

Supplementary Information:

A Study of the Spiropyran-Merocyanine System Using Ion Mobility-Mass Spectrometry: Experimental Support for the *Cisoid* Conformation

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Experimental

Ion Mobility Instrumentation. All ion mobility data was obtained using a Waters SYNAPT G2 equipped with traveling wave ion mobility (TWIM) in positive ion mode. Both the MassLynx and Driftscope software were used for instrument operation and ion mobility data acquisition. The TWIM N₂ gas flow was set to 120 mL/min and the He gas flow was set to 10 mL/min. Wave velocity and height were set to 750 m/s and 35 V, respectively. The source gas flow was set to 0.0 mL/min and the trap gas flow was set to 0.4 mL/min. Mobility data was obtained over an approximate 30 second period for each drift time measurement. The ESI injection rate was set to 6.00 μ L/min.

Sample Preparation

Equilibrated Samples. All samples were recrystallized prior to use. Each sample was then dissolved in methanol to an approximate concentration of 0.5 mg/mL and equilibrated for at least 24 hours in the dark prior to use. After equilibration, each solution was further diluted by a factor of 50 to a total volume per sample of 1 mL in a quartz cuvette and approximately 50 μ L were immediately placed into a 100 μ L syringe for injection into the ESI source. All samples were prepared at room temperature.

Irradiated Samples. Methanol solutions of SP-1—SP-3 were irradiated in the same quartz cuvette as the equilibrated samples were diluted in using either a Dolan Jenner DC-950 or MH-100 light source. Band selection was performed by filtering the light source output with colored glass filters from Edmund Optics (Models UG-11 or GG-400). Irradiation times were approximately 3 minutes with stirring at room temperature. This amount of time has been determined to be sufficient for reaching a photostationary state (PSS) within the system; a state at which no change in absorbance at a specified wavelength increases or decreases with continued irradiation.

Computational Work

DFT-B3LYP Calculations. ^[1,2] Sheng, et. al. ^[3] identified ground, singlet, triplet and excited state geometries for a model spiropyran. In order to accurately assess the ground state structures of the three spiropyran derivatives used in this study, the Cartesian coordinates provided by Sheng, et. al. for the ground state conformations of the various merocyanine isomers were used as foundational structures from which we modified and computed the geometries of our derivatives according to the DFT-B3LYP method using the 6-31++G(d,p) basis set. All structures were calculated in the protonated form to accurately reflect the product of electrospray ionization. The proton resides on the indoline nitrogen or the phenolate oxygen for the ring-closed and ring-opened isomers, respectively.

Theoretical Collision Cross-Section Calculations. All theoretical collision cross-sections (CCS) were calculated with the MOBCAL program developed by Martin Jarrold's group at Indiana University—Bloomington, available for free online. ^[4] References can be found in the manuscript. Cartesian coordinates from DFT-B3LYP results were imported into the program for each structure. Only the projection approximation method (PA) and Trajectory method (TJ) results are reported for these small molecule systems as suggested by a review of the accepted methods for calculating theoretical CCS values.

Isomer Population Determination. The software OriginPro 8.5 was used to evaluate plots of drift time vs. % relative intensity using the peak finding function incorporated into the program based on a Gaussian distribution about the peak center. The resulting area under each peak after deconvolution was determined by the software from which a total area could be obtained. The fraction of the total area represented by each peak is then equal to the mole fraction of each isomer in the sample. Please note that we assume all isomers have similar ionization efficiency.

Data and Results

N-methyl Spiropyran (SP-1)

Table S1: Experimental drift times and isomer populations for N-methyl spiropyran at equilibrium, UV-irradiated and Vis-irradiated PSS's.

	Drift Time (msec.)	Mole Fraction EQ	Mole Fraction UV	Mole Fraction Vis
Peak 1	3.749	.15	.08	.20
Peak 2	3.969	.64	.12	.64
Peak 3	4.410	.21	.80	.16

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Methoxyspiropyran (SP-2)

Table S2: Experimental drift times and isomer populations for Methoxyspiropyran (SP-2) at equilibrium, UV-irradiated and Vis-irradiated PSS's.

	Drift Time (msec.)	Mole Fraction EQ	Mole Fraction UV	Mole Fraction Vis
Peak 1	4.177	.06	.07	.12
Peak 2	4.449	.14	.16	.31
Peak 3	4.883	.80	.77	.57

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Chlorospiropyran (SP-3)

Table S3: Experimental drift times and isomer populations for Chlorospiropyran at equilibrium, UV-irradiated and Vis-irradiated PSS's.

	Drift Time (msec.)	Mole Fraction EQ	Mole Fraction UV	Mole Fraction Vis
Peak 1	3.601	.03	.03	.03
Peak 2	3.809	.83	.84	.80
Peak 3	4.155	.14	.13	.17

Mass Spectra and Detailed Chromatographs for Each Species Investigated

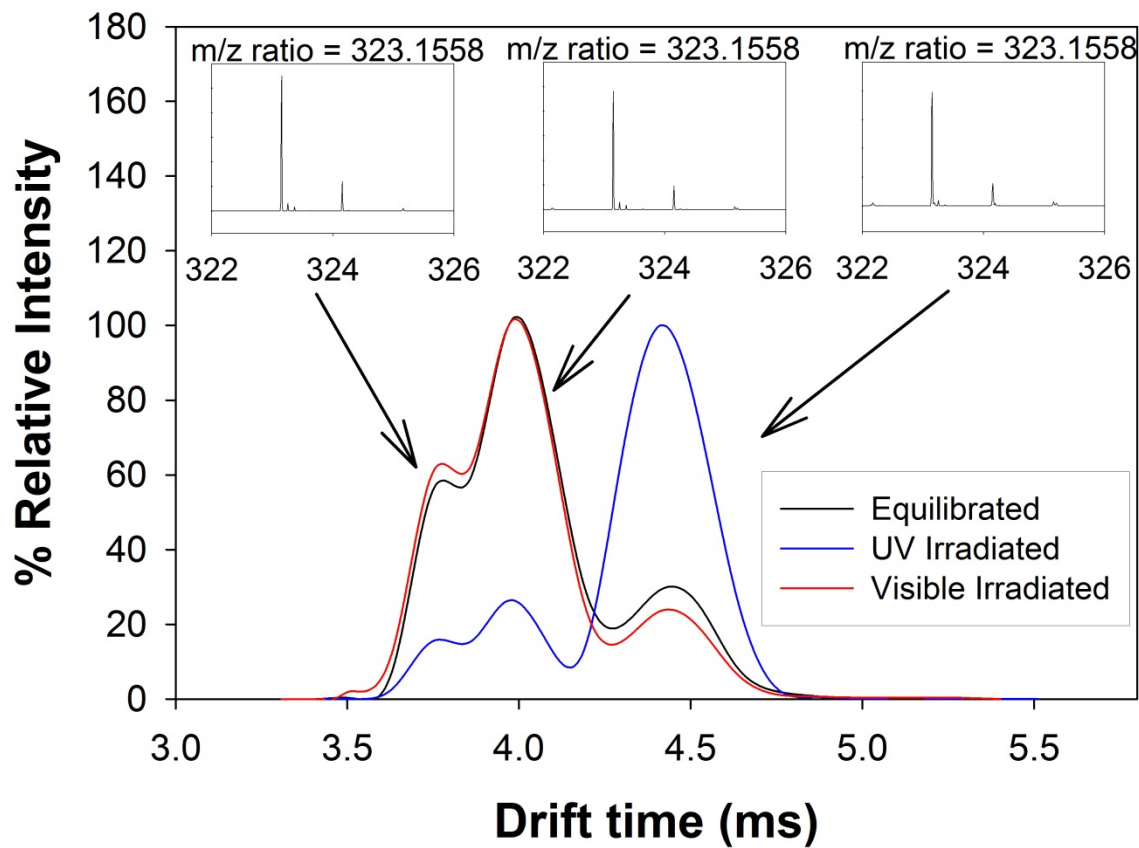


Figure S1: IM-MS Spectra and Chromatographs for N-methyl Spiropyran (SP-1)

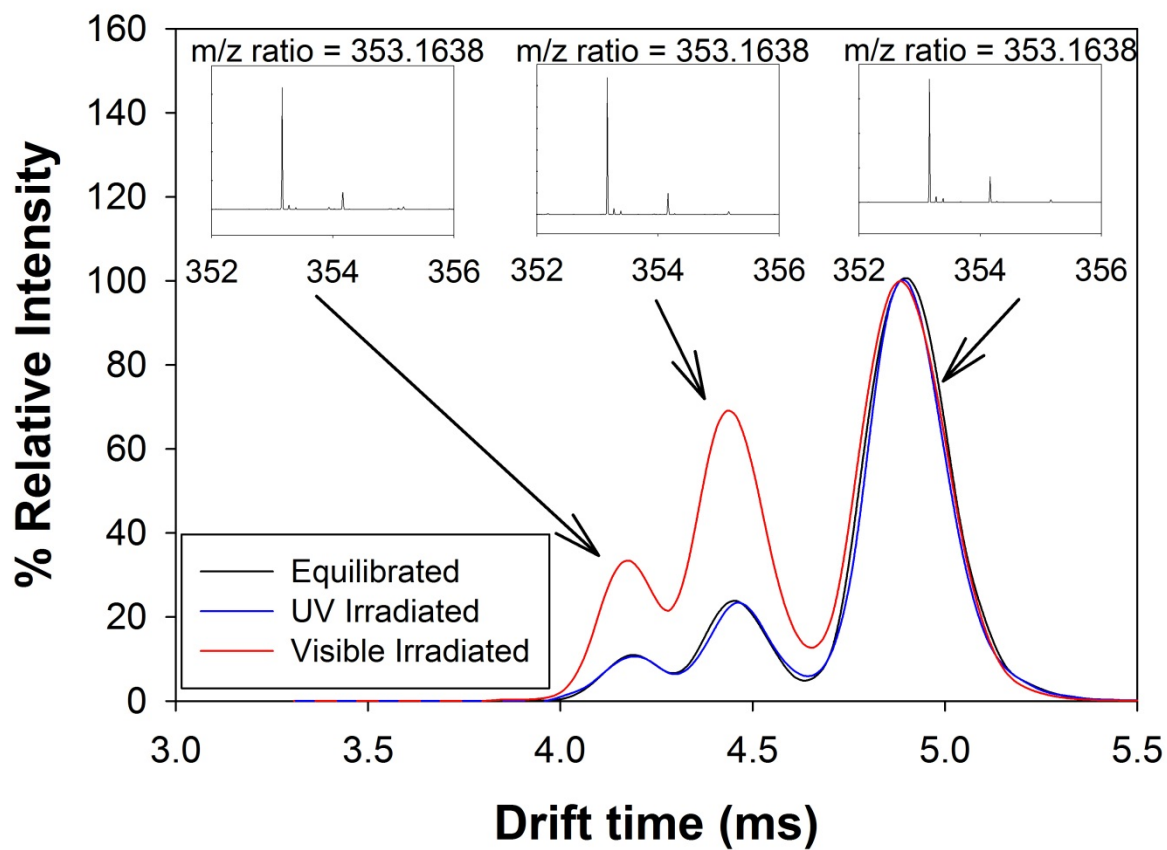


Figure S2: IM-MS Spectra and Chromatographs for Methoxyspiropyran (SP-2)

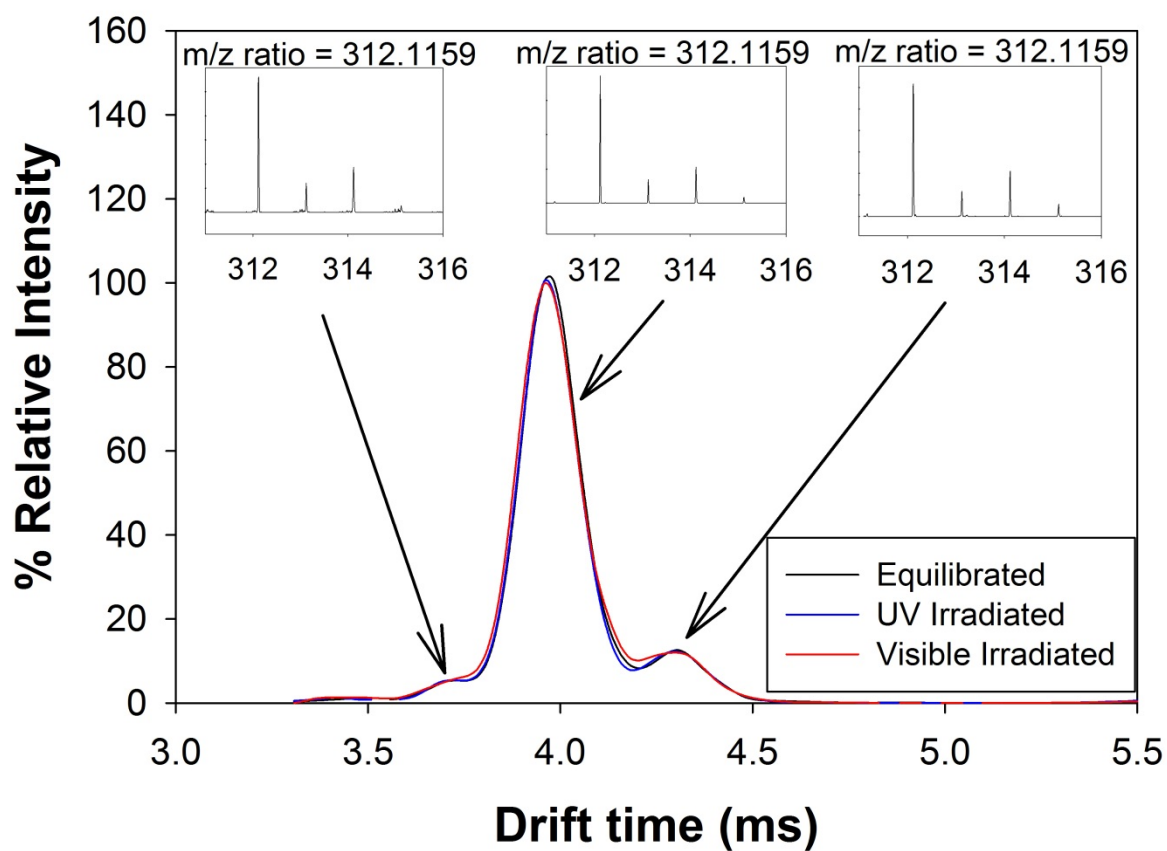


Figure S3: IM-MS Spectra and Chromatographs for Chlorospiropyran (SP-3)

Example Deconvolution Plot for Isomer Population Statistics

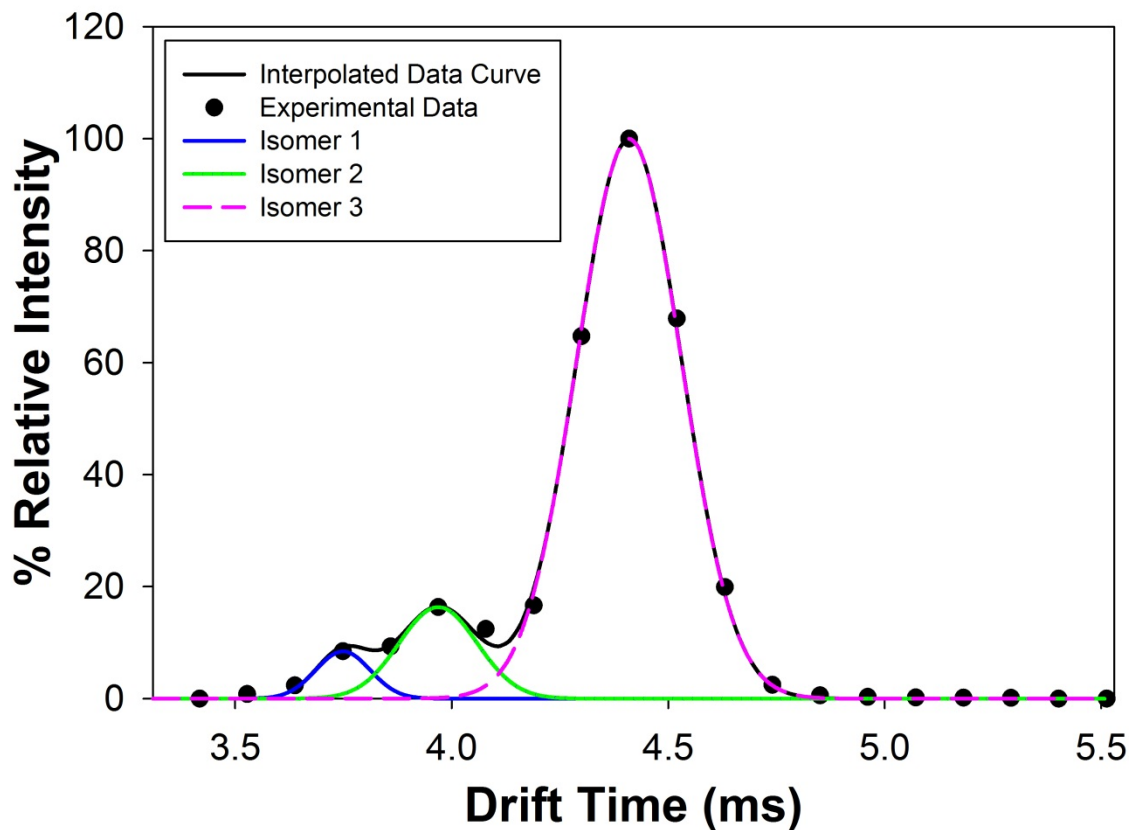


Figure S4: Example of a deconvoluted ion mobility chromatograph. Integration of each resultant Gaussian curve gave individual areas from which the isomer mole fraction could be determined.

DFT-B3LYP Optimized Geometries for Protonated SP and MC isomers

SP-1: N-methylspiropyran

SP

C(1)	-2.8592	-3.9484	-0.367
C(2)	-2.8592	-2.5504	-0.367
C(3)	-1.6232	-1.9144	-0.367
C(4)	-0.4062	-2.5894	-0.36
C(5)	-0.4232	-3.9854	-0.359
C(6)	-1.6502	-4.6554	-0.364
H(7)	-3.8022	-4.4844	-0.363
H(8)	-3.7922	-1.9944	-0.361
H(9)	0.5038	-4.5504	-0.35
H(10)	-1.6662	-5.7404	-0.36
C(11)	0.7918	-1.6544	-0.393
C(12)	0.1778	-0.3014	0.114
N(13)	-1.4312	-0.4554	-0.358
C(14)	1.9478	-2.1074	0.524
H(15)	2.4118	-3.0064	0.109
H(16)	2.7218	-1.3364	0.576
H(17)	1.6198	-2.3404	1.539
C(18)	1.3398	-1.5374	-1.838
H(19)	2.1868	-0.8484	-1.879
H(20)	1.6828	-2.5234	-2.161
H(21)	0.5888	-1.2014	-2.555
H(22)	-1.9682	-0.0374	0.407
C(23)	-1.8282	0.2406	-1.628
H(24)	-2.8992	0.0916	-1.777
H(25)	-1.6082	1.3046	-1.536
H(26)	-1.2782	-0.1894	-2.461
O(27)	0.7178	0.7746	-0.567
C(28)	0.0978	-0.1344	1.598
C(29)	0.8068	2.0376	-0.009
C(30)	0.2748	1.0696	2.17
C(31)	0.5958	2.2336	1.366
H(32)	-0.1322	-1.0164	2.185
H(33)	0.1978	1.1836	3.248
C(34)	1.1638	3.0796	-0.863
C(35)	0.7388	3.5276	1.886
C(36)	1.2998	4.3616	-0.337
C(37)	1.0808	4.5656	1.028
H(38)	1.3398	2.8826	-1.915

H(39)	1.5738	5.2016	-0.965
H(40)	0.5908	3.7276	2.941
N(41)	1.2228	5.9286	1.582
O(42)	1.0238	6.0696	2.787
O(43)	1.5288	6.8246	0.8

CCC

C(1)	3.1564	-2.134	-0.8795
C(2)	2.737	-0.8448	-0.567
C(3)	3.5379	0.0856	0.0977
C(4)	4.8274	-0.2714	0.475
C(5)	5.2777	-1.5648	0.1764
C(6)	4.4546	-2.4816	-0.4904
H(7)	2.5212	-2.8476	-1.3924
H(8)	5.4789	0.4285	0.9893
H(9)	6.2805	-1.8614	0.4659
H(10)	4.8264	-3.4769	-0.7099
C(11)	2.7658	1.3808	0.2476
C(12)	1.4203	0.9936	-0.3631
N(13)	1.4755	-0.2351	-0.847
C(14)	0.4544	-0.9139	-1.6445
H(15)	-0.0791	-1.6439	-1.0311
H(16)	-0.2468	-0.1797	-2.0353
H(17)	0.9469	-1.4248	-2.4734
C(18)	0.3149	1.9111	-0.4687
C(19)	-1.0323	1.7539	-0.3417
H(20)	0.6409	2.931	-0.6625
H(21)	-1.5979	2.6494	-0.594
C(22)	-1.8986	0.6686	0.1127
C(23)	-1.5405	-0.355	1.0282
C(24)	-3.2426	0.7141	-0.3132
C(25)	-2.4853	-1.2939	1.4648
C(26)	-4.1538	-0.2397	0.1085
C(27)	-3.7943	-1.2495	1.0037
H(28)	-4.5342	-1.9707	1.3296
C(29)	3.4184	2.5204	-0.586
H(30)	2.8442	3.4474	-0.5044
H(31)	4.4207	2.7129	-0.1948
H(32)	3.5117	2.2495	-1.6413
C(33)	2.6033	1.8237	1.7215
H(34)	1.9951	2.7298	1.7905
H(35)	2.1344	1.0434	2.3249
H(36)	3.5885	2.0415	2.1424

H(37)	-3.5783	1.4967	-0.9845
H(38)	-2.1896	-2.0612	2.1756
O(39)	-0.2601	-0.3846	1.4888
H(40)	-0.1777	-1.0253	2.2105
N(41)	-5.5429	-0.171	-0.3847
O(42)	-5.8194	0.7343	-1.1697
O(43)	-6.3255	-1.0265	0.0217

CCT

C(1)	2.7326	1.4367	1.6712
C(2)	2.334	0.3752	0.8652
C(3)	3.0622	-0.0709	-0.2389
C(4)	4.2568	0.5596	-0.5667
C(5)	4.6859	1.6315	0.2277
C(6)	3.9346	2.064	1.3283
H(7)	2.1492	1.781	2.5178
H(8)	4.8496	0.2383	-1.4175
H(9)	5.6143	2.1378	-0.0153
H(10)	4.2855	2.9005	1.9232
C(11)	2.3282	-1.2318	-0.8774
C(12)	1.0917	-1.329	0.0149
N(13)	1.1628	-0.4358	0.9892
C(14)	0.2442	-0.2912	2.1189
H(15)	-0.4185	0.5626	1.954
H(16)	-0.346	-1.1997	2.223
H(17)	0.8334	-0.1282	3.0225
C(18)	0.066	-2.3294	-0.1691
C(19)	-1.2927	-2.258	-0.1044
H(20)	0.4712	-3.2927	-0.4715
H(21)	-1.807	-3.2097	-0.213
C(22)	-2.1883	-1.1108	-0.0055
C(23)	-1.8259	0.185	-0.4046
C(24)	-3.5323	-1.3235	0.4107
C(25)	-2.7511	1.2181	-0.3689
C(26)	-4.4547	-0.2676	0.4343
C(27)	-4.0705	1.0085	0.0436
H(28)	-4.7711	1.835	0.0497
C(29)	3.1551	-2.5444	-0.806
H(30)	2.6091	-3.3801	-1.2524
H(31)	4.08	-2.4093	-1.3725
H(32)	3.422	-2.7999	0.2232

C(33)	1.9135	-0.9347	-2.3416
H(34)	1.3165	-1.7543	-2.7511
H(35)	1.3411	-0.0061	-2.4185
H(36)	2.8124	-0.8268	-2.9545
O(37)	-3.8591	-2.5794	0.7893
H(38)	-4.8003	-2.6539	1.0039
H(39)	-5.4752	-0.4495	0.7594
H(40)	-0.8365	0.3971	-0.7878
N(41)	-2.324	2.562	-0.7887
O(42)	-3.1734	3.4481	-0.8083
O(43)	-1.1347	2.7126	-1.0833

CTC

C(1)	1.4213	-4.0969	0.4651
C(2)	1.4213	-2.7049	0.4651
C(3)	2.5873	-1.9379	0.4651
C(4)	3.8233	-2.5739	0.4751
C(5)	3.8553	-3.9749	0.4791
C(6)	2.6713	-4.7239	0.4731
H(7)	0.5103	-4.6839	0.4491
H(8)	4.7493	-2.0069	0.4781
H(9)	4.8113	-4.4879	0.4851
H(10)	2.7213	-5.8079	0.4701
C(11)	2.2143	-0.4709	0.4531
N(12)	0.2973	-1.8219	0.4621
C(13)	0.6873	-0.5509	0.4181
C(14)	-1.0707	-2.3329	0.5821
H(15)	-1.0517	-3.2199	1.2161
H(16)	-1.7037	-1.5779	1.0481
H(17)	-1.4717	-2.6029	-0.3989
C(18)	-0.1357	0.6201	0.3571
C(19)	2.7513	0.2591	-0.8049
C(20)	2.6883	0.2521	1.7421
H(21)	2.3913	1.3051	1.7401
H(22)	3.7803	0.2171	1.7871
H(23)	2.2973	-0.2279	2.6431
H(24)	3.8443	0.2421	-0.7899
H(25)	2.4163	-0.2269	-1.7249
H(26)	2.4293	1.3041	-0.8219
C(27)	-1.3787	0.7191	-0.2139
H(28)	0.3793	1.5261	0.6591
H(29)	-1.7917	-0.1619	-0.6979
C(30)	-2.1977	1.9011	-0.3759

C(31)	-3.1717	1.8711	-1.3999
C(32)	-2.0817	3.0951	0.3951
C(33)	-3.9187	2.9971	-1.6879
C(34)	-2.8447	4.2251	0.0771
C(35)	-3.7567	4.1881	-0.9679
H(36)	-4.3587	5.0521	-1.2219
H(37)	-2.7207	5.1181	0.6811
H(38)	-3.3237	0.9751	-1.9919
O(39)	-1.2537	3.2141	1.4611
N(40)	-4.9107	2.9361	-2.7769
O(41)	-5.0327	1.8641	-3.3699
O(42)	-5.5457	3.9591	-3.0179
H(43)	-1.0277	2.3501	1.8341

CTT

C(1)	1.3403	-4.2327	-0.2303
C(2)	1.3403	-2.8407	-0.2303
C(3)	2.5083	-2.0767	-0.2303
C(4)	3.7433	-2.7137	-0.2413
C(5)	3.7743	-4.1147	-0.2473
C(6)	2.5893	-4.8617	-0.2393
H(7)	0.4293	-4.8197	-0.2143
H(8)	4.6693	-2.1467	-0.2453
H(9)	4.7303	-4.6287	-0.2543
H(10)	2.6373	-5.9457	-0.2373
C(11)	2.1383	-0.6087	-0.2203
N(12)	0.2183	-1.9547	-0.2293
C(13)	0.6113	-0.6827	-0.1853
C(14)	-1.1527	-2.4557	-0.3413
H(15)	-1.1337	-3.3977	-0.8883
H(16)	-1.5877	-2.6227	0.6487
H(17)	-1.7577	-1.7377	-0.8963
C(18)	-0.2007	0.4923	-0.1273
C(19)	2.6153	0.1093	-1.5113
C(20)	2.6803	0.1203	1.0357
H(21)	2.3653	1.1673	1.0507
H(22)	3.7733	0.0973	1.0217
H(23)	2.3413	-0.3617	1.9567
H(24)	3.7073	0.0743	-1.5543
H(25)	2.2233	-0.3747	-2.4103
H(26)	2.3153	1.1613	-1.5163
C(27)	-1.4887	0.5993	0.3167
H(28)	0.3343	1.3953	-0.4033

H(29)	-1.9997	-0.2767	0.6967
C(30)	-2.2657	1.8203	0.3947
C(31)	-3.5697	1.7753	0.9647
C(32)	-1.7967	3.0613	-0.0773
C(33)	-4.3547	2.9333	1.0557
C(34)	-2.5877	4.1903	0.0237
H(35)	-0.8187	3.1623	-0.5303
C(36)	-3.8687	4.1453	0.5877
H(37)	-5.3467	2.8803	1.4947
H(38)	-4.4597	5.0513	0.6477
O(39)	-4.0077	0.5743	1.4077
N(40)	-2.0647	5.4733	-0.4803
O(41)	-0.9327	5.4723	-0.9653
O(42)	-2.7937	6.4573	-0.3803
H(43)	-4.8977	0.6413	1.7837

TTC

C(1)	0.8133	-4.5883	-0.0153
C(2)	0.8133	-3.1953	-0.0153
C(3)	1.9803	-2.4313	-0.0153
C(4)	3.2163	-3.0673	-0.0043
C(5)	3.2473	-4.4683	-0.0023
C(6)	2.0623	-5.2163	-0.0093
C(7)	1.6173	-0.9583	-0.0193
N(8)	-0.3017	-2.3093	-0.0233
C(9)	0.0833	-1.0313	-0.0593
C(10)	-1.6787	-2.8163	-0.0123
C(11)	2.1193	-0.2883	1.2907
C(12)	2.1933	-0.2523	-1.2723
C(13)	-0.8627	0.0347	-0.1613
C(14)	-0.5517	1.3687	-0.0773
C(15)	-1.4447	2.5047	-0.1393
C(16)	-0.9837	3.7107	0.4387
C(17)	-2.7577	2.4977	-0.6973
C(18)	-1.8217	4.8037	0.5377
C(19)	-3.5907	3.6157	-0.5753
C(20)	-3.1347	4.7677	0.0497
O(21)	-3.2697	1.4367	-1.3703
N(22)	-1.3167	6.0367	1.1707
O(23)	-0.1537	6.0277	1.5747
O(24)	-2.0907	6.9857	1.2517
H(25)	-0.0977	-5.1753	-0.0273
H(26)	4.1423	-2.5003	-0.0013
H(27)	4.2033	-4.9823	0.0027

H(28)	2.1113	-6.3003	-0.0113
H(29)	-2.0107	-3.0313	-1.0333
H(30)	-1.7057	-3.7333	0.5747
H(31)	-2.3467	-2.0953	0.4547
H(32)	3.2053	-0.3993	1.3477
H(33)	1.8933	0.7787	1.3247
H(34)	1.6853	-0.7643	2.1747
H(35)	1.9283	0.8077	-1.3013
H(36)	3.2843	-0.3243	-1.2523
H(37)	1.8413	-0.7243	-2.1933
H(38)	-1.9027	-0.2523	-0.2533
H(39)	0.4793	1.6397	0.1237
H(40)	0.0203	3.7797	0.8427
H(41)	-4.5847	3.5667	-1.0033
H(42)	-3.7647	5.6447	0.1447
H(43)	-2.5667	0.8957	-1.7573

TTT

C(1)	0	0	0
C(2)	0	1.397	0
C(3)	1.197	2.13	0
C(4)	2.416	1.468	0
C(5)	2.438	0.064	0
C(6)	1.239	-0.654	0
H(7)	-0.919	-0.577	0
H(8)	3.35	2.026	0
H(9)	3.387	-0.464	0
H(10)	1.262	-1.74	0
C(11)	0.883	3.62	0
N(12)	-1.083	2.283	0
C(13)	-0.655	3.605	0
C(14)	-2.477	1.887	0
H(15)	-2.991	2.267	-0.891
H(16)	-2.548	0.8	0
H(17)	-2.991	2.267	0.891
C(18)	1.454	4.293	1.273
H(19)	2.545	4.198	1.285
H(20)	1.205	5.356	1.313
H(21)	1.062	3.816	2.176
C(22)	1.454	4.293	-1.273
H(23)	1.205	5.356	-1.313
H(24)	2.545	4.198	-1.285
H(25)	1.062	3.816	-2.176
C(26)	-1.547	4.668	0

C(27)	-1.238	6.036	0
H(28)	-2.599	4.399	0
H(29)	-0.203	6.348	0
C(30)	-2.2	7.103	0
C(31)	-1.756	8.462	0
C(32)	-3.6	6.908	0
C(33)	-2.651	9.532	0
C(34)	-4.476	7.989	-0.001
C(35)	-4.028	9.312	0
H(36)	-4.736	10.13	-0.001
H(37)	-4.022	5.913	0
N(38)	-5.919	7.728	-0.001
O(39)	-6.299	6.553	-0.001
O(40)	-6.682	8.698	-0.001
O(41)	-0.405	8.664	0
H(42)	-2.269	10.55	0
H(43)	-0.212	9.611	0

SP-2: Methoxyspiropyran

SP

C(1)	3.1925	1.2795	0.1415
C(2)	1.8323	1.2418	-0.1694
C(3)	1.2136	-0.0027	-0.3846
C(4)	1.9399	-1.2187	-0.2944
C(5)	3.3118	-1.1569	0.0146
C(6)	3.906	0.0828	0.2263
C(7)	1.221	-2.4394	-0.5034
C(8)	-0.1559	-2.3766	-0.7779
C(9)	-0.8234	-1.1768	-0.8543
O(10)	-0.1236	0.0062	-0.6709
C(11)	-2.9746	-0.1109	1.1369
C(12)	-2.9365	0.101	-0.2755
C(13)	-2.2736	-0.9176	-1.2382
C(14)	-3.6604	0.815	1.9483
C(15)	-4.2989	1.9278	1.4043
C(16)	-4.2565	2.1508	0.0314
C(17)	-3.5756	1.2385	-0.7804
H(18)	-3.5544	1.4313	-1.846
H(19)	-4.74	3.0165	-0.4102
H(20)	-4.819	2.6189	2.0617
H(21)	-3.6935	0.6632	3.0205

H(22)	-0.718	-3.2901	-0.9291
H(23)	1.7369	-3.3902	-0.4387
H(24)	3.9013	-2.0616	0.0943
H(25)	3.6775	2.2296	0.3235
N(26)	5.3372	0.1388	0.552
O(27)	5.9524	-0.9287	0.6234
O(28)	5.8462	1.2477	0.7343
C(29)	0.6397	2.8767	-1.4364
H(30)	0.1479	3.8291	-1.235
H(31)	1.4745	3.0321	-2.1305
H(32)	-0.0817	2.1763	-1.8654
O(33)	1.1245	2.4121	-0.1668
C(34)	-3.0995	-2.2303	-1.2328
H(35)	-4.1196	-1.997	-1.5492
H(36)	-2.692	-2.9619	-1.9386
H(37)	-3.1544	-2.6839	-0.2409
C(38)	-2.2398	-0.4127	-2.7082
H(39)	-1.7377	-1.1584	-3.3318
H(40)	-3.252	-0.2776	-3.1001
H(41)	-1.699	0.532	-2.8046
C(42)	-2.2266	-1.3553	3.159
H(43)	-3.2015	-1.4539	3.6487
H(44)	-1.6597	-2.2659	3.3663
H(45)	-1.6971	-0.5038	3.6141
N(46)	-2.3821	-1.2323	1.7187
H(47)	-1.6144	-1.6252	1.1931

CCC

C(1)	-3.3169	1.5291	-1.6994
C(2)	-2.9516	0.4489	-0.9025
C(3)	-3.7549	-0.0596	0.1197
C(4)	-4.9905	0.5258	0.3709
C(5)	-5.3852	1.6182	-0.4139
C(6)	-4.5606	2.112	-1.4329
H(7)	-2.6797	1.9167	-2.4867
H(8)	-5.6418	0.1528	1.1554
H(9)	-6.3452	2.0892	-0.2298
H(10)	-4.8882	2.9592	-2.0262
C(11)	-3.0493	-1.2371	0.7603
C(12)	-1.7332	-1.2482	-0.0149
N(13)	-1.7515	-0.3242	-0.9595
C(14)	-0.7504	-0.1145	-2.0046
H(15)	-0.1366	0.7575	-1.7665
H(16)	-0.1196	-0.9976	-2.0835

H(17)	-1.2685	0.0502	-2.9508
C(18)	-0.6932	-2.216	0.2215
C(19)	0.6666	-2.1274	0.2296
H(20)	-1.09	-3.198	0.4712
H(21)	1.1635	-3.0891	0.3451
C(22)	1.6176	-1.0209	0.1833
C(23)	1.3505	0.3019	0.5908
C(24)	2.9446	-1.337	-0.195
C(25)	2.3769	1.28	0.6064
C(26)	3.9178	-0.3581	-0.1979
C(27)	3.6636	0.9605	0.204
H(28)	4.471	1.6808	0.1995
C(29)	-3.8263	-2.5607	0.5127
H(30)	-3.2995	-3.4147	0.9477
H(31)	-4.8046	-2.4912	0.9953
H(32)	-3.9855	-2.7443	-0.5535
C(33)	-2.7978	-1.0394	2.2749
H(34)	-2.2332	-1.8805	2.6867
H(35)	-2.2435	-0.1191	2.4708
H(36)	-3.7578	-0.985	2.7952
H(37)	3.2084	-2.3458	-0.4898
O(38)	0.1159	0.6647	1.0106
H(39)	0.174	1.5802	1.3407
N(40)	5.2873	-0.7109	-0.6194
O(41)	5.4917	-1.8713	-0.9704
O(42)	6.1318	0.183	-0.5932
O(43)	1.9498	2.4945	1.049
C(44)	2.9096	3.5552	1.2055
H(45)	3.3505	3.8182	0.2391
H(46)	2.3485	4.4016	1.5986
H(47)	3.69	3.2623	1.9144

CCT

C(1)	3.2093	1.4559	1.7133
C(2)	2.8458	0.3835	0.9051
C(3)	3.6199	-0.0744	-0.1623
C(4)	4.8259	0.5546	-0.4484
C(5)	5.22	1.6377	0.3491
C(6)	4.4231	2.082	1.4121
H(7)	2.5903	1.8095	2.5302
H(8)	5.4537	0.2241	-1.2701
H(9)	6.1565	2.1435	0.1378
H(10)	4.7473	2.927	2.0101
C(11)	2.9146	-1.2441	-0.8169

C(12)	1.6405	-1.3307	0.0221
N(13)	1.6713	-0.4275	0.9898
C(14)	0.7094	-0.2752	2.0817
H(15)	0.054	0.5773	1.8852
H(16)	0.1148	-1.1828	2.1676
H(17)	1.2637	-0.1076	3.0065
C(18)	0.621	-2.3291	-0.1954
C(19)	-0.7394	-2.2505	-0.1874
H(20)	1.034	-3.2966	-0.4731
H(21)	-1.254	-3.2008	-0.3079
C(22)	-1.6323	-1.0996	-0.1386
C(23)	-1.246	0.2036	-0.5135
C(24)	-2.9861	-1.3198	0.1979
C(25)	-2.1806	1.2218	-0.5249
C(26)	-3.9274	-0.258	0.1724
C(27)	-3.5283	1.0198	-0.188
H(28)	-4.2138	1.856	-0.2246
C(29)	3.7375	-2.5551	-0.6905
H(30)	3.2103	-3.3977	-1.1464
H(31)	4.6858	-2.429	-1.2192
H(32)	3.9601	-2.7946	0.353
C(33)	2.5653	-0.9675	-2.3018
H(34)	1.989	-1.7943	-2.7263
H(35)	1.994	-0.0422	-2.4164
H(36)	3.4904	-0.8652	-2.8754
O(37)	-3.3863	-2.5527	0.5559
H(38)	-4.3461	-2.5401	0.7185
H(39)	-0.2395	0.4219	-0.8424
N(40)	-1.7456	2.5721	-0.9156
O(41)	-2.6029	3.4505	-0.9784
O(42)	-0.5447	2.7398	-1.1452
O(43)	-5.1805	-0.6435	0.5217
C(44)	-6.243	0.3253	0.4921
H(45)	-7.1396	-0.2159	0.7895
H(46)	-6.0436	1.1337	1.2025
H(47)	-6.3668	0.726	-0.5188

CTC

C(1)	1.721	-4.667	0.406
C(2)	1.721	-3.275	0.406
C(3)	2.888	-2.509	0.406
C(4)	4.124	-3.145	0.417
C(5)	4.155	-4.546	0.421
C(6)	2.971	-5.295	0.413

H(7)	0.81	-5.254	0.39
H(8)	5.05	-2.578	0.42
H(9)	5.111	-5.06	0.426
H(10)	3.02	-6.378	0.41
C(11)	2.516	-1.041	0.396
N(12)	0.598	-2.391	0.404
C(13)	0.989	-1.119	0.362
C(14)	-0.77	-2.902	0.527
H(15)	-0.751	-3.787	1.164
H(16)	-1.402	-2.145	0.99
H(17)	-1.172	-3.174	-0.453
C(18)	0.167	0.05	0.302
C(19)	3.052	-0.311	-0.862
C(20)	2.995	-0.321	1.685
H(21)	2.701	0.732	1.685
H(22)	4.086	-0.361	1.729
H(23)	2.602	-0.802	2.586
H(24)	4.145	-0.326	-0.849
H(25)	2.716	-0.797	-1.782
H(26)	2.727	0.733	-0.88
C(27)	-1.078	0.146	-0.267
H(28)	0.681	0.958	0.603
H(29)	-1.486	-0.737	-0.751
C(30)	-1.905	1.322	-0.431
C(31)	-2.875	1.279	-1.463
C(32)	-1.786	2.502	0.348
C(33)	-3.619	2.405	-1.737
C(34)	-2.56	3.652	0.036
C(35)	-3.472	3.597	-1.014
H(36)	-4.092	4.444	-1.278
H(37)	-3.016	0.386	-2.06
O(38)	-0.965	2.618	1.415
N(39)	-4.611	2.357	-2.828
O(40)	-4.733	1.294	-3.436
O(41)	-5.25	3.382	-3.056
H(42)	-0.737	1.748	1.773
O(43)	-2.344	4.722	0.822
C(44)	-3.099	5.919	0.583
H(45)	-2.756	6.629	1.333
H(46)	-2.898	6.313	-0.419
H(47)	-4.171	5.735	0.71

CTT

C(1)	1.9109	-4.5661	-0.4281
C(2)	1.9109	-3.1741	-0.4281
C(3)	3.0799	-2.4101	-0.4281
C(4)	4.3149	-3.0471	-0.4401
C(5)	4.3459	-4.4491	-0.4441
C(6)	3.1609	-5.1951	-0.4371
H(7)	0.9999	-5.1531	-0.4111
H(8)	5.2409	-2.4811	-0.4431
H(9)	5.3009	-4.9631	-0.4511
H(10)	3.2079	-6.2791	-0.4341
C(11)	2.7099	-0.9421	-0.4171
N(12)	0.7899	-2.2891	-0.4251
C(13)	1.1829	-1.0161	-0.3781
C(14)	-0.5811	-2.7901	-0.5391
H(15)	-0.5621	-3.7261	-1.0951
H(16)	-1.0141	-2.9671	0.4499
H(17)	-1.1881	-2.0681	-1.0861
C(18)	0.3709	0.1569	-0.3091
C(19)	3.1809	-0.2261	-1.7121
C(20)	3.2579	-0.2111	0.8339
H(21)	2.9409	0.8359	0.8499
H(22)	4.3499	-0.2321	0.8129
H(23)	2.9249	-0.6921	1.7579
H(24)	4.2729	-0.2601	-1.7591
H(25)	2.7869	-0.7121	-2.6091
H(26)	2.8789	0.8249	-1.7181
C(27)	-0.9131	0.2609	0.1479
H(28)	0.9009	1.0629	-0.5831
H(29)	-1.4221	-0.6191	0.5239
C(30)	-1.6851	1.4809	0.2479
C(31)	-2.9761	1.4139	0.8199
C(32)	-1.2171	2.7369	-0.2011
C(33)	-3.7791	2.5769	0.9449
C(34)	-2.0201	3.8489	-0.0681
H(35)	-0.2421	2.8549	-0.6541
C(36)	-3.3041	3.7999	0.5019
H(37)	-3.8831	4.7119	0.5769
O(38)	-3.4571	0.2339	1.2529
N(39)	-1.5141	5.1509	-0.5411
O(40)	-0.3851	5.1789	-1.0311
O(41)	-2.2551	6.1249	-0.4151
H(42)	-4.3491	0.3749	1.6159
O(43)	-4.9861	2.3359	1.5179
C(44)	-5.8951	3.4339	1.7149
H(45)	-5.4491	4.1849	2.3739

H(46)	-6.1681	3.8819	0.7549
H(47)	-6.7761	3.0019	2.1869

TTC

C(1)	1.3171	-4.993	0.0971
C(2)	1.3171	-3.6	0.0971
C(3)	2.4851	-2.837	0.0971
C(4)	3.7201	-3.474	0.1071
C(5)	3.7511	-4.875	0.1091
C(6)	2.5661	-5.622	0.1031
C(7)	2.1231	-1.363	0.0961
N(8)	0.2031	-2.714	0.0891
C(9)	0.5891	-1.435	0.0511
C(10)	-1.1769	-3.211	0.0991
C(11)	2.6211	-0.697	1.4091
C(12)	2.7051	-0.653	-1.1529
C(13)	-0.3569	-0.371	-0.0569
C(14)	-0.0459	0.964	0.0221
C(15)	-0.9339	2.103	-0.0519
C(16)	-0.4659	3.308	0.5311
C(17)	-2.2309	2.081	-0.6259
C(18)	-1.3109	4.393	0.6061
C(19)	-3.0859	3.21	-0.5219
C(20)	-2.6179	4.364	0.1021
O(21)	-2.7319	1.02	-1.3009
N(22)	-0.8239	5.635	1.2361
O(23)	0.3311	5.639	1.6611
O(24)	-1.6049	6.582	1.2951
H(25)	0.4061	-5.58	0.0841
H(26)	4.6471	-2.908	0.1111
H(27)	4.7071	-5.389	0.1141
H(28)	2.6141	-6.706	0.1011
H(29)	-1.5319	-3.368	-0.9239
H(30)	-1.2009	-4.158	0.6361
H(31)	-1.8299	-2.51	0.6171
H(32)	3.7071	-0.801	1.4661
H(33)	2.3871	0.369	1.4471
H(34)	2.1881	-1.179	2.2901
H(35)	2.4401	0.406	-1.1789
H(36)	3.7951	-0.726	-1.1299
H(37)	2.3551	-1.122	-2.0769
H(38)	-1.3959	-0.66	-0.1529
H(39)	0.9841	1.234	0.2311
H(40)	0.5321	3.377	0.9471

H(41)	-3.2279	5.254	0.1891
H(42)	-2.0169	0.483	-1.6719
O(43)	-4.3049	3.065	-1.0729
C(44)	-5.2179	4.17	-1.0299
H(45)	-5.4549	4.441	0.0041
H(46)	-4.8089	5.035	-1.5639
H(47)	-6.1169	3.819	-1.5339

TTT

C(1)	0	0	0
C(2)	0	1.397	0
C(3)	1.197	2.13	0
C(4)	2.416	1.468	0
C(5)	2.438	0.064	0
C(6)	1.239	-0.654	0
H(7)	-0.919	-0.576	0
H(8)	3.349	2.026	0
H(9)	3.387	-0.464	0
H(10)	1.261	-1.74	0
C(11)	0.884	3.62	0
N(12)	-1.083	2.283	0
C(13)	-0.653	3.606	0
C(14)	-2.477	1.887	0
H(15)	-2.991	2.267	-0.891
H(16)	-2.547	0.8	0
H(17)	-2.991	2.268	0.89
C(18)	1.456	4.293	1.273
H(19)	2.547	4.197	1.286
H(20)	1.207	5.356	1.312
H(21)	1.062	3.816	2.176
C(22)	1.456	4.293	-1.273
H(23)	1.207	5.356	-1.312
H(24)	2.547	4.197	-1.286
H(25)	1.062	3.816	-2.176
C(26)	-1.545	4.67	0
C(27)	-1.236	6.038	0
H(28)	-2.597	4.402	0
H(29)	-0.201	6.352	0
C(30)	-2.2	7.104	-0.001
C(31)	-1.752	8.452	-0.001
C(32)	-3.603	6.907	-0.001
C(33)	-2.653	9.533	-0.001
C(34)	-4.468	7.99	-0.001
C(35)	-4.026	9.322	-0.001

H(36)	-4.747	10.126	-0.001
H(37)	-4.027	5.913	-0.001
N(38)	-5.911	7.743	-0.001
O(39)	-6.304	6.572	-0.001
O(40)	-6.667	8.721	-0.001
O(41)	-0.415	8.702	-0.001
H(42)	-0.291	9.665	-0.001
O(43)	-2.037	10.761	-0.001
C(44)	-2.855	11.93	-0.002
H(45)	-3.484	11.967	-0.898
H(46)	-3.484	11.968	0.894
H(47)	-2.166	12.776	-0.002

SP-3: Chlorospiropyran

SP

C(1)	0.611	2.544	1.459
C(2)	0.327	1.37	2.261
C(3)	0.996	4.91	1.136
C(4)	1.248	4.695	-0.226
C(5)	0.686	3.847	1.979
C(6)	1.18	3.406	-0.753
C(7)	0.853	2.351	0.091
C(8)	0.196	0.158	1.687
C(9)	-1.728	0.549	-1.552
C(10)	1.435	-1.227	-1.757
C(11)	2.046	-1.82	0.596
N(12)	-1.344	-0.149	-0.283
C(13)	0.293	0.003	0.206
C(14)	0.889	-1.351	-0.313
C(15)	-1.556	-4.35	-0.289
C(16)	-0.33	-3.678	-0.282
C(17)	-0.313	-2.281	-0.283
C(18)	-1.53	-1.605	-0.291
C(19)	-2.765	-2.245	-0.291
C(20)	-2.765	-3.643	-0.291
H(21)	0.505	4.02	3.035
H(22)	-3.708	-4.179	-0.287
H(23)	-2.798	0.408	-1.714
H(24)	-1.879	0.27	0.483
Cl(25)	1.082	6.528	1.783
H(26)	-1.501	1.61	-1.458
H(27)	1.498	5.533	-0.867

H(28)	0.237	1.479	3.338
H(29)	-0.01	-0.73	2.272
H(30)	-1.173	0.117	-2.381
H(31)	0.683	-0.884	-2.471
H(32)	1.774	-2.212	-2.088
H(33)	2.283	-0.54	-1.795
H(34)	1.721	-2.058	1.611
H(35)	2.825	-1.054	0.651
H(36)	2.501	-2.719	0.172
H(37)	-1.571	-5.435	-0.285
H(38)	1.386	3.22	-1.802
O(39)	0.834	1.075	-0.462
H(40)	0.597	-4.241	-0.273
H(41)	-3.698	-1.689	-0.285

CCC

C(1)	2.9642	-2.1543	-0.7659
C(2)	2.5297	-0.8564	-0.5171
C(3)	3.3178	0.1113	0.1083
C(4)	4.6088	-0.2145	0.5078
C(5)	5.0743	-1.5157	0.2722
C(6)	4.2638	-2.4706	-0.3547
H(7)	2.3383	-2.8976	-1.2471
H(8)	5.25	0.5152	0.9927
H(9)	6.0785	-1.7879	0.5803
H(10)	4.6461	-3.4715	-0.5255
C(11)	2.5312	1.4033	0.1977
C(12)	1.1942	0.9772	-0.4078
N(13)	1.265	-0.2731	-0.8341
C(14)	0.257	-0.9967	-1.6071
H(15)	-0.2886	-1.6892	-0.9618
H(16)	-0.4378	-0.2858	-2.0495
H(17)	0.7627	-1.5537	-2.3974
C(18)	0.084	1.8774	-0.5621
C(19)	-1.2663	1.7096	-0.4575
H(20)	0.4031	2.8943	-0.7809
H(21)	-1.833	2.5895	-0.7583
C(22)	-2.1295	0.6403	0.0285
C(23)	-1.7723	-0.3428	0.9834
C(24)	-3.4756	0.668	-0.4108
C(25)	-2.7229	-1.2586	1.4469
C(26)	-4.4031	-0.2611	0.0347
C(27)	-4.0306	-1.2306	0.9741

H(28)	-4.7594	-1.9466	1.3376
C(29)	3.1815	2.5175	-0.6692
H(30)	2.5959	3.4402	-0.6297
H(31)	4.1769	2.7367	-0.2741
H(32)	3.2904	2.2085	-1.7125
C(33)	2.3472	1.8974	1.6528
H(34)	1.7275	2.7978	1.6818
H(35)	1.8793	1.1339	2.2782
H(36)	3.3248	2.1417	2.0771
H(37)	-3.784	1.4325	-1.1165
H(38)	-2.4378	-1.999	2.1902
O(39)	-0.4903	-0.355	1.4586
H(40)	-0.4251	-0.9503	2.2191
Cl(41)	-6.0448	-0.2095	-0.5564

CCT

C(1)	-2.67	1.5382	-1.5806
C(2)	-2.2538	0.449	-0.8216
C(3)	-3.0032	-0.0911	0.2248
C(4)	-4.2368	0.4673	0.539
C(5)	-4.6836	1.5656	-0.2086
C(6)	-3.9112	2.0932	-1.2512
H(7)	-2.0713	1.9542	-2.3832
H(8)	-4.847	0.07	1.3444
H(9)	-5.6426	2.0163	0.0251
H(10)	-4.2768	2.9467	-1.8123
C(11)	-2.2457	-1.2594	0.8214
C(12)	-0.9674	-1.2463	-0.0177
N(13)	-1.0447	-0.303	-0.947
C(14)	-0.1039	-0.0684	-2.0425
H(15)	0.5455	0.7793	-1.8079
H(16)	0.5026	-0.9597	-2.1932
H(17)	-0.6768	0.1442	-2.9461
C(18)	0.0933	-2.2029	0.1569
C(19)	1.451	-2.0757	0.0873
H(20)	-0.2717	-3.1875	0.4409
H(21)	2.002	-3.0111	0.1533
C(22)	2.3003	-0.8962	0.0289
C(23)	1.9095	0.3626	0.5345
C(24)	3.6244	-1.039	-0.4584
C(25)	2.7895	1.4352	0.5339
C(26)	4.502	0.0506	-0.4565
C(27)	4.0906	1.2852	0.0362

H(28)	4.7758	2.1257	0.0447
C(29)	-3.0103	-2.5964	0.6197
H(30)	-2.4484	-3.4392	1.0319
H(31)	-3.9652	-2.5409	1.1488
H(32)	-3.2178	-2.7882	-0.4366
C(33)	-1.9166	-1.05	2.3207
H(34)	-1.3044	-1.8712	2.7036
H(35)	-1.3877	-0.1079	2.49
H(36)	-2.8474	-1.0214	2.8935
O(37)	3.9745	-2.2608	-0.939
H(38)	4.9116	-2.2888	-1.1782
H(39)	0.9293	0.484	0.9809
H(40)	5.5121	-0.066	-0.8399
Cl(41)	2.2792	2.9788	1.1814

CTC

C(1)	1.168	-3.955	0.314
C(2)	1.168	-2.563	0.314
C(3)	2.334	-1.796	0.314
C(4)	3.57	-2.431	0.325
C(5)	3.602	-3.833	0.329
C(6)	2.418	-4.582	0.322
H(7)	0.256	-4.541	0.298
H(8)	4.496	-1.864	0.327
H(9)	4.558	-4.346	0.334
H(10)	2.468	-5.665	0.319
C(11)	1.961	-0.329	0.302
N(12)	0.044	-1.679	0.311
C(13)	0.434	-0.408	0.267
C(14)	-1.324	-2.191	0.432
H(15)	-1.305	-3.077	1.066
H(16)	-1.957	-1.436	0.898
H(17)	-1.725	-2.46	-0.55
C(18)	-0.389	0.762	0.206
C(19)	2.498	0.401	-0.956
C(20)	2.435	0.395	1.592
H(21)	2.138	1.448	1.59
H(22)	3.527	0.359	1.636
H(23)	2.044	-0.085	2.493
H(24)	3.591	0.384	-0.941
H(25)	2.163	-0.085	-1.876
H(26)	2.176	1.446	-0.972
C(27)	-1.632	0.861	-0.364
H(28)	0.126	1.669	0.509

H(29)	-2.045	-0.019	-0.848
C(30)	-2.451	2.044	-0.526
C(31)	-3.426	2.013	-1.55
C(32)	-2.335	3.238	0.245
C(33)	-4.172	3.139	-1.838
C(34)	-3.098	4.368	-0.073
C(35)	-4.01	4.33	-1.119
H(36)	-4.612	5.195	-1.372
H(37)	-2.974	5.26	0.53
H(38)	-3.577	1.117	-2.142
O(39)	-1.507	3.356	1.31
H(40)	-1.281	2.492	1.683
Cl(41)	-5.356	3.066	-3.139

CTT

C(1)	1.247	-3.9479	-0.261
C(2)	1.247	-2.5559	-0.261
C(3)	2.415	-1.7919	-0.261
C(4)	3.65	-2.4289	-0.272
C(5)	3.681	-3.8299	-0.278
C(6)	2.496	-4.5769	-0.27
H(7)	0.336	-4.5349	-0.245
H(8)	4.576	-1.8619	-0.275
H(9)	4.636	-4.3439	-0.284
H(10)	2.544	-5.6609	-0.268
C(11)	2.045	-0.3239	-0.25
N(12)	0.125	-1.6699	-0.259
C(13)	0.518	-0.3979	-0.216
C(14)	-1.246	-2.1709	-0.372
H(15)	-1.227	-3.1129	-0.918
H(16)	-1.681	-2.3369	0.618
H(17)	-1.851	-1.4529	-0.927
C(18)	-0.294	0.7771	-0.158
C(19)	2.522	0.3941	-1.542
C(20)	2.587	0.4051	1.006
H(21)	2.272	1.4521	1.021
H(22)	3.68	0.3821	0.991
H(23)	2.248	-0.0769	1.927
H(24)	3.613	0.3591	-1.585
H(25)	2.13	-0.0899	-2.441
H(26)	2.222	1.4461	-1.547
C(27)	-1.582	0.8841	0.286
H(28)	0.241	1.6801	-0.434

H(29)	-2.093	0.0081	0.666
C(30)	-2.359	2.1051	0.364
C(31)	-3.663	2.0611	0.934
C(32)	-1.89	3.3461	-0.108
C(33)	-4.448	3.2181	1.026
C(34)	-2.681	4.4751	-0.007
H(35)	-0.912	3.4481	-0.56
C(36)	-3.962	4.4311	0.557
H(37)	-5.44	3.1651	1.465
H(38)	-4.554	5.3361	0.618
O(39)	-4.102	0.8591	1.377
H(40)	-4.991	0.9261	1.753
Cl(41)	-2.057	6.0071	-0.608

TTC

C(1)	0.756	-4.277	0.051
C(2)	0.756	-2.884	0.051
C(3)	1.923	-2.12	0.051
C(4)	3.159	-2.756	0.062
C(5)	3.19	-4.157	0.064
C(6)	2.006	-4.905	0.057
C(7)	1.56	-0.647	0.047
N(8)	-0.359	-1.998	0.043
C(9)	0.026	-0.72	0.006
C(10)	-1.736	-2.504	0.053
C(11)	2.062	0.023	1.357
C(12)	2.137	0.06	-1.206
C(13)	-0.92	0.347	-0.095
C(14)	-0.609	1.68	-0.011
C(15)	-1.502	2.817	-0.073
C(16)	-1.041	4.022	0.505
C(17)	-2.814	2.809	-0.631
C(18)	-1.879	5.116	0.603
C(19)	-3.647	3.927	-0.51
C(20)	-3.192	5.079	0.116
H(21)	2.054	-5.988	0.054
O(22)	-3.327	1.748	-1.304
H(23)	-0.155	-4.864	0.038
H(24)	4.085	-2.189	0.065
H(25)	4.146	-4.67	0.069
H(26)	1.836	1.091	1.39
H(27)	-2.068	-2.719	-0.967
H(28)	-1.763	-3.422	0.64
H(29)	-2.404	-1.784	0.521

H(30)	3.148	-0.087	1.414
H(31)	1.628	-0.452	2.24
H(32)	1.871	1.119	-1.235
H(33)	3.227	-0.013	-1.187
H(34)	1.784	-0.412	-2.128
H(35)	-1.96	0.059	-0.187
H(36)	0.422	1.952	0.19
H(37)	-0.037	4.091	0.908
H(38)	-4.642	3.879	-0.938
H(39)	-3.822	5.956	0.211
H(40)	-2.624	1.207	-1.692
Cl(41)	-1.276	6.586	1.359

TTT

C(1)	0	0	0
C(2)	0	1.397	0
C(3)	1.197	2.13	0
C(4)	2.416	1.468	0
C(5)	2.438	0.064	0
C(6)	1.239	-0.654	0
H(7)	-0.919	-0.577	0
H(8)	3.35	2.026	0
H(9)	3.387	-0.464	0
H(10)	1.262	-1.74	0
C(11)	0.883	3.62	0
N(12)	-1.083	2.283	0
C(13)	-0.655	3.605	0
C(14)	-2.477	1.887	0
H(15)	-2.991	2.267	-0.891
H(16)	-2.548	0.8	0
H(17)	-2.991	2.267	0.891
C(18)	1.454	4.293	1.273
H(19)	2.545	4.198	1.285
H(20)	1.205	5.356	1.313
H(21)	1.062	3.816	2.176
C(22)	1.454	4.293	-1.273
H(23)	1.205	5.356	-1.313
H(24)	2.545	4.198	-1.285
H(25)	1.062	3.816	-2.176
C(26)	-1.547	4.668	0
C(27)	-1.238	6.036	0
H(28)	-2.599	4.399	0
H(29)	-0.203	6.348	0
C(30)	-2.2	7.103	0

C(31)	-1.756	8.462	0
C(32)	-3.6	6.908	0
C(33)	-2.651	9.532	0
C(34)	-4.476	7.989	-0.001
C(35)	-4.028	9.312	0
H(36)	-4.736	10.13	-0.001
H(37)	-4.022	5.913	0
O(38)	-0.405	8.664	0
H(39)	-2.269	10.55	0
H(40)	-0.212	9.611	0
Cl(41)	-6.208	7.676	-0.001

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