	-3.182404114	5.527413320	0.386697356
H	-4.861195383	5.060682579	0.181164081
H	-4.717690048	5.602518388	-2.274883230
H	-3.027411998	6.071420602	-2.068910373
H	-4.305478127	7.007284008	-1.284885721

Merocyanine 1 in DCM, excited state

N	3.765542207	0.854749598	-0.171598597
C	4.982470753	0.230366903	-0.096526117
C	6.283382655	0.727104960	-0.160274053
C	7.319904094	-0.192707605	-0.053375479
C	7.072163732	-1.561489559	0.114879544
C	5.777033213	-2.062951128	0.182312839
C	4.733285971	-1.146580183	0.075233301
N	3.370275304	-1.316231700	0.117799898
C	2.748041368	-0.084628014	-0.042229597
C	1.394074594	0.242887523	-0.096369433
C	0.284323970	-0.619414273	-0.170613403
C	-1.066212743	-0.224490351	-0.110799073
C	-2.046440777	-1.288888074	-0.210676082
N	-3.398760227	-0.926050311	-0.204173180
C	-3.859085325	0.353632076	-0.008962178
N	-2.910393339	1.336324449	0.130145223
C	-1.520885243	1.138537562	0.036700510
O	-1.731316683	-2.477166271	-0.317185128
O	-0.771759725	2.120762393	0.097010598
S	-5.515833069	0.698173406	0.057174308
C	3.571493349	2.285849116	-0.352979090
C	3.379494884	3.037639242	0.962856679
C	3.183239706	4.535079388	0.739253319
C	2.996096034	5.301920363	2.044420473
C	2.728320583	-2.596678301	0.393092892
C	2.427202731	-3.405422378	-0.867886519
C	1.632749567	-4.671397617	-0.553807831
C	1.389660282	-5.530236269	-1.790598452
C	-4.341672163	-2.045338104	-0.379810553
C	-4.697150107	-2.722114344	0.937963991

C	-5.663814947	-3.886145380	0.733841138
C	-6.025724136	-4.585717073	2.040248943
C	-3.316674676	2.736382942	0.350478269
C	-3.457915020	3.514805575	-0.951635200
C	-3.885987627	4.959252414	-0.704087020
C	-4.021774096	5.761402111	-1.994523747
H	6.481702678	1.785086896	-0.280849502
H	8.344710553	0.158972066	-0.098898326
H	7.909038236	-2.246594869	0.193037531
H	5.591804507	-3.123182538	0.305234279
H	1.165496206	1.300408707	-0.089950456
H	0.413557663	-1.683316872	-0.296706966
H	2.714299624	2.432890122	-1.014436083
H	4.446399902	2.664432548	-0.886464186
H	4.251839081	2.865126745	1.603651962
H	2.512682219	2.625054770	1.491117758
H	2.311965521	4.692179297	0.092416803
H	4.046790808	4.937899810	0.196212590
H	3.866368269	5.186457719	2.697816663
H	2.119927553	4.940021059	2.590864596
H	2.856513194	6.370111208	1.859683865
H	1.821942986	-2.404377829	0.966738067
H	3.398043742	-3.155494413	1.051479089
H	3.370537871	-3.662692677	-1.362885818
H	1.865668950	-2.783314958	-1.573580984
H	0.671088061	-4.388142853	-0.109549218
H	2.165406172	-5.258711173	0.203993605
H	2.334132428	-5.854006383	-2.238791129
H	0.833677718	-4.974016708	-2.551375268
H	0.812463812	-6.424963235	-1.543878201
H	-3.850145775	-2.754142268	-1.044544205
H	-5.230785775	-1.650105798	-0.865118689
H	-5.144601772	-1.983255553	1.611263971
H	-3.777186562	-3.082470837	1.410383948
H	-5.218891061	-4.610504688	0.040623115
H	-6.576418790	-3.518479965	0.249141964
H	-6.501562012	-3.891172283	2.739535949
H	-5.134154787	-4.989430688	2.530233737
H	-6.717786482	-5.414999932	1.870862798
H	-2.542726617	3.183655131	0.972128531
H	-4.256912134	2.720357428	0.895949392
H	-4.194534625	3.015210758	-1.589912304
H	-2.499136472	3.496879992	-1.480244679
H	-3.157580981	5.446198106	-0.044104728
H	-4.841166913	4.966604607	-0.165063451
H	-4.767441393	5.313853945	-2.658965252
H	-3.072442859	5.795508802	-2.538199003
H	-4.328893098	6.791410066	-1.794226269

Merocyanine 1 in ethanol, ground state

N	3.774687708	0.715030458	-0.263024352
C	4.966034990	0.002523318	-0.221075785
C	6.285931596	0.394110547	-0.411273457
C	7.255118722	-0.593662212	-0.304269341
C	6.917566398	-1.922465200	-0.015923777
C	5.598274863	-2.310724717	0.172517195
C	4.629781203	-1.319966887	0.064139873
N	3.245622396	-1.364993277	0.207269572
C	2.738355731	-0.121740632	-0.000104006
C	1.386555165	0.325923967	0.068449254
C	0.289398288	-0.465424416	-0.125105128
C	-1.079617602	-0.107821559	-0.076427861

C	-2.021390230	-1.156896361	-0.325678388
N	-3.394550273	-0.800875899	-0.311286979
C	-3.859422940	0.451029629	-0.014390163
N	-2.933049338	1.418449498	0.253948211
C	-1.524245889	1.214991207	0.207407995
O	-1.722803941	-2.329991796	-0.555498774
O	-0.791170529	2.183043597	0.418634799
S	-5.522360947	0.787746207	0.019679006
C	3.669824060	2.140943859	-0.563705975
C	3.788103716	3.017531507	0.679317514
C	3.705654673	4.503045675	0.336613142
C	3.823729754	5.394011492	1.568919075
C	2.524065472	-2.559280234	0.641711882
C	2.171608664	-3.503175815	-0.505825869
C	1.242194992	-4.624979919	-0.048257948
C	0.937386330	-5.620319541	-1.162868328
C	-4.325427173	-1.901653473	-0.611740700
C	-4.705663315	-2.700600225	0.628840502
C	-5.673548422	-3.834465131	0.299400196
C	-6.056393344	-4.656827245	1.525870739
C	-3.350976384	2.790361254	0.587247800
C	-3.453000530	3.684762358	-0.642231116
C	-3.889829020	5.101970179	-0.279559245
C	-3.983837490	6.018415457	-1.495470268
H	6.551759819	1.421710865	-0.628158435
H	8.296946539	-0.329451350	-0.446092113
H	7.703260943	-2.665520409	0.060191143
H	5.341685494	-3.340643505	0.389682034
H	1.237665468	1.380581876	0.247565900
H	0.425241229	-1.509350201	-0.380060599
H	2.719998514	2.306096474	-1.074637356
H	4.461295691	2.375033797	-1.279381193
H	4.738024631	2.802917985	1.181986967
H	2.992487723	2.753768277	1.385371941
H	2.756448946	4.704384881	-0.173871356
H	4.498828270	4.754699864	-0.377503678
H	4.777644211	5.233900422	2.080751651
H	3.023211452	5.183673125	2.284681465
H	3.762124220	6.451597361	1.300107627
H	1.631469477	-2.229128527	1.173906796
H	3.159505593	-3.065919633	1.372237544
H	3.092674846	-3.922302289	-0.926033954
H	1.695211559	-2.938112501	-1.314702843
H	0.306534798	-4.182711080	0.312748031
H	1.693070551	-5.149323150	0.802829098
H	1.852051848	-6.095313696	-1.530865632
H	0.455902704	-5.123205983	-2.010575540
H	0.266840295	-6.410306665	-0.815181492
H	-3.815259442	-2.543921102	-1.327424243
H	-5.206523046	-1.468541041	-1.078897439
H	-5.160012663	-2.028846898	1.365136293
H	-3.794418097	-3.109343342	1.078301787
H	-5.221893708	-4.489754023	-0.455497536
H	-6.578019922	-3.416906122	-0.159609555
H	-6.539339764	-4.031684205	2.283423055
H	-5.173261483	-5.111035689	1.986017022
H	-6.749130073	-5.462005742	1.266701736
H	-2.598628611	3.179842314	1.270727489
H	-4.307291438	2.726878246	1.100940127
H	-4.167161963	3.246746183	-1.347895936
H	-2.477672185	3.712747447	-1.139706986
H	-3.183950872	5.525407685	0.445505420

H	-4.862030953	5.062940203	0.226848233
H	-4.706923276	5.634835190	-2.222058206
H	-3.017167867	6.099531503	-2.002383088
H	-4.297995989	7.026702908	-1.212588409

Merocyanine 1 in ethanol, excited state

N	3.764005873	0.854643625	-0.171226882
C	4.983023172	0.236121554	-0.092623667
C	6.281958269	0.738930791	-0.154663337
C	7.322167702	-0.175793248	-0.044521775
C	7.080357724	-1.546014426	0.125303655
C	5.787857693	-2.053531916	0.191213588
C	4.739789760	-1.142098047	0.081118295
N	3.378024771	-1.318032495	0.121817387
C	2.750160008	-0.089397167	-0.041828699
C	1.396437561	0.233685384	-0.097062639
C	0.284885123	-0.629464619	-0.158176139
C	-1.064287072	-0.233060135	-0.101801896
C	-2.046915115	-1.295298940	-0.204619322
N	-3.398592965	-0.929922307	-0.205022938
C	-3.856948697	0.350960754	-0.017539111
N	-2.908000193	1.331427236	0.128977226
C	-1.518176443	1.130462439	0.048071093
O	-1.734428409	-2.484763367	-0.307731983
O	-0.767853826	2.111076709	0.119682811
S	-5.515201285	0.700293629	0.030721901
C	3.563250218	2.284885505	-0.353356192
C	3.348124727	3.033459414	0.960769377
C	3.144049209	4.529661724	0.736050580
C	2.934699651	5.293649482	2.039545835
C	2.740711591	-2.601976927	0.391597401
C	2.434316334	-3.402164535	-0.873536936
C	1.647390177	-4.673782153	-0.563612114
C	1.393601181	-5.521076475	-1.806241074
C	-4.342603732	-2.048410994	-0.380826478
C	-4.702960045	-2.720569459	0.938050628
C	-5.673789674	-3.881443884	0.735450239
C	-6.040072248	-4.576396092	2.043102071
C	-3.312317546	2.732385389	0.348709492
C	-3.435833200	3.515836391	-0.952154255
C	-3.860102964	4.961354539	-0.703906502
C	-3.979375399	5.768555265	-1.992809975
H	6.475497810	1.797612062	-0.276543308
H	8.345439389	0.180430767	-0.088739699
H	7.920332414	-2.226992281	0.205942571
H	5.607643153	-3.114355100	0.315754847
H	1.167851082	1.290958549	-0.103677092
H	0.414235237	-1.694359362	-0.275015615
H	2.714877819	2.427419011	-1.027150027
H	4.443054067	2.669823959	-0.873563114
H	4.213264134	2.866687733	1.612538605
H	2.477518486	2.614105077	1.477461937
H	2.280233243	4.681387997	0.077885759
H	4.011677558	4.938949608	0.204726401
H	3.797621186	5.183654768	2.703504736
H	2.054521927	4.924624070	2.574839204
H	2.789678272	6.361045608	1.854207187
H	1.837646300	-2.416000329	0.972607675
H	3.415431427	-3.163900632	1.041781344
H	3.375203198	-3.652498368	-1.376372043
H	1.865835931	-2.777017299	-1.571066423
H	0.689823428	-4.398556934	-0.105358913

H	2.190271624	-5.266576832	0.182357015
H	2.334421036	-5.836824474	-2.267486909
H	0.827949687	-4.959234882	-2.555824929
H	0.822362342	-6.420458190	-1.562361124
H	-3.850516902	-2.759708530	-1.042308002
H	-5.229355097	-1.653539782	-0.870451039
H	-5.148129850	-1.978590548	1.609601333
H	-3.785276629	-3.082984515	1.413250115
H	-5.230694534	-4.609110671	0.044593076
H	-6.584306071	-3.511692309	0.248345360
H	-6.514389797	-3.878443332	2.740061634
H	-5.150660751	-4.982141372	2.535283580
H	-6.734865995	-5.403521919	1.874557593
H	-2.544616399	3.175137177	0.981156269
H	-4.258453600	2.718070123	0.883748940
H	-4.167135790	3.021978511	-1.601014506
H	-2.471619266	3.495589588	-1.470623433
H	-3.136235314	5.442653359	-0.034938128
H	-4.820467764	4.971294286	-0.174145884
H	-4.720418269	5.326832070	-2.666310254
H	-3.024484822	5.800231603	-2.526760683
H	-4.283735012	6.799187013	-1.791677487

Merocyanine 2 in vacuum, ground state

N	5.056005880	0.849451063	-0.232931332
C	6.217730386	0.089922392	-0.213179655
C	7.551455442	0.437390105	-0.359883787
C	8.489351947	-0.590161694	-0.296753696
C	8.101772899	-1.913708454	-0.089624131
C	6.760619305	-2.259345485	0.058476331
C	5.829567708	-1.235127481	-0.005994162
N	4.442499643	-1.242481669	0.119580210
C	3.964164501	0.038558141	-0.024261563
C	2.658421883	0.517889990	0.036218376
C	1.465967932	-0.208994041	-0.060727991
C	0.200801194	0.336070820	0.027083668
C	-0.921152490	-0.487202579	-0.123034461
C	-2.265587676	-0.167701650	-0.074401294
C	-3.202948002	-1.257092237	-0.275200928
N	-4.572303483	-0.922872560	-0.272532571
C	-5.069416914	0.333306989	-0.004733869
N	-4.152165895	1.332774019	0.228747389
C	-2.748283979	1.172643644	0.162629753
O	-2.870597787	-2.421056469	-0.456185559
O	-2.033732225	2.154788919	0.318965777
S	-6.719035234	0.630165245	0.035019963
C	5.006649709	2.279223859	-0.490700170
C	5.056455887	3.125214034	0.779304422
C	5.011718856	4.621256893	0.477518035
C	5.064944303	5.477236892	1.738792005
C	3.696809936	-2.417777962	0.547027033
C	3.271908423	-3.327170366	-0.603343716
C	2.468552207	-4.531120354	-0.116254582
C	2.055698611	-5.461334851	-1.252175445
C	-5.486922476	-2.045888766	-0.536313368
C	-5.867274921	-2.798543652	0.732629423
C	-6.823442487	-3.952262352	0.441296296
C	-7.206645346	-4.731174463	1.695642722
C	-4.605912515	2.701096546	0.527277112
C	-4.760470478	3.551147235	-0.727728500
C	-5.241569434	4.962316615	-0.400166019
C	-5.389481894	5.837401330	-1.640852726

H	7.858381580	1.465788557	-0.510835029
H	9.541449188	-0.353456413	-0.409250068
H	8.856629745	-2.690633579	-0.044596232
H	6.462888574	-3.290062960	0.211745903
H	2.561622404	1.592937002	0.125961572
H	1.512515596	-1.276440460	-0.256185216
H	0.062642525	1.393907956	0.210076963
H	-0.738607279	-1.545590635	-0.304651830
H	4.099563221	2.487253686	-1.063742639
H	5.851261594	2.519096805	-1.142878985
H	5.970038073	2.882344812	1.334791539
H	4.217338354	2.850687874	1.428578093
H	4.097795631	4.850925190	-0.083533530
H	5.848384563	4.884821533	-0.181510749
H	5.983653592	5.291938334	2.303651877
H	4.220243458	5.259153295	2.398900093
H	5.031563114	6.542259976	1.496967326
H	2.835473620	-2.077160463	1.124200806
H	4.339665576	-2.968648584	1.240805765
H	4.165387452	-3.665629838	-1.141083132
H	2.682163473	-2.753277989	-1.326974739
H	1.574071023	-4.180630683	0.412950842
H	3.059675860	-5.088805784	0.620874400
H	2.930384428	-5.853097998	-1.780497210
H	1.431988149	-4.938124684	-1.982756549
H	1.482708957	-6.312629012	-0.877436067
H	-4.960934483	-2.710367482	-1.220436108
H	-6.370517405	-1.639694923	-1.023964771
H	-6.334359094	-2.100808987	1.435639800
H	-4.954310708	-3.182026234	1.200894322
H	-6.362435915	-4.632361164	-0.285830435
H	-7.728901803	-3.559146109	-0.036830057
H	-7.698097496	-4.081564865	2.426492437
H	-6.322605114	-5.160342430	2.177665109
H	-7.891931947	-5.551552957	1.465121175
H	-3.851270663	3.135627036	1.181341847
H	-5.551813736	2.622274631	1.058818417
H	-5.473517569	3.065635402	-1.402291780
H	-3.794516572	3.598025593	-1.242070742
H	-4.539239489	5.433320736	0.298940006
H	-6.203454824	4.903645198	0.123594631
H	-6.110140131	5.405688953	-2.342211959
H	-4.435430475	5.937111765	-2.168050995
H	-5.735348757	6.842595899	-1.384391846

Merocyanine 2 in vacuum, excited state

N	4.977291706	0.914693617	-0.195893575
C	6.195064719	0.271023261	-0.136960645
C	7.498040872	0.745625778	-0.235224006
C	8.525571007	-0.189107484	-0.137170989
C	8.260554913	-1.546161881	0.056704539
C	6.955916508	-2.023259485	0.158677313
C	5.928703192	-1.092750897	0.059163965
N	4.555716602	-1.237231516	0.134469155
C	3.954536671	-0.002957755	-0.026708303
C	2.597826759	0.337726719	-0.032855645
C	1.467581304	-0.481617915	-0.127938005
C	0.167544937	0.042619945	-0.046038883
C	-0.973178408	-0.752675265	-0.145805692
C	-2.314810251	-0.333999926	-0.095610104
C	-3.319289864	-1.365891513	-0.246377012
N	-4.664173893	-0.953781660	-0.243940163

C	-5.086371827	0.335104417	-0.014765516
N	-4.105697115	1.280836827	0.172801818
C	-2.717439407	1.036651812	0.093994560
O	-3.048717393	-2.556273311	-0.387769657
O	-1.939099373	1.985454300	0.204307516
S	-6.719854189	0.732506712	0.033012521
C	4.802594733	2.339726191	-0.421082641
C	4.700351069	3.147842421	0.871355773
C	4.516829726	4.639971336	0.603850567
C	4.414389832	5.458200957	1.887021860
C	3.906090690	-2.492828372	0.484481183
C	3.616071886	-3.383485192	-0.722177907
C	2.922127517	-4.683534678	-0.320939428
C	2.639740100	-5.590879346	-1.513956906
C	-5.641778419	-2.032174809	-0.462390592
C	-6.040847757	-2.725671479	0.834236185
C	-7.057217544	-3.838472357	0.591548572
C	-7.461711214	-4.557126092	1.874904950
C	-4.469426611	2.683303940	0.432511599
C	-4.577892955	3.502006746	-0.848001932
C	-4.960120106	4.952049518	-0.562580526
C	-5.061856173	5.794992907	-1.829958725
H	7.710792405	1.798993727	-0.373926704
H	9.554012491	0.146956229	-0.210400295
H	9.086415916	-2.245199667	0.128382061
H	6.754867413	-3.078329591	0.301847861
H	2.398680469	1.402719710	0.027462856
H	1.566245015	-1.548912661	-0.293315045
H	0.033757796	1.108847125	0.099924863
H	-0.849652246	-1.823683942	-0.284729803
H	3.912004732	2.479683212	-1.039775582
H	5.653483343	2.679488820	-1.018110727
H	5.604700874	2.981885350	1.468472179
H	3.861571114	2.770110541	1.467157973
H	3.614642367	4.791842831	-0.000969760
H	5.355391078	5.007039956	-0.000958707
H	5.316016481	5.350421099	2.497621004
H	3.562532045	5.135754924	2.492939722
H	4.284124386	6.521037216	1.669613711
H	2.992442467	-2.259477742	1.032317639
H	4.567995737	-3.010883622	1.185265188
H	4.557141518	-3.604314055	-1.239403006
H	2.994215894	-2.834105348	-1.437874462
H	1.981149279	-4.449492011	0.191847315
H	3.542757765	-5.217220512	0.409609066
H	3.565257297	-5.868014552	-2.027938602
H	1.990898280	-5.094562772	-2.241486007
H	2.142753386	-6.512146986	-1.201064273
H	-5.161715544	-2.743961131	-1.132982333
H	-6.509886234	-1.592250468	-0.948653022
H	-6.462471106	-1.983343174	1.520346731
H	-5.141158135	-3.139766117	1.301976617
H	-6.640207351	-4.563500472	-0.118503844
H	-7.948427651	-3.415865808	0.111729432
H	-7.910401979	-3.860885681	2.590191001
H	-6.593566462	-5.014455449	2.359917611
H	-8.189938009	-5.349158005	1.679241064
H	-3.682851367	3.088227746	1.067998907
H	-5.415268543	2.680412616	0.969885857
H	-5.328540942	3.043876713	-1.500777333
H	-3.615559965	3.467004253	-1.369816553
H	-4.220534341	5.396837511	0.115008795

H	-5.918326502	4.975112607	-0.029381076
H	-5.817154268	5.390574010	-2.510824039
H	-4.108817890	5.812969005	-2.368077154
H	-5.336705724	6.829049438	-1.603798597

Merocyanine 2 in n-hexane, ground state

N	5.041521320	0.839086899	-0.249974665
C	6.203045982	0.078447666	-0.235391636
C	7.535324585	0.422471180	-0.412866466
C	8.470164403	-0.605117931	-0.344308431
C	8.083359488	-1.925588250	-0.103037264
C	6.746582667	-2.266976025	0.074775343
C	5.816373361	-1.240389699	0.004321767
N	4.431426509	-1.240387752	0.152904880
C	3.960318515	0.034611090	-0.008075236
C	2.646498466	0.521097123	0.070418368
C	1.466366318	-0.201236918	-0.044694901
C	0.189172873	0.342963436	0.048887836
C	-0.922526202	-0.472326634	-0.121171126
C	-2.278685416	-0.155396550	-0.073460845
C	-3.207774930	-1.237706172	-0.299383636
N	-4.582383310	-0.908637909	-0.292873769
C	-5.080484736	0.339437543	-0.007847002
N	-4.169643550	1.334622038	0.244454230
C	-2.761272397	1.173630211	0.185470941
O	-2.877459988	-2.400910443	-0.504904025
O	-2.051621036	2.158039962	0.366872992
S	-6.738091383	0.634258251	0.030299401
C	4.993034375	2.267999914	-0.528412673
C	5.101650942	3.128742440	0.727323886
C	5.072202916	4.620701013	0.403922988
C	5.183803577	5.493058392	1.650021389
C	3.685804118	-2.411100460	0.600256168
C	3.271668399	-3.341938899	-0.536462136
C	2.479543028	-4.545106376	-0.029422274
C	2.079515990	-5.498578187	-1.150525300
C	-5.491603313	-2.030366870	-0.579479468
C	-5.868376774	-2.811534800	0.673218841
C	-6.815780054	-3.966146058	0.357475235
C	-7.195372653	-4.772270638	1.595671631
C	-4.624515058	2.697592276	0.564155230
C	-4.767242677	3.571521994	-0.675813101
C	-5.247175294	4.977830943	-0.326156123
C	-5.383866794	5.875543368	-1.551929691
H	7.840640701	1.446867475	-0.590812656
H	9.520809318	-0.374105268	-0.479314109
H	8.838519553	-2.701945505	-0.054858832
H	6.450383375	-3.293543285	0.255257625
H	2.556130026	1.594193887	0.188083002
H	1.514991135	-1.264815304	-0.260318755
H	0.054972156	1.397485316	0.251766777
H	-0.737690098	-1.526461644	-0.322555735
H	4.066377775	2.474642725	-1.068304777
H	5.813366735	2.488636775	-1.216591630
H	6.030247067	2.878549648	1.253619120
H	4.281084501	2.879347484	1.409732684
H	4.143580645	4.858071999	-0.128774585
H	5.890435951	4.858934034	-0.286820761
H	6.118102397	5.298881245	2.185596518
H	4.358444065	5.299389891	2.341535052
H	5.160875095	6.554917790	1.393356648
H	2.820985181	-2.061068585	1.165862931

H	4.327913491	-2.944686427	1.307314629
H	4.168818436	-3.681833023	-1.066799394
H	2.677275695	-2.786469135	-1.270676841
H	1.580662079	-4.194435049	0.491794920
H	3.075352043	-5.083651481	0.717804675
H	2.959982417	-5.889832530	-1.669527111
H	1.452710698	-4.994193866	-1.891711275
H	1.514591468	-6.349379102	-0.762461541
H	-4.963475666	-2.677910195	-1.277744818
H	-6.376992470	-1.619409861	-1.059228498
H	-6.340695197	-2.132130623	1.390561518
H	-4.953665175	-3.197761250	1.135654647
H	-6.348383402	-4.628256881	-0.381991770
H	-7.723228494	-3.570468883	-0.114701418
H	-7.693042636	-4.140723812	2.338110724
H	-6.308943663	-5.204346916	2.070679778
H	-7.874127143	-5.592861327	1.347344417
H	-3.875627061	3.118892207	1.233000130
H	-5.574593387	2.610602548	1.086568901
H	-5.475415993	3.100796886	-1.365892593
H	-3.797422120	3.625048627	-1.182021311
H	-4.548606180	5.433999036	0.386339612
H	-6.212873915	4.912387482	0.189734645
H	-6.100770466	5.458595512	-2.266010483
H	-4.425694694	5.982125699	-2.070261410
H	-5.728862526	6.876763922	-1.279349395

Merocyanine 2 in n-hexane, excited state

N	4.967896778	0.920949450	-0.172330710
C	6.190111673	0.287615744	-0.119369969
C	7.489419093	0.775348299	-0.210249081
C	8.524287488	-0.150983189	-0.123189755
C	8.271013837	-1.514154966	0.052287678
C	6.971616086	-2.004371170	0.146410249
C	5.935813694	-1.081337904	0.058840013
N	4.565103932	-1.239236770	0.129770251
C	3.953693946	-0.008654189	-0.017984284
C	2.594554904	0.322662494	-0.025556680
C	1.466281290	-0.500655503	-0.107885924
C	0.166219258	0.027859434	-0.040880370
C	-0.978562956	-0.763697170	-0.127944590
C	-2.320623178	-0.342707134	-0.086658302
C	-3.327281700	-1.374756846	-0.214557611
N	-4.672655741	-0.962827437	-0.219954884
C	-5.092693278	0.330338347	-0.022536804
N	-4.113429549	1.278698888	0.144557567
C	-2.724855117	1.030772854	0.074837177
O	-3.059908905	-2.569849592	-0.330627082
O	-1.947186720	1.982733144	0.168476710
S	-6.730192725	0.730819679	0.012392290
C	4.784354300	2.350015069	-0.371786840
C	4.672142085	3.131848578	0.935737732
C	4.488030937	4.628293405	0.694603259
C	4.375802397	5.421960253	1.992268277
C	3.926870295	-2.511425179	0.441428116
C	3.636597957	-3.361466471	-0.793954356
C	2.972770959	-4.688332702	-0.432082687
C	2.690198019	-5.555140567	-1.654809697
C	-5.650939747	-2.046710218	-0.411580962
C	-6.049626014	-2.708846754	0.901481596
C	-7.062537839	-3.830385121	0.685491186
C	-7.467315307	-4.516735014	1.986327427

C	-4.474620575	2.687712886	0.374845001
C	-4.565093041	3.485050774	-0.920343823
C	-4.941863332	4.941924431	-0.663373451
C	-5.026181540	5.763407587	-1.946029341
H	7.692957914	1.832000555	-0.336213806
H	9.549797383	0.194986846	-0.190814169
H	9.103215601	-2.206475889	0.115106487
H	6.780529123	-3.063144792	0.274649484
H	2.392258908	1.387498820	0.022947779
H	1.564282577	-1.570752383	-0.250499445
H	0.038628169	1.097242141	0.083547963
H	-0.854684097	-1.836609377	-0.246175794
H	3.896966695	2.496768155	-0.992937416
H	5.635779771	2.705560722	-0.958044923
H	5.573467034	2.956792008	1.534582838
H	3.830239735	2.742022225	1.519168423
H	3.589925450	4.789981100	0.086452365
H	5.330445557	5.007254257	0.102974520
H	5.273693266	5.303567904	2.606439097
H	3.520522891	5.086614847	2.586357609
H	4.245502850	6.488591560	1.793856924
H	3.017090427	-2.305626147	1.006059493
H	4.598158237	-3.047277708	1.118672359
H	4.575173159	-3.545929167	-1.329314988
H	2.995484972	-2.798556824	-1.481641305
H	2.035492946	-4.491963074	0.102625034
H	3.614524942	-5.236741501	0.268394599
H	3.613528449	-5.794282116	-2.191303419
H	2.022224837	-5.043786341	-2.354167010
H	2.215322007	-6.497186192	-1.370391864
H	-5.172583438	-2.774019652	-1.066148533
H	-6.518870077	-1.619705644	-0.908985202
H	-6.473640768	-1.951543463	1.569538260
H	-5.149879141	-3.108484069	1.381492156
H	-6.641978136	-4.572033169	-0.004896521
H	-7.953898179	-3.422880163	0.193151332
H	-7.919190661	-3.803553618	2.682690888
H	-6.598874639	-4.959457046	2.484160264
H	-8.193129424	-5.315194457	1.809180903
H	-3.694932441	3.100711725	1.013261468
H	-5.425494099	2.698430593	0.902486175
H	-5.310583895	3.020635047	-1.574605831
H	-3.598108864	3.435901485	-1.431932416
H	-4.206274348	5.393773045	0.013726721
H	-5.904976207	4.979578890	-0.139995399
H	-5.777340136	5.351909039	-2.627263254
H	-4.067735516	5.766900739	-2.474689658
H	-5.297105274	6.802508183	-1.739570551

Merocyanine 2 in DCM, ground state

N	5.018557943	0.832926186	-0.282460272
C	6.184648447	0.078861061	-0.268843220
C	7.511838852	0.423976828	-0.493169268
C	8.449227717	-0.596242247	-0.406359521
C	8.073724758	-1.911079639	-0.103720278
C	6.746633733	-2.252862540	0.118909827
C	5.810141664	-1.230347317	0.029360457
N	4.429061393	-1.227677623	0.208477277
C	3.959595897	0.033018251	0.011576339
C	2.628387094	0.520719725	0.110803914
C	1.473074656	-0.200808449	-0.044267389
C	0.173060528	0.337698358	0.059673194

C	-0.923094105	-0.463835151	-0.143827076
C	-2.298871924	-0.148330871	-0.090871460
C	-3.218399899	-1.215830038	-0.356517108
N	-4.600762339	-0.892563388	-0.335451979
C	-5.097032087	0.341031068	-0.014138084
N	-4.193368228	1.326105613	0.268028135
C	-2.778708623	1.161412254	0.211723054
O	-2.893991586	-2.375957127	-0.608001899
O	-2.074010816	2.145833658	0.434588696
S	-6.767043623	0.634448173	0.031952445
C	4.958110634	2.258502135	-0.594991008
C	5.126047008	3.143184100	0.636749067
C	5.098160939	4.627390237	0.279578061
C	5.266204799	5.525084040	1.501134708
C	3.689055451	-2.391389396	0.692035035
C	3.303478323	-3.366693642	-0.416504510
C	2.535683151	-4.568516781	0.129358120
C	2.159162463	-5.565587002	-0.961568175
C	-5.504710822	-2.009263620	-0.655984787
C	-5.867028748	-2.838532418	0.569948218
C	-6.804615313	-3.991230658	0.219189065
C	-7.169677923	-4.843233810	1.430777100
C	-4.645449543	2.679380958	0.629723472
C	-4.778498679	3.595350903	-0.580787139
C	-5.249439321	4.992941388	-0.186253992
C	-5.376415079	5.931493702	-1.382149145
H	7.807601361	1.441319110	-0.719753503
H	9.495590000	-0.368389693	-0.575098700
H	8.835016664	-2.680449589	-0.043152434
H	6.460707041	-3.272314271	0.348100594
H	2.539631745	1.587189835	0.281877065
H	1.531967511	-1.255335093	-0.298955159
H	0.044058316	1.384923389	0.300486732
H	-0.735561186	-1.509189304	-0.382766746
H	4.008371788	2.452434352	-1.096358320
H	5.746678760	2.457856858	-1.324280300
H	6.072919497	2.895751587	1.130047241
H	4.330768540	2.918926116	1.356849213
H	4.151885515	4.861659926	-0.222226076
H	5.892024223	4.840456175	-0.446286923
H	6.218829487	5.332074841	2.003873674
H	4.466383497	5.354521429	2.228079444
H	5.243777294	6.581401153	1.221839020
H	2.812636616	-2.028310635	1.229890245
H	4.328478843	-2.887748749	1.426868925
H	4.210254703	-3.706276715	-0.929485238
H	2.700465978	-2.850502328	-1.172060671
H	1.629135631	-4.218985238	0.637670878
H	3.142264480	-5.069432837	0.893301119
H	3.049910958	-5.954716222	-1.464232723
H	1.526004213	-5.097677599	-1.721370886
H	1.610641531	-6.415282201	-0.547709126
H	-4.978617004	-2.627155312	-1.381642564
H	-6.395903678	-1.588968654	-1.115852009
H	-6.340658472	-2.190913886	1.315601820
H	-4.946341891	-3.231124347	1.014575077
H	-6.334341948	-4.622389470	-0.544924744
H	-7.718328206	-3.589354473	-0.235488979
H	-7.670524715	-4.243070984	2.196846006
H	-6.276440591	-5.282068496	1.886372782
H	-7.840865496	-5.661682363	1.156632249
H	-3.899438016	3.075700755	1.316326280

H	-5.597428179	2.580259111	1.145996718
H	-5.486272276	3.153374757	-1.290345211
H	-3.807257668	3.658696553	-1.083006300
H	-4.549513856	5.419957106	0.542580219
H	-6.216625728	4.918014625	0.325690291
H	-6.094556179	5.543904970	-2.111484598
H	-4.416017386	6.048326937	-1.894041386
H	-5.714780220	6.925301752	-1.076593444

Merocyanine 2 in DCM, excited state

N	4.957266824	0.926978033	-0.143041406
C	6.184995481	0.308022016	-0.100031656
C	7.478844174	0.814032785	-0.182096694
C	8.524134397	-0.100331033	-0.111561544
C	8.287582377	-1.471368250	0.038895168
C	6.995675923	-1.979807751	0.124214865
C	5.947583548	-1.067906068	0.054327210
N	4.580677184	-1.244499263	0.122002315
C	3.953687061	-0.018514416	-0.005690539
C	2.594876220	0.300545299	-0.010974669
C	1.463945269	-0.529043161	-0.063221559
C	0.170032752	0.004925064	-0.016207340
C	-0.985145075	-0.782626666	-0.081866924
C	-2.323286247	-0.356784905	-0.056828461
C	-3.336350121	-1.386331170	-0.157297000
N	-4.680246069	-0.970770652	-0.183840513
C	-5.094195565	0.328308438	-0.033702398
N	-4.115976283	1.277772828	0.110345467
C	-2.727708155	1.022211840	0.062113872
O	-3.075752244	-2.587326178	-0.233686205
O	-1.948585129	1.975077716	0.136142499
S	-6.736626620	0.737132954	-0.026787053
C	4.759792570	2.359991389	-0.306376248
C	4.626687934	3.103072141	1.021435352
C	4.435184641	4.604176845	0.819252484
C	4.302849137	5.359979363	2.137508011
C	3.958493541	-2.536863672	0.382009381
C	3.652534014	-3.325616824	-0.889536044
C	3.028047148	-4.684899892	-0.582402415
C	2.729569007	-5.489407704	-1.843398218
C	-5.660798425	-2.058658823	-0.347160724
C	-6.062169790	-2.685978486	0.982051007
C	-7.073228966	-3.814335456	0.793389322
C	-7.481173718	-4.465158457	2.111369201
C	-4.472447107	2.695802709	0.296008998
C	-4.539610320	3.459823858	-1.020497491
C	-4.908834543	4.925603519	-0.805279389
C	-4.971207332	5.714441652	-2.109462374
H	7.668938136	1.875024137	-0.290201442
H	9.545298477	0.259304790	-0.172899536
H	9.128563985	-2.154027512	0.088603063
H	6.818860024	-3.043030426	0.233188621
H	2.388639632	1.365224914	0.012016131
H	1.560392421	-1.603043170	-0.166433292
H	0.050522555	1.078569492	0.072768884
H	-0.860975522	-1.858125644	-0.168137153
H	3.878732448	2.515384838	-0.933828651
H	5.613618093	2.739051001	-0.872908686
H	5.522975586	2.918488179	1.624544753
H	3.780569867	2.691896450	1.583733207
H	3.543175794	4.776542660	0.205207572
H	5.282276976	5.004203968	0.249057366

H	5.195071592	5.229739867	2.757591144
H	3.443690561	5.001326651	2.712434359
H	4.167325950	6.431152968	1.967990948
H	3.060394970	-2.370215130	0.977215856
H	4.648280070	-3.098864325	1.016813015
H	4.581004866	-3.461493825	-1.455709069
H	2.981527578	-2.742346685	-1.530209585
H	2.102913223	-4.540212979	-0.011438883
H	3.702545582	-5.255092050	0.067626125
H	3.642742594	-5.676251459	-2.416750083
H	2.031569293	-4.955290670	-2.495133606
H	2.284151610	-6.457104402	-1.599322520
H	-5.184909780	-2.803015851	-0.983597004
H	-6.526751008	-1.644978838	-0.858162379
H	-6.487535005	-1.912864935	1.631064556
H	-5.163970310	-3.071195192	1.476222398
H	-6.649386353	-4.573700236	0.124849091
H	-7.963348915	-3.422146464	0.286542423
H	-7.937149084	-3.734173204	2.786344905
H	-6.613676150	-4.892518516	2.623967803
H	-8.204642522	-5.269396219	1.952676283
H	-3.701878252	3.121676172	0.936484157
H	-5.429420383	2.726872505	0.810898252
H	-5.278243407	2.984780595	-1.675039831
H	-3.567297868	3.391249874	-1.519365351
H	-4.178294355	5.388899481	-0.130758708
H	-5.877645737	4.983906268	-0.294386759
H	-5.717208402	5.291507272	-2.789477121
H	-4.006199113	5.697914653	-2.625661154
H	-5.236735537	6.760039909	-1.931637746

Merocyanine 2 in ethanol, ground state

N	5.012955702	0.831766568	-0.289736089
C	6.180968707	0.080853280	-0.273433813
C	7.506660323	0.427359803	-0.507162157
C	8.446082287	-0.589583425	-0.412987157
C	8.074832114	-1.902671097	-0.094429438
C	6.750202822	-2.245773221	0.137193637
C	5.810847481	-1.225883606	0.040020943
N	4.430546804	-1.224215312	0.223855692
C	3.959692408	0.032192505	0.016144021
C	2.623921764	0.518538332	0.118160419
C	1.474821898	-0.203626260	-0.047335118
C	0.169316277	0.333039874	0.059641365
C	-0.923843722	-0.464961127	-0.151611626
C	-2.304051575	-0.149095002	-0.096269275
C	-3.222462546	-1.212055078	-0.371979172
N	-4.606330152	-0.889325019	-0.346309447
C	-5.101245439	0.340632151	-0.014728483
N	-4.198471238	1.322396890	0.274988722
C	-2.782610321	1.155942011	0.218544615
O	-2.900201147	-2.370988618	-0.635904886
O	-2.078267455	2.139203982	0.452292650
S	-6.774084591	0.634352984	0.034659623
C	4.947414586	2.255442750	-0.613361713
C	5.125308816	3.148758384	0.610593010
C	5.090659539	4.630174275	0.242728247
C	5.268052236	5.536899404	1.456289529
C	3.692306447	-2.386840943	0.714351842
C	3.316456681	-3.372012524	-0.388670171
C	2.555484631	-4.575053390	0.163858290
C	2.187316190	-5.581313515	-0.921505488

C	-5.509850509	-2.003988051	-0.675219300
C	-5.867959041	-2.845435144	0.543695962
C	-6.804976847	-3.996126621	0.184746598
C	-7.165203676	-4.860094345	1.389287900
C	-4.648473235	2.673525220	0.647438654
C	-4.776261995	3.600619805	-0.555203599
C	-5.246296352	4.995446693	-0.149795814
C	-5.367989625	5.944740543	-1.337730235
H	7.798935978	1.442805680	-0.746169571
H	9.491283873	-0.361385338	-0.588268414
H	8.838565009	-2.669173484	-0.028527637
H	6.467968517	-3.263259085	0.379128276
H	2.534247038	1.582825266	0.302717203
H	1.536816490	-1.255522131	-0.311932534
H	0.041583966	1.378198043	0.310228711
H	-0.735892086	-1.507899308	-0.400144064
H	3.992772124	2.443518583	-1.107264192
H	5.728932377	2.449762732	-1.351309965
H	6.077493229	2.907174761	1.096280108
H	4.337348139	2.927989695	1.339750136
H	4.139175609	4.858479068	-0.251919557
H	5.877429091	4.839441038	-0.491741404
H	6.225888500	5.349447042	1.951162090
H	4.475554848	5.369525826	2.192031742
H	5.240593991	6.591210247	1.169704467
H	2.811841146	-2.022017919	1.244160854
H	4.330223159	-2.874192810	1.456246973
H	4.226812600	-3.709499844	-0.896423614
H	2.712017933	-2.865149748	-1.149345468
H	1.645987158	-4.227956496	0.668521324
H	3.164406092	-5.067052974	0.931550738
H	3.081610062	-5.967803305	-1.419838223
H	1.553015626	-5.121960421	-1.685685819
H	1.643453754	-6.432032672	-0.503389110
H	-4.985015064	-2.614161455	-1.408145232
H	-6.402620842	-1.580963043	-1.129415859
H	-6.340019703	-2.205796134	1.297289943
H	-4.945681769	-3.240810238	0.982456039
H	-6.336087757	-4.619238997	-0.586731890
H	-7.720573029	-3.591453550	-0.263708393
H	-7.664619150	-4.268062300	2.162613985
H	-6.269986216	-5.302005402	1.837931812
H	-7.836010136	-5.676765661	1.109150952
H	-3.903594074	3.062109615	1.339551948
H	-5.601641859	2.572599832	1.160990537
H	-5.481992449	3.166304536	-1.271576363
H	-3.803566482	3.666945537	-1.054146650
H	-4.548062281	5.414781329	0.585019721
H	-6.215118473	4.917660786	0.358678004
H	-6.084464663	5.564947174	-2.072822750
H	-4.405777049	6.064615065	-1.845449971
H	-5.705680382	6.936230374	-1.024165499

Merocyanine 2 in ethanol, excited state

N	4.957853851	0.928054523	-0.143778759
C	6.185673040	0.310459250	-0.099171304
C	7.479216450	0.817933076	-0.180850584
C	8.525185978	-0.095145576	-0.108278343
C	8.289943037	-1.466685131	0.043778516
C	6.998813839	-1.976585072	0.128643055
C	5.949571984	-1.065834948	0.056668932
N	4.583239841	-1.243992502	0.123284555

C	3.954906550	-0.018564428	-0.006411498
C	2.596947293	0.299618058	-0.013547663
C	1.464685334	-0.531054844	-0.059755785
C	0.172696044	0.003486542	-0.016227912
C	-0.984771867	-0.783899962	-0.079004983
C	-2.321936274	-0.358203441	-0.054764857
C	-3.335825283	-1.387201111	-0.155108344
N	-4.679610511	-0.971572440	-0.182676277
C	-5.092838966	0.327231358	-0.033466116
N	-4.115539188	1.276784568	0.110121921
C	-2.727260810	1.021022636	0.063141056
O	-3.075981902	-2.588651021	-0.230686019
O	-1.948355657	1.974066728	0.137269214
S	-6.736907084	0.736260034	-0.026939718
C	4.759106243	2.361145122	-0.306803998
C	4.617917456	3.102352302	1.021160349
C	4.425283793	4.603290806	0.819109024
C	4.285299228	5.357737080	2.137365737
C	3.962156188	-2.537535864	0.380985640
C	3.654538701	-3.322836474	-0.892253687
C	3.034103814	-4.684444403	-0.587409062
C	2.733399663	-5.485436652	-1.850134930
C	-5.660119226	-2.059639944	-0.346852639
C	-6.061548483	-2.688270019	0.981697088
C	-7.074249484	-3.815080823	0.792295068
C	-7.482035801	-4.466914209	2.109823776
C	-4.471939546	2.695206390	0.295024293
C	-4.537987254	3.459089418	-1.021629756
C	-4.908958260	4.924562321	-0.806984615
C	-4.970277684	5.713165911	-2.111353463
H	7.668144529	1.878969851	-0.290236312
H	9.546023555	0.265454000	-0.169257128
H	9.131688935	-2.148268026	0.095093160
H	6.823244469	-3.039808567	0.239141468
H	2.390630101	1.364390042	0.001814878
H	1.561122061	-1.605628730	-0.155566290
H	0.054368828	1.077676289	0.067450872
H	-0.859685282	-1.859459092	-0.162544264
H	3.881383187	2.516002758	-0.938960776
H	5.615501488	2.741895429	-0.867982448
H	5.511469844	2.918739507	1.628501089
H	3.769354135	2.689543527	1.578545868
H	3.536113654	4.774677210	0.200677661
H	5.274798040	5.004745231	0.253678002
H	5.174803490	5.228211370	2.761502859
H	3.423973311	4.997037601	2.707874512
H	4.148961610	6.428924708	1.968194692
H	3.065357039	-2.373263689	0.978764737
H	4.653444760	-3.100813920	1.012733133
H	4.581952909	-3.455166775	-1.460860943
H	2.980474325	-2.739244828	-1.529469663
H	2.110596819	-4.543600698	-0.012838147
H	3.712333906	-5.255017611	0.058252573
H	3.645335854	-5.668320891	-2.426714417
H	2.032414029	-4.950492678	-2.498096099
H	2.290909553	-6.455033890	-1.607956459
H	-5.184549945	-2.803118104	-0.984415540
H	-6.525872362	-1.645876740	-0.857948528
H	-6.485128518	-1.915631685	1.632447989
H	-5.163779108	-3.075094826	1.475309493
H	-6.651939951	-4.574100347	0.122456873
H	-7.964207928	-3.421261653	0.286383596

H	-7.936748603	-3.736229561	2.786006401
H	-6.614688889	-4.895893170	2.621295812
H	-8.206488874	-5.270077969	1.950452696
H	-3.702303790	3.121147624	0.936446115
H	-5.428950579	2.726763547	0.809657966
H	-5.274789949	2.983374936	-1.677814323
H	-3.565095094	3.391440653	-1.519473848
H	-4.179854729	5.388549007	-0.131473415
H	-5.878430136	4.982084343	-0.297187504
H	-5.714928178	5.289535060	-2.792458749
H	-4.004499253	5.697587515	-2.626094301
H	-5.237027537	6.758443805	-1.933721403

Merocyanine 3 in vacuum, ground state

N	6.327841429	0.872355209	-0.240717830
C	7.453301159	0.060330286	-0.227137453
C	8.800655651	0.347137257	-0.374713349
C	9.692561626	-0.722318526	-0.318364014
C	9.246506481	-2.026963022	-0.116357011
C	7.890174655	-2.311820971	0.033048661
C	7.006094524	-1.247306771	-0.024907056
N	5.620264136	-1.193831166	0.103792898
C	5.196269247	0.110936858	-0.032383175
C	3.918629566	0.645800480	0.030761765
C	2.684106860	-0.027360799	-0.044773736
C	1.453039867	0.569804144	0.056375253
C	0.251253424	-0.157747511	-0.070236877
C	-1.016476834	0.360206152	0.017072606
C	-2.131879968	-0.485942939	-0.125712241
C	-3.475470052	-0.185318414	-0.074558389
C	-4.401486036	-1.289969035	-0.272982279
N	-5.773949539	-0.974823610	-0.267273749
C	-6.288824767	0.274067353	0.004481514
N	-5.385344522	1.287590442	0.236195750
C	-3.980837532	1.150912811	0.163052354
O	-4.051710675	-2.447279022	-0.454284074
O	-3.281008510	2.142613244	0.314323701
S	-7.941017053	0.545943182	0.050697062
C	6.343657584	2.301524542	-0.497059133
C	6.427852013	3.144893919	0.773154811
C	6.449608871	4.641633879	0.472706968
C	6.539075652	5.494099548	1.734338211
C	4.828655363	-2.333054409	0.541290016
C	4.354126688	-3.226634791	-0.602286610
C	3.512200409	-4.399344678	-0.104701744
C	3.049005403	-5.313611582	-1.234237976
C	-6.673297227	-2.111071205	-0.529706394
C	-7.038099217	-2.871227248	0.739296347
C	-7.977989767	-4.038506453	0.448832546
C	-8.345774411	-4.824806440	1.703172079
C	-5.859277941	2.648959632	0.538042788
C	-6.031422423	3.498101492	-0.715242934
C	-6.532606936	4.901295614	-0.383363563
C	-6.699093348	5.775672857	-1.622174960
H	9.153676673	1.361358766	-0.521089281
H	10.753946404	-0.532085597	-0.432068633
H	9.965148658	-2.837784934	-0.076123096
H	7.546718035	-3.328869190	0.182418877
H	3.872240999	1.725488864	0.105856466
H	2.679169869	-1.096663454	-0.235167772
H	1.390048941	1.639928899	0.239370631
H	0.345734420	-1.229751088	-0.252378863

H	-1.173517681	1.416258096	0.194533232
H	-1.930547980	-1.541060359	-0.304040414
H	7.199904633	2.504923454	-1.146673535
H	5.448473145	2.551275333	-1.072837397
H	5.576689988	2.906448444	1.421115149
H	7.328855868	2.861825674	1.330077665
H	7.297932443	4.868422663	-0.185049558
H	5.547801196	4.912125983	-0.090027184
H	6.552790709	6.559782992	1.493357993
H	5.685341719	5.312804957	2.394077410
H	7.448217935	5.268242015	2.299830196
H	5.452317618	-2.911001734	1.230875330
H	3.987920723	-1.954857372	1.125681238
H	3.778398537	-2.630463194	-1.319365350
H	5.227132029	-3.599151677	-1.150877732
H	4.091166252	-4.979465048	0.624551828
H	2.639648785	-4.015263126	0.438209335
H	2.447327522	-6.141796784	-0.852507972
H	2.439537884	-4.766966399	-1.959939643
H	3.901343128	-5.740021075	-1.771891311
H	-7.564182366	-1.716892999	-1.013832874
H	-6.140243808	-2.766483004	-1.217102190
H	-6.118205269	-3.242050835	1.204094463
H	-7.513227307	-2.181767677	1.445084248
H	-8.890571226	-3.658130725	-0.026064694
H	-7.508990767	-4.710579980	-0.280586187
H	-9.019448482	-5.654887462	1.473280315
H	-7.454024756	-5.241543906	2.181807127
H	-8.844692776	-4.183709568	2.436475731
H	-6.801730133	2.554569244	1.073041580
H	-5.109399616	3.094174433	1.190384185
H	-5.068425226	3.560683528	-1.233356129
H	-6.739638909	3.002917446	-1.387880913
H	-7.491205384	4.827227611	0.144483885
H	-5.834391159	5.381864758	0.313269480
H	-7.059108347	6.775046317	-1.362580695
H	-5.748904797	5.890743085	-2.153115756
H	-7.416113704	5.334101590	-2.321130818

Merocyanine 3 in vacuum, excited state

N	6.229928398	0.952174702	-0.200693744
C	7.433785895	0.277359359	-0.149631304
C	8.746459487	0.718700366	-0.257331472
C	9.751247224	-0.241300015	-0.167402552
C	9.453132151	-1.590758908	0.027862683
C	8.137158770	-2.033564079	0.138806065
C	7.134431225	-1.077456939	0.047643837
N	5.756179978	-1.186159736	0.133163223
C	5.186455205	0.061863589	-0.024080162
C	3.842396603	0.439659633	-0.015502899
C	2.690741695	-0.353069167	-0.098393673
C	1.401937136	0.177387720	-0.019882888
C	0.228635361	-0.573105702	-0.120221551
C	-1.051802982	-0.019687099	-0.048261626
C	-2.206544793	-0.796984012	-0.157033299
C	-3.539503796	-0.373329623	-0.098640466
C	-4.552649131	-1.397967201	-0.249566019
N	-5.896029883	-0.973806817	-0.240738404
C	-6.306659840	0.316898297	-0.003473363
N	-5.319049990	1.254726968	0.185568713
C	-3.931320967	1.000182069	0.100020909
O	-4.297481793	-2.589394748	-0.397334764

O	-3.148837078	1.942460506	0.212096512
S	-7.936186405	0.726411288	0.052238524
C	6.091398896	2.379779385	-0.433454724
C	6.024285568	3.198944327	0.854167038
C	5.881312300	4.694118588	0.579025915
C	5.815112438	5.523226522	1.857599250
C	5.080333857	-2.423412774	0.496915934
C	4.753635090	-3.312796648	-0.701115727
C	4.037440458	-4.595888495	-0.284728292
C	3.718968640	-5.502324921	-1.469359757
C	-6.883247031	-2.042873720	-0.460984177
C	-7.284012171	-2.739557074	0.833457850
C	-8.310900678	-3.842169401	0.588607288
C	-8.716998496	-4.564202960	1.869571552
C	-5.671453250	2.658515722	0.453033334
C	-5.779498068	3.484139378	-0.823092220
C	-6.150699768	4.935352472	-0.529213445
C	-6.251246250	5.785203287	-1.792076391
H	8.984935807	1.766413713	-0.397623142
H	10.787135608	0.068933207	-0.248532006
H	10.260914554	-2.311139539	0.093340178
H	7.910471619	-3.083377402	0.282860933
H	3.675237914	1.510046275	0.042049434
H	2.770141365	-1.422380073	-0.260692812
H	1.299949498	1.251132754	0.130080132
H	0.318183716	-1.649700660	-0.264540350
H	-1.162998452	1.048820745	0.096274860
H	-2.090287769	-1.867959313	-0.304513482
H	6.945188075	2.692703562	-1.040957986
H	5.199275450	2.539462371	-1.045129528
H	5.181349349	2.848670036	1.460925593
H	6.929123312	3.011095595	1.443932685
H	6.724230855	5.032964471	-0.035984607
H	4.978532458	4.868711954	-0.018950403
H	5.712964877	6.587930512	1.634514574
H	4.961014886	5.229098679	2.474768421
H	6.719505726	5.393765319	2.459721758
H	5.738396818	-2.954809726	1.191315314
H	4.180403825	-2.165445961	1.056674387
H	4.135250373	-2.753403039	-1.412175107
H	5.682486278	-3.556768283	-1.229766661
H	4.656437919	-5.139845527	0.439467373
H	3.109459877	-4.339586538	0.241272404
H	3.205767072	-6.410933634	-1.145789524
H	3.072912843	-4.995145633	-2.191991228
H	4.631310281	-5.802682964	-1.993508981
H	-7.749309841	-1.593625636	-0.942370498
H	-6.411413334	-2.755443869	-1.136470067
H	-6.386317261	-3.163929107	1.295696109
H	-7.696759153	-1.997314919	1.525013191
H	-9.200174578	-3.409337782	0.114274774
H	-7.902735524	-4.566994094	-0.126772821
H	-9.452779984	-5.348915695	1.672458462
H	-7.851032472	-5.031507297	2.348918445
H	-9.156988317	-3.867910308	2.590220767
H	-6.614851929	2.660291228	0.994733782
H	-4.879282698	3.054910625	1.086872945
H	-4.819405414	3.445199283	-1.348681902
H	-6.535706962	3.034444509	-1.475302534
H	-7.106774940	4.962439426	0.007685347
H	-5.405503053	5.371694712	0.147689586
H	-6.518163096	6.820061468	-1.559956881

H	-5.300018553	5.799180763	-2.333467469
H	-7.011727668	5.389241647	-2.472186200

Merocyanine 3 in n-hexane, ground state

N	6.312817875	0.863059946	-0.254565930
C	7.437115637	0.048447963	-0.262478420
C	8.781523618	0.330806971	-0.453137757
C	9.668857078	-0.740431834	-0.407779829
C	9.223933473	-2.043199794	-0.175964192
C	7.873862713	-2.322995988	0.015278194
C	6.992106517	-1.253987612	-0.031789852
N	5.610474515	-1.192280449	0.134169955
C	5.194216405	0.107066403	-0.008048257
C	3.909894268	0.651011775	0.085755058
C	2.687400332	-0.016349772	0.001328999
C	1.445522307	0.583004360	0.112423263
C	0.257743350	-0.140816607	-0.028324172
C	-1.023764383	0.373621612	0.060710075
C	-2.125772580	-0.466557072	-0.102566432
C	-3.482491303	-0.171739896	-0.059729069
C	-4.396450486	-1.271527843	-0.283137453
N	-5.774944445	-0.964017620	-0.283035126
C	-6.294439338	0.277409335	-0.004431208
N	-5.400577312	1.289372589	0.245337890
C	-3.990591015	1.153049338	0.190484409
O	-4.046001969	-2.428930643	-0.481150166
O	-3.298343970	2.148976288	0.367540761
S	-7.955654836	0.544131835	0.029134400
C	6.327358978	2.293750272	-0.521270401
C	6.465568963	3.141544529	0.740668694
C	6.498535753	4.635492576	0.427141796
C	6.640588517	5.495169915	1.678939772
C	4.821361507	-2.329268363	0.590255258
C	4.338879790	-3.232361044	-0.542060741
C	3.510591647	-4.406265284	-0.024511181
C	3.039048447	-5.330565310	-1.142334377
C	-6.665447253	-2.101618369	-0.567636327
C	-7.033985393	-2.883119300	0.687246716
C	-7.962063014	-4.053802962	0.373219572
C	-8.333337000	-4.860241874	1.613726656
C	-5.879259780	2.646715101	0.556201876
C	-6.030194096	3.512202626	-0.688734001
C	-6.535617531	4.911784310	-0.347955419
C	-6.681422956	5.801127976	-1.578764111
H	9.133071252	1.341465231	-0.624237745
H	10.727324820	-0.556641829	-0.554032281
H	9.941923069	-2.854977056	-0.145940047
H	7.531896839	-3.336703791	0.187591945
H	3.871602631	1.728734705	0.188654002
H	2.680851716	-1.082568469	-0.205109907
H	1.385470907	1.650383044	0.311249309
H	0.353205124	-1.209866194	-0.226873815
H	-1.180033023	1.426832883	0.253848575
H	-1.919487212	-1.518012467	-0.295253248
H	7.160100661	2.485314336	-1.203264666
H	5.413504319	2.544939282	-1.064873216
H	5.632955711	2.921112703	1.418514846
H	7.380830758	2.850157786	1.269023422
H	7.328683462	4.844317121	-0.258841026
H	5.582908932	4.914190992	-0.108291151
H	6.662099149	6.558678176	1.429004161
H	5.805551528	5.331088455	2.366562617

H	7.564035678	5.259680345	2.216667668
H	5.452687777	-2.898645641	1.279158711
H	3.986650957	-1.944299042	1.178327278
H	3.750470879	-2.646083332	-1.257047955
H	5.207249040	-3.604719494	-1.097743478
H	4.103314669	-4.977427117	0.700441867
H	2.642837078	-4.023707646	0.526694417
H	2.448141306	-6.160132141	-0.746950996
H	2.416402498	-4.792424640	-1.863248726
H	3.887380914	-5.754559902	-1.688174629
H	-7.555440041	-1.706822867	-1.052349045
H	-6.124816174	-2.743501974	-1.261519863
H	-6.114981415	-3.252937440	1.154511666
H	-7.519424978	-2.208164911	1.400012905
H	-8.873895211	-3.674453028	-0.103915421
H	-7.481653999	-4.711759760	-0.361565368
H	-8.998196618	-5.692485982	1.366632531
H	-7.441924483	-5.276196253	2.093715985
H	-8.843548324	-4.233331546	2.351569633
H	-6.830165684	2.546492433	1.074540855
H	-5.140967319	3.083415239	1.226940569
H	-5.059005214	3.580174613	-1.190489528
H	-6.726748680	3.026600012	-1.380334448
H	-7.502547716	4.832445918	0.163677163
H	-5.848195964	5.383026037	0.365510108
H	-7.044522158	6.797656209	-1.312621885
H	-5.722644217	5.921372976	-2.092899031
H	-7.387741548	5.368791275	-2.294258240

Merocyanine 3 in n-hexane, excited state

N	6.218995172	0.958855835	-0.181018275
C	7.428962762	0.296318021	-0.130946079
C	8.737989846	0.752707418	-0.229270511
C	9.751095085	-0.197541119	-0.144195164
C	9.465768163	-1.553219381	0.036509568
C	8.155120368	-2.010866794	0.137669529
C	7.142824082	-1.063359298	0.052236453
N	5.766034846	-1.186687585	0.130326320
C	5.186288980	0.055880108	-0.018390439
C	3.836467601	0.422940956	-0.013347545
C	2.692496770	-0.375338227	-0.094052443
C	1.399310898	0.156338713	-0.027856870
C	0.228865712	-0.593926017	-0.120519550
C	-1.053930788	-0.035288734	-0.056223284
C	-2.210190649	-0.807274382	-0.150615982
C	-3.546024800	-0.381051058	-0.096541203
C	-4.560010235	-1.404762667	-0.226386864
N	-5.904554294	-0.980773208	-0.219524079
C	-6.311970662	0.313474144	-0.008269737
N	-5.325545640	1.253079988	0.160671169
C	-3.937179340	0.993696854	0.080125033
O	-4.308794222	-2.600951984	-0.354561750
O	-3.154666209	1.938973545	0.177468348
S	-7.945773404	0.726356989	0.040951975
C	6.069381153	2.390552015	-0.390670080
C	5.990051186	3.185322230	0.911162380
C	5.840611108	4.683908494	0.659808193
C	5.762473325	5.490776685	1.951805649
C	5.100194795	-2.440477126	0.457745939
C	4.780644630	-3.294627807	-0.767328199
C	4.086976671	-4.601347705	-0.388563253
C	3.774193779	-5.472525098	-1.600804883

C	-6.893046071	-2.054534903	-0.413901320
C	-7.289969013	-2.723858110	0.896077336
C	-8.314851621	-3.833917983	0.677395669
C	-8.717964879	-4.527161642	1.975106826
C	-5.673972451	2.663003938	0.403109254
C	-5.766269589	3.469953808	-0.886003876
C	-6.128886341	4.928263090	-0.617185453
C	-6.214113353	5.758874602	-1.893907239
H	8.966364173	1.803828338	-0.359485403
H	10.784157186	0.123693589	-0.217769248
H	10.280877766	-2.265640493	0.097874112
H	7.939107358	-3.064342976	0.270160269
H	3.662809308	1.492391160	0.041655041
H	2.773949309	-1.446294001	-0.241395112
H	1.298407925	1.232272644	0.106529949
H	0.316437604	-1.672228317	-0.249721503
H	-1.157589668	1.035757693	0.072991586
H	-2.094803476	-1.880196146	-0.281130190
H	6.923731736	2.719819863	-0.987917783
H	5.180222619	2.554099261	-1.004947242
H	5.145418071	2.820807256	1.506979910
H	6.892872924	2.992794799	1.502208377
H	6.685630656	5.036781781	0.056028144
H	4.940505103	4.863286405	0.059435449
H	5.656089436	6.558602927	1.745891706
H	4.906334154	5.181426487	2.558707717
H	6.664140291	5.355463364	2.556777771
H	5.763919884	-2.986293883	1.134471893
H	4.200333714	-2.207936947	1.028261971
H	4.149918183	-2.722944502	-1.457506319
H	5.710843300	-3.507532711	-1.306629334
H	4.720020402	-5.159040993	0.312395211
H	3.159160130	-4.376893899	0.151888409
H	3.277689621	-6.399540607	-1.304236871
H	3.115397992	-4.951370715	-2.301745706
H	4.687618355	-5.740324346	-2.140507303
H	-7.760275505	-1.616464481	-0.902890610
H	-6.424733519	-2.780655583	-1.076881782
H	-6.391018631	-3.135922502	1.366914243
H	-7.702590158	-1.968243784	1.573065491
H	-9.205428091	-3.413972935	0.194106988
H	-7.905732202	-4.573811951	-0.021704161
H	-9.452482269	-5.317270896	1.796191480
H	-7.850600134	-4.982088084	2.463716644
H	-9.158541029	-3.815449305	2.680185202
H	-6.621138660	2.678057967	0.937343943
H	-4.886796930	3.065435643	1.039000221
H	-4.802876885	3.415976458	-1.403798078
H	-6.519688238	3.016331471	-1.538772969
H	-7.088341633	4.970843808	-0.087438811
H	-5.385109355	5.369294364	0.058085279
H	-6.474689650	6.798968463	-1.679105044
H	-5.258972333	5.757422116	-2.428495421
H	-6.973025073	5.358296314	-2.573089617

Merocyanine 3 in DCM, ground state

N	6.282849456	0.857153037	-0.292589507
C	7.414496168	0.052257511	-0.303724126
C	8.750922250	0.338059193	-0.556345251
C	9.643101122	-0.723042403	-0.490170092
C	9.215833833	-2.020656848	-0.180760345
C	7.880127960	-2.303370725	0.069603438

C	6.988624478	-1.239603500	0.001259494
N	5.613077009	-1.176408910	0.208481028
C	5.196312920	0.103662816	0.021169102
C	3.888942563	0.649420296	0.144613027
C	2.700908561	-0.020393246	0.010849309
C	1.427632104	0.572335988	0.136014974
C	0.271122317	-0.145075611	-0.045207410
C	-1.040807430	0.363360410	0.058467403
C	-2.123085545	-0.456791864	-0.142100466
C	-3.506034960	-0.164038210	-0.088777257
C	-4.407319262	-1.245411612	-0.356497934
N	-5.795949024	-0.945608814	-0.334716932
C	-6.313008591	0.278565579	-0.012519002
N	-5.426235212	1.277970851	0.269842846
C	-4.007947293	1.136426833	0.214982160
O	-4.064876488	-2.400292798	-0.610310493
O	-3.321214720	2.133203493	0.440618851
S	-7.989001575	0.543431416	0.034555685
C	6.278029022	2.285494752	-0.600093837
C	6.487722810	3.159186525	0.633267541
C	6.518129811	4.644282247	0.279706684
C	6.725915967	5.531361194	1.502895693
C	4.832192596	-2.307252219	0.706350576
C	4.383293017	-3.263536151	-0.394975952
C	3.567234229	-4.427300551	0.163392648
C	3.130160836	-5.407130537	-0.920602357
C	-6.680550448	-2.077213873	-0.655902447
C	-7.028443161	-2.913424324	0.569496989
C	-7.945255868	-4.082487195	0.218030564
C	-8.295418381	-4.941503089	1.429073065
C	-5.900336381	2.623436033	0.631707971
C	-6.044666406	3.538759286	-0.578095701
C	-6.540766214	4.927573816	-0.183417366
C	-6.679707575	5.865463706	-1.378512195
H	9.087452945	1.341067650	-0.789574731
H	10.694723215	-0.541918107	-0.681241909
H	9.943210875	-2.823280016	-0.137589280
H	7.553567494	-3.309564872	0.302869895
H	3.851226736	1.718793592	0.316419510
H	2.706991411	-1.076236948	-0.243505743
H	1.367208228	1.629975736	0.381729346
H	0.370319694	-1.203758362	-0.290452812
H	-1.190790656	1.408097098	0.298523331
H	-1.917208808	-1.498571215	-0.380916524
H	7.070068772	2.455225624	-1.332913933
H	5.334405496	2.519028229	-1.096277377
H	5.687876637	2.965664474	1.357215049
H	7.426135209	2.872422035	1.121296258
H	7.317660806	4.827235628	-0.448075427
H	5.580561872	4.917707851	-0.218684250
H	6.744963014	6.588382059	1.226110121
H	5.922337507	5.391248976	2.232216785
H	7.671683137	5.299086884	2.001900319
H	5.463494370	-2.831636762	1.428577120
H	3.983467871	-1.906534917	1.261623936
H	3.794516641	-2.719554211	-1.142217995
H	5.264935753	-3.646217976	-0.921125121
H	4.159480352	-4.955032400	0.920369964
H	2.684772576	-4.035197175	0.683052648
H	2.547835649	-6.229532203	-0.497944277
H	2.510050298	-4.911308151	-1.673511630
H	3.994974862	-5.838430051	-1.433897426

H	-7.579010971	-1.672151708	-1.115323704
H	-6.143939370	-2.685593097	-1.381852504
H	-6.100949434	-3.289628093	1.014112941
H	-7.513709017	-2.274639342	1.315320192
H	-8.865890347	-3.696768887	-0.236743333
H	-7.463618686	-4.704809493	-0.546261218
H	-8.951813809	-5.771708050	1.154391522
H	-7.394590424	-5.364498536	1.884703879
H	-8.807075312	-4.350756273	2.195325034
H	-6.852073940	2.508808213	1.145164967
H	-5.162414074	3.030871716	1.320568112
H	-5.072895191	3.619399041	-1.076770025
H	-6.742198486	3.085976726	-1.290976922
H	-7.508260132	4.835490555	0.325171982
H	-5.850690294	5.365512281	0.548323819
H	-7.036071727	6.852964281	-1.072903380
H	-5.719698710	5.999343856	-1.886938054
H	-7.388592624	5.466607838	-2.110842426

Merocyanine 3 in DCM, excited state

N	6.202267297	0.969864409	-0.158667731
C	7.421020447	0.326322914	-0.114506279
C	8.723294964	0.805461103	-0.205320282
C	9.750487008	-0.129152910	-0.130427886
C	9.486436768	-1.493037455	0.032573783
C	8.184211517	-1.973357694	0.125834429
C	7.156411079	-1.040586065	0.051242260
N	5.782901419	-1.187403673	0.124302650
C	5.184138785	0.047697196	-0.010673585
C	3.831149751	0.396847565	-0.007566364
C	2.692091536	-0.414631108	-0.069990617
C	1.400269799	0.113803924	-0.017602684
C	0.225887540	-0.641186731	-0.093105573
C	-1.050396180	-0.075231159	-0.041648869
C	-2.218134828	-0.838378717	-0.118620864
C	-3.550068719	-0.402015747	-0.077145531
C	-4.572994737	-1.418856097	-0.185893193
N	-5.914811654	-0.986428531	-0.194285996
C	-6.311065664	0.314399468	-0.020651002
N	-5.322401534	1.250727790	0.130425000
C	-3.935264094	0.978349449	0.067108234
O	-4.332166229	-2.621399335	-0.284075864
O	-3.147187834	1.921212473	0.150273686
S	-7.948149145	0.741703294	0.005852580
C	6.032298634	2.404317566	-0.341332357
C	5.926374177	3.168960816	0.976387837
C	5.762147616	4.670419486	0.753929442
C	5.657089263	5.448042342	2.061893832
C	5.136490824	-2.461746855	0.412523196
C	4.817282143	-3.274104827	-0.840519059
C	4.162495794	-4.611497420	-0.502283010
C	3.848886809	-5.440076160	-1.743861147
C	-6.909944446	-2.059505565	-0.365517944
C	-7.310543636	-2.699719621	0.957818705
C	-8.340188998	-3.809785188	0.761444045
C	-8.747123551	-4.473608090	2.073244732
C	-5.660849967	2.669603916	0.339996361
C	-5.731893600	3.453471175	-0.964598191
C	-6.079942261	4.920630206	-0.724956892
C	-6.145489965	5.728617252	-2.017220223
H	8.934679156	1.861435823	-0.323314087
H	10.778407940	0.209327040	-0.198417807

H	10.312962153	-2.192839192	0.085780685
H	7.985595949	-3.031752966	0.244477387
H	3.646499007	1.465043057	0.029970404
H	2.779245611	-1.487988596	-0.189881635
H	1.296932822	1.192742484	0.090013826
H	0.312709563	-1.721776495	-0.196909513
H	-1.143330680	0.999428373	0.062889482
H	-2.107162300	-1.914155265	-0.224556021
H	6.888509381	2.757766370	-0.920763524
H	5.148838159	2.567577701	-0.963281455
H	5.078131628	2.782597129	1.552967768
H	6.824575562	2.975783941	1.573933776
H	6.611373594	5.045293068	0.170053775
H	4.867987986	4.851278574	0.145396290
H	5.540693870	6.519033487	1.877723946
H	4.796827347	5.114697971	2.650289926
H	6.552553690	5.309598566	2.675454833
H	5.814972576	-3.022077954	1.060973147
H	4.241165152	-2.264026216	1.002654666
H	4.161662991	-2.692713341	-1.498657481
H	5.744242216	-3.444050814	-1.399883722
H	4.823019065	-5.180254809	0.163115218
H	3.239867958	-4.432400491	0.063104947
H	3.381428804	-6.391290099	-1.477279742
H	3.164741945	-4.906864152	-2.410904326
H	4.758980907	-5.661440793	-2.309706987
H	-7.774010618	-1.628339372	-0.865223075
H	-6.447652979	-2.801018122	-1.015002567
H	-6.414423294	-3.105553528	1.439111361
H	-7.718851245	-1.929706091	1.621290192
H	-9.228404385	-3.396794344	0.267928538
H	-7.933561686	-4.565625859	0.078361956
H	-9.484183267	-5.264311054	1.909106909
H	-7.882051731	-4.921599632	2.572138484
H	-9.186140268	-3.745716693	2.762664160
H	-6.612194083	2.704412487	0.865080488
H	-4.879244618	3.077395075	0.978799943
H	-4.765565322	3.379709306	-1.474228273
H	-6.483008264	2.997387237	-1.618416775
H	-7.042598388	4.984143303	-0.203148477
H	-5.336534641	5.364920238	-0.051713139
H	-6.395508012	6.774953076	-1.822035285
H	-5.186143938	5.706911777	-2.543670743
H	-6.903888436	5.324980426	-2.695260657

Merocyanine 3 in ethanol, ground state

N	6.272792866	0.855486118	-0.300820182
C	7.408497626	0.056644111	-0.309702296
C	8.741889988	0.347118730	-0.575694464
C	9.639384657	-0.707888571	-0.500490652
C	9.221088457	-2.004205431	-0.169667129
C	7.889607007	-2.291507804	0.093533715
C	6.991648197	-1.232977196	0.015620942
N	5.617315137	-1.173577684	0.230343402
C	5.195856267	0.100301884	0.029817338
C	3.881787574	0.642350154	0.159910417
C	2.703260764	-0.030565509	0.011158422
C	1.421586657	0.558064495	0.142176432
C	0.272006721	-0.157584650	-0.050434719
C	-1.046619818	0.350466918	0.058796580
C	-2.126842555	-0.462177240	-0.152391884
C	-3.515222471	-0.166445607	-0.095595729

C	-4.416789995	-1.240542748	-0.375904626
N	-5.806768530	-0.939284971	-0.348440709
C	-6.320308220	0.281105712	-0.012936835
N	-5.432617089	1.274805149	0.278899892
C	-4.013035861	1.128937456	0.222966309
O	-4.078780144	-2.394543287	-0.645339217
O	-3.324936699	2.123424049	0.461204099
S	-7.999056949	0.549032815	0.038710813
C	6.258706062	2.281525277	-0.623154122
C	6.494509402	3.165768295	0.597634052
C	6.513316838	4.647668891	0.230296703
C	6.746591398	5.545562247	1.440965186
C	4.840713080	-2.304860311	0.736099518
C	4.404624909	-3.273667033	-0.359225660
C	3.598447156	-4.440481245	0.206944562
C	3.172111907	-5.432015521	-0.870665805
C	-6.692716286	-2.066597297	-0.680666672
C	-7.037044672	-2.917657546	0.535551438
C	-7.955378235	-4.082261056	0.173250464
C	-8.301226154	-4.955888720	1.375042300
C	-5.902106743	2.618052739	0.654660225
C	-6.041915690	3.546850284	-0.545408406
C	-6.533743079	4.933194451	-0.136813855
C	-6.667676254	5.884148796	-1.322110970
H	9.070673475	1.348748874	-0.825092431
H	10.688811406	-0.524214749	-0.700850297
H	9.953696310	-2.801646129	-0.119803792
H	7.570646796	-3.295860155	0.344301537
H	3.841225349	1.708171539	0.353091821
H	2.715023750	-1.082423358	-0.258973509
H	1.360229502	1.612227978	0.402553287
H	0.371953149	-1.212616535	-0.309953807
H	-1.193297369	1.392555019	0.312799164
H	-1.923340448	-1.501197119	-0.404578387
H	7.033928559	2.444397880	-1.375062663
H	5.303816353	2.508022316	-1.100106900
H	5.711667652	2.976736296	1.341072836
H	7.444690704	2.885558146	1.066144363
H	7.295946917	4.825746682	-0.516665071
H	5.563952480	4.914421411	-0.248929460
H	6.757002061	6.600268915	1.154782351
H	5.959968307	5.409818387	2.189419336
H	7.703969828	5.319384377	1.920260240
H	5.471665767	-2.817465417	1.466701642
H	3.986253772	-1.903569640	1.281800422
H	3.812500846	-2.741442025	-1.112230441
H	5.291273381	-3.652503882	-0.879491741
H	4.194917140	-4.957054592	0.968162300
H	2.711793599	-4.052343989	0.722308969
H	2.596850956	-6.256892466	-0.442953589
H	2.548751644	-4.947040156	-1.628010240
H	4.041853261	-5.858771625	-1.379417326
H	-7.592380793	-1.656305062	-1.132984969
H	-6.158609328	-2.666201645	-1.415574436
H	-6.108286476	-3.299300463	0.972781695
H	-7.519192510	-2.288057732	1.291236817
H	-8.877575268	-3.691109728	-0.273726551
H	-7.476678622	-4.695209381	-0.600356066
H	-8.958735977	-5.782493952	1.092474386
H	-7.398805850	-5.384588116	1.822080413
H	-8.809973880	-4.374556380	2.150407972
H	-6.854368876	2.502212823	1.166753616

H	-5.163369610	3.015427900	1.348368877
H	-5.069419698	3.629362951	-1.042320983
H	-6.739659759	3.104156886	-1.264489209
H	-7.502195284	4.839276464	0.369670126
H	-5.843269695	5.360861660	0.600540521
H	-7.020991234	6.869476569	-1.006297946
H	-5.706462665	6.020132691	-1.827662857
H	-7.376912623	5.495705495	-2.059713526

Merocyanine 3 in ethanol, excited state

N	6.200109365	0.971859445	-0.156924970
C	7.420267216	0.331826224	-0.112480491
C	8.721297902	0.814901784	-0.203029441
C	9.751028250	-0.116662362	-0.127785348
C	9.490846349	-1.481648004	0.035282909
C	8.190199793	-1.965886151	0.128262508
C	7.159524810	-1.036035389	0.053318953
N	5.786736049	-1.186961651	0.125876935
C	5.184442749	0.046609505	-0.009291150
C	3.831565261	0.392835329	-0.006925268
C	2.692377218	-0.421337891	-0.062275062
C	1.402092698	0.106589489	-0.013563064
C	0.225754930	-0.649889274	-0.084424698
C	-1.048044284	-0.082677679	-0.036499086
C	-2.218870151	-0.844316377	-0.110917002
C	-3.549429108	-0.406080502	-0.072532227
C	-4.574328565	-1.421177412	-0.180388128
N	-5.915437459	-0.986969720	-0.191362652
C	-6.309271541	0.314466987	-0.021236800
N	-5.320371557	1.249952292	0.127847782
C	-3.933595508	0.975304304	0.067086594
O	-4.335561986	-2.624596365	-0.275710904
O	-3.144353576	1.917437455	0.148409355
S	-7.947317278	0.744226564	0.003619646
C	6.026166634	2.406276395	-0.337993016
C	5.911177053	3.167931942	0.980631717
C	5.743949210	4.669249205	0.759668618
C	5.630120750	5.444261582	2.068466288
C	5.143838566	-2.464517056	0.408620861
C	4.823726892	-3.270250326	-0.848442144
C	4.177682906	-4.613397716	-0.516377325
C	3.864267949	-5.435396805	-1.762393405
C	-6.911838107	-2.059247131	-0.362321131
C	-7.313804479	-2.698609799	0.960980106
C	-8.345593909	-3.806751589	0.764654627
C	-8.753709056	-4.469598127	2.076577051
C	-5.657048675	2.670108476	0.333583477
C	-5.726137739	3.451215536	-0.972798210
C	-6.075274759	4.918741080	-0.736679872
C	-6.138730202	5.724066010	-2.030697574
H	8.929473745	1.871474315	-0.321160522
H	10.777984016	0.224781755	-0.195557576
H	10.319413988	-2.179003456	0.088792674
H	7.994812947	-3.024794772	0.247311317
H	3.645186356	1.460909024	0.023082486
H	2.780522426	-1.495419371	-0.173396786
H	1.298151555	1.186253919	0.086548617
H	0.312768742	-1.730973056	-0.181838764
H	-1.139015092	0.992671489	0.062601137
H	-2.108517750	-1.920514896	-0.212729301
H	6.884220029	2.763396800	-0.912134685
H	5.145450054	2.567844232	-0.964170425

H	5.060777307	2.778413946	1.551853601
H	6.806943111	2.976403639	1.582268598
H	6.595239350	5.047232190	0.180910982
H	4.852313862	4.848408052	0.146974457
H	5.511639499	6.515330463	1.885671072
H	4.767867445	5.107233397	2.651928640
H	6.522984006	5.307114291	2.686135186
H	5.825457165	-3.026800941	1.051782863
H	4.249859519	-2.272663855	1.002680511
H	4.162269973	-2.688267680	-1.500207161
H	5.749525522	-3.431810114	-1.412102461
H	4.844205692	-5.182571394	0.142552830
H	3.256132660	-4.443240513	0.053425189
H	3.403260218	-6.391166377	-1.500605393
H	3.174716804	-4.901418394	-2.423316474
H	4.773675472	-5.647609741	-2.332862630
H	-7.774998168	-1.627611468	-0.862994688
H	-6.450553082	-2.801301121	-1.011777153
H	-6.418746249	-3.105938716	1.442908594
H	-7.720352839	-1.927974162	1.624817407
H	-9.233011879	-3.392280838	0.270910774
H	-7.940462157	-4.563345412	0.081581217
H	-9.492082137	-5.258979831	1.912276659
H	-7.889448994	-4.919054237	2.575535061
H	-9.191539676	-3.740888696	2.765911906
H	-6.608396495	2.707579613	0.858318047
H	-4.875940028	3.078396892	0.972549989
H	-4.759162812	3.376844124	-1.481123886
H	-6.475545065	2.993569160	-1.627539209
H	-7.038845568	4.982935995	-0.216588326
H	-5.333421068	5.364641679	-0.062870713
H	-6.389632980	6.770562546	-1.837781795
H	-5.178320693	5.701901897	-2.555149582
H	-6.895619354	5.318787782	-2.709483375