Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Triphenyl moieties as building blocks for obtaining molecular glasses with nonlinear optical activity

Kaspars Traskovskis,*[a] Igors Mihailovs,[a,b] Andrejs Tokmakovs,[b] Andrejs Jurgis,[b] Valdis Kokars[a] and Martins Rutkis[b]

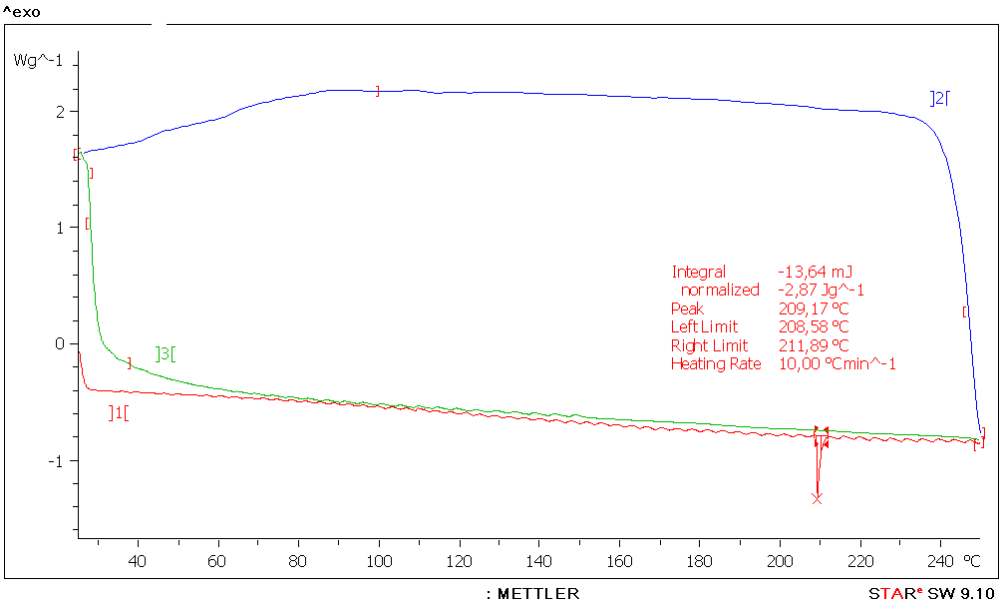
[a] *Riga Technical University, Faculty of Materials Science and Applied Chemistry, 14/24 Azenes Street, Riga, LV-1048, Latvia. Tel: +371 29148070; E-mail: kaspars.traskovskis@rtu.lv*

[b] *Institute of Solid State Physics, University of Latvia, 8 Kengaraga Street, Riga, LV-1063, Latvia.*

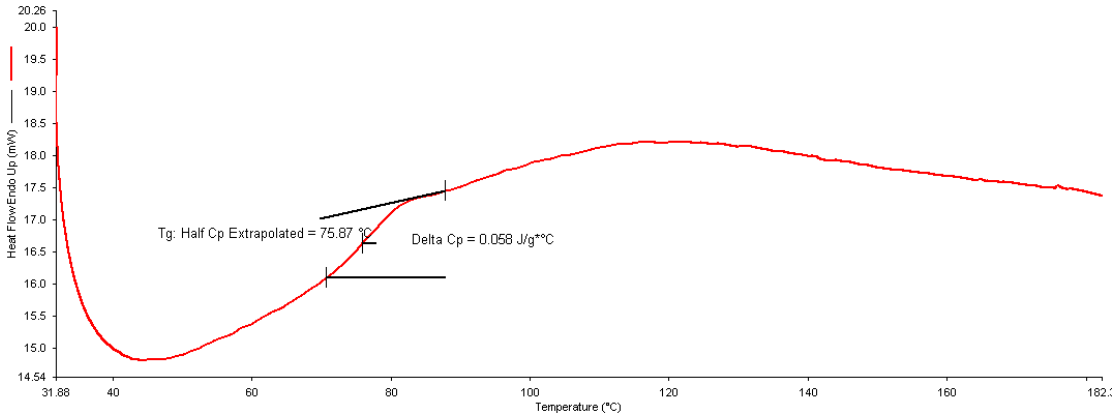
Electronic Supplementary Information

DSC thermograms. In all the cases heating [1]-cooling [2]-heating [3] cycles are given. The first heating [1] represents melting of crystalline material.

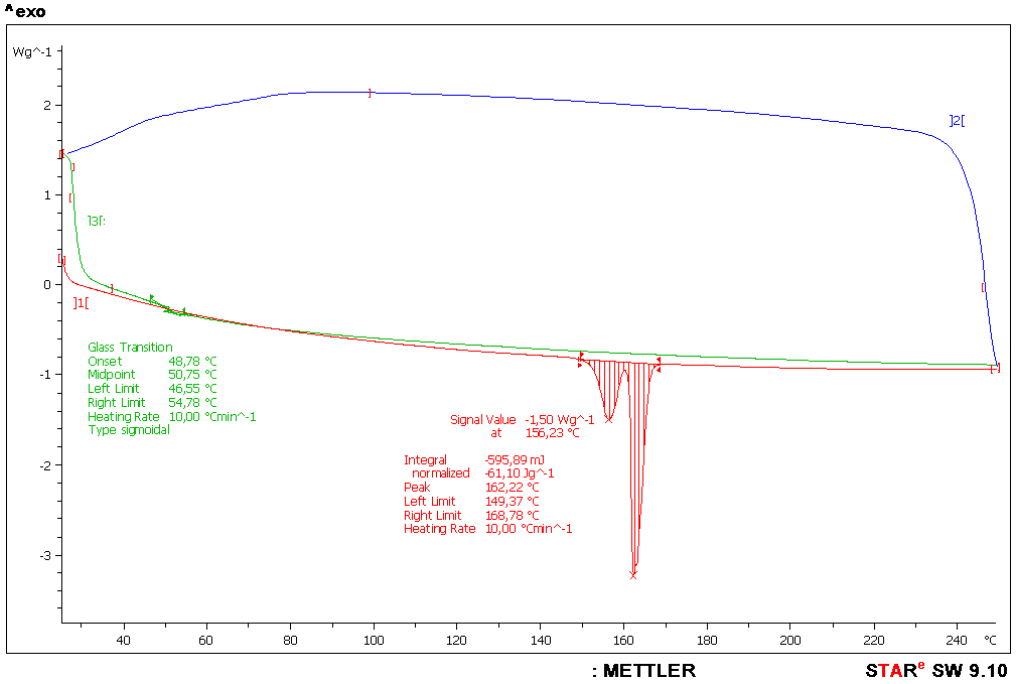
- **A-1:**



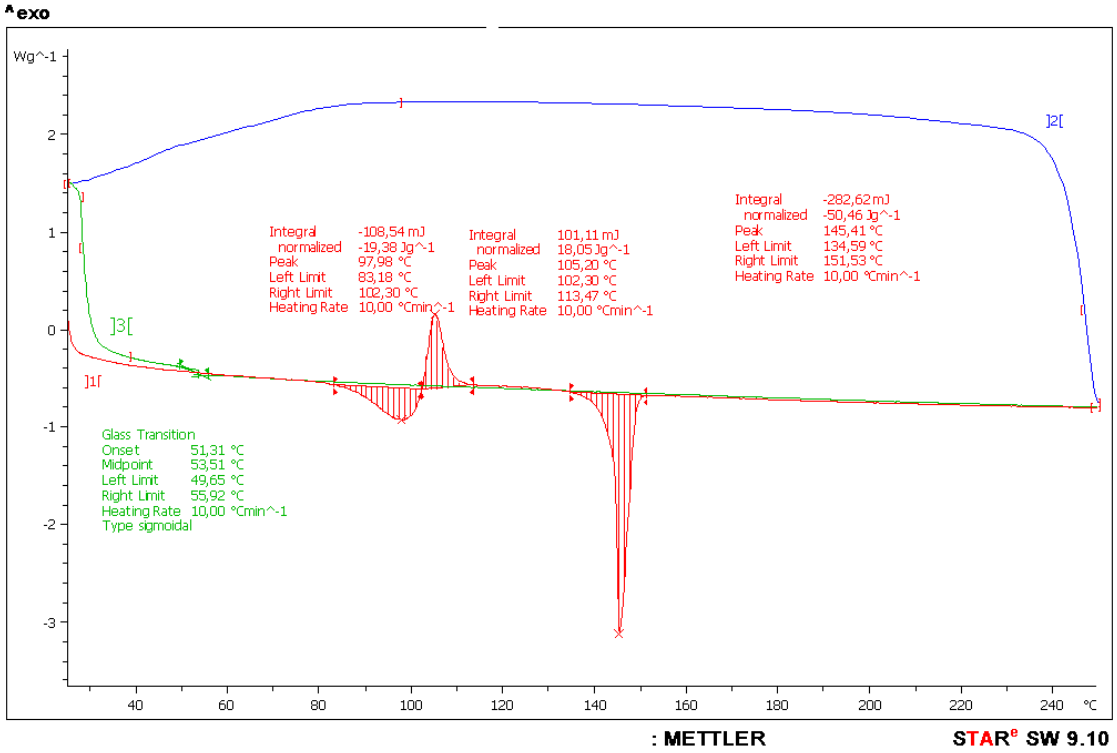
DSC thermogram showing T_g peak for **A-1**:



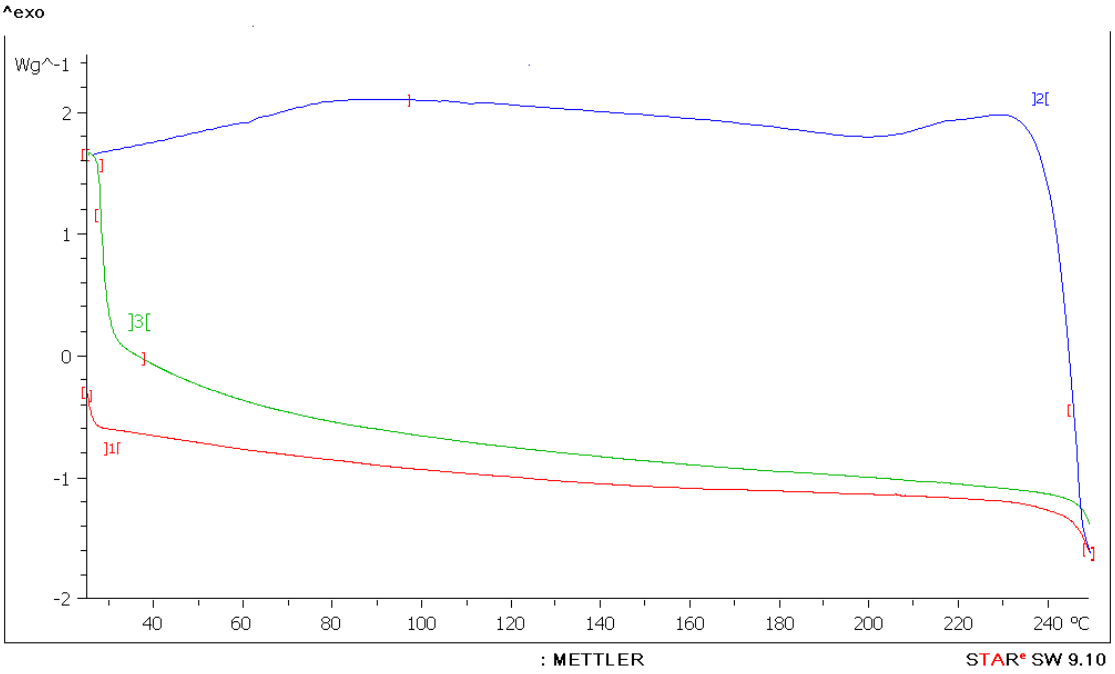
- **A-2:**



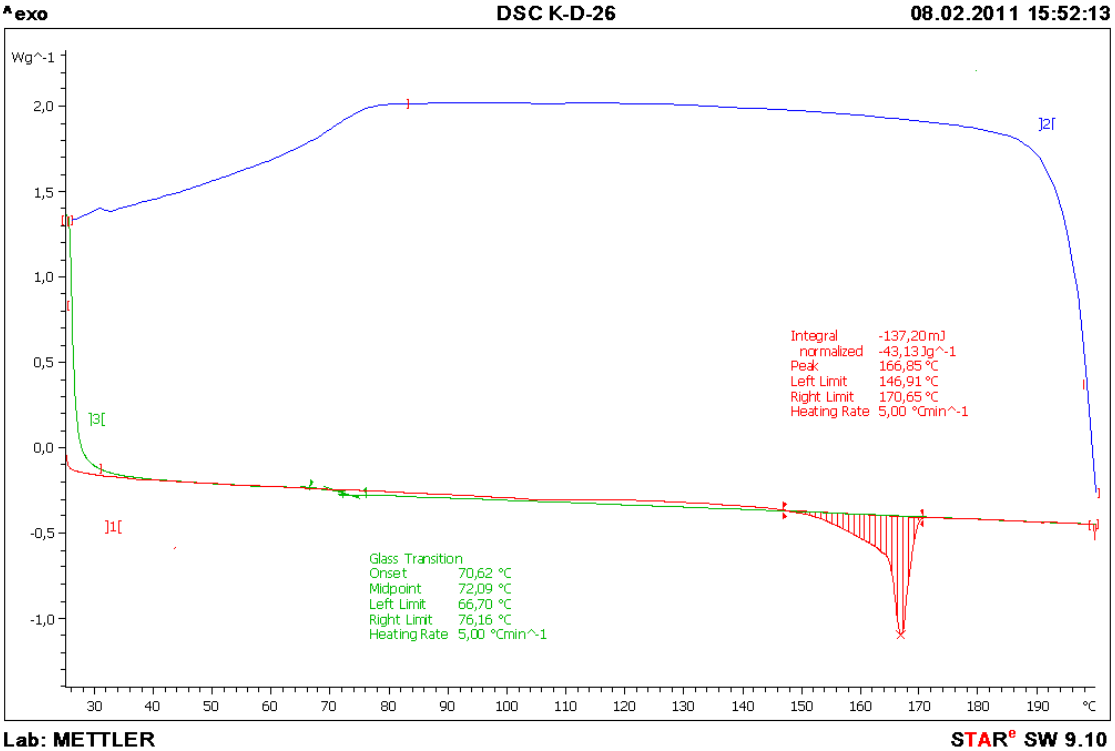
- **A-3:**



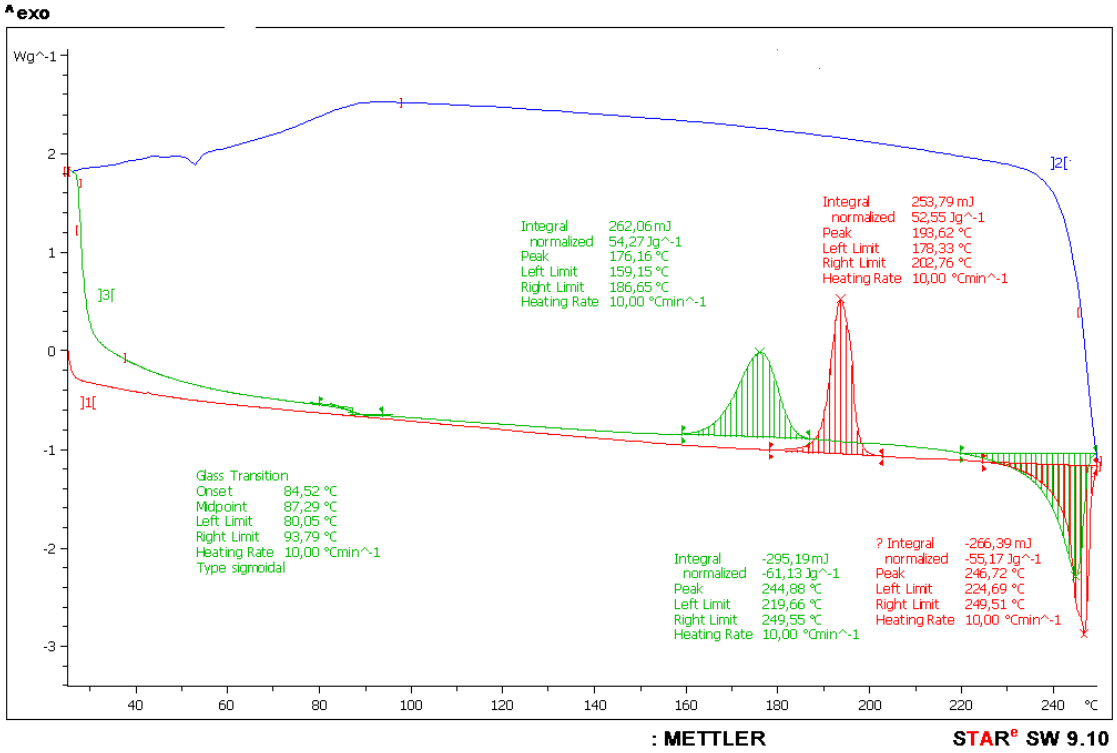
- **A-4** (no T_g peaks were observed)**:**



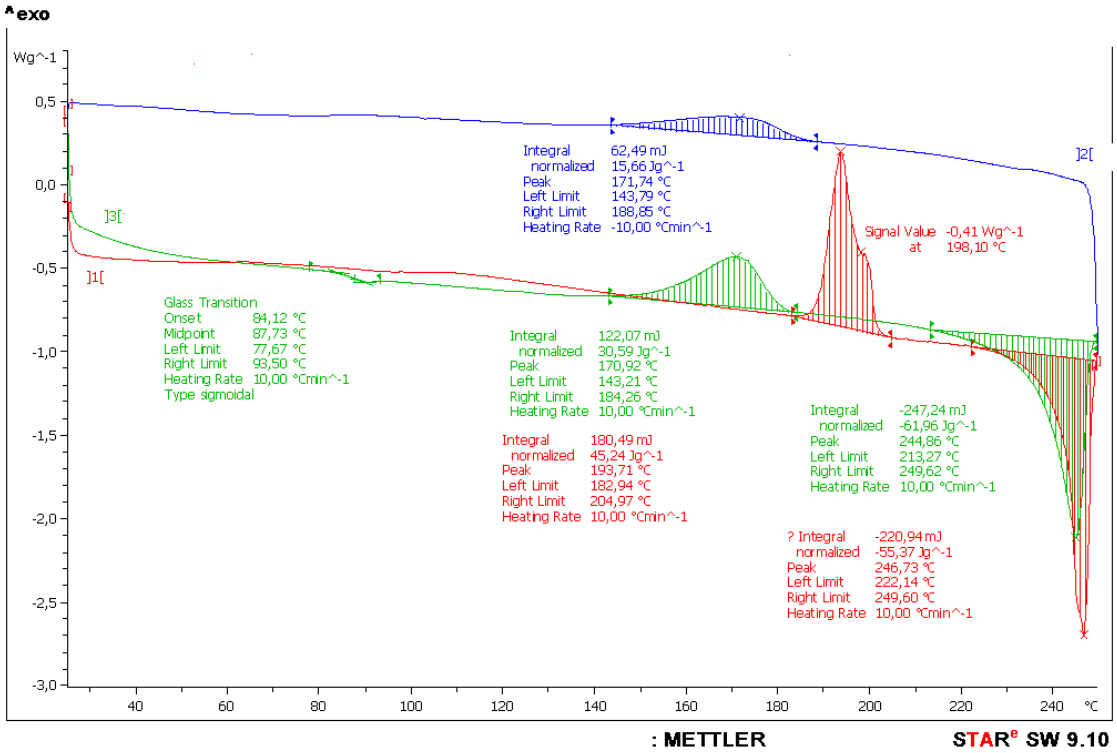
- **A-5:**



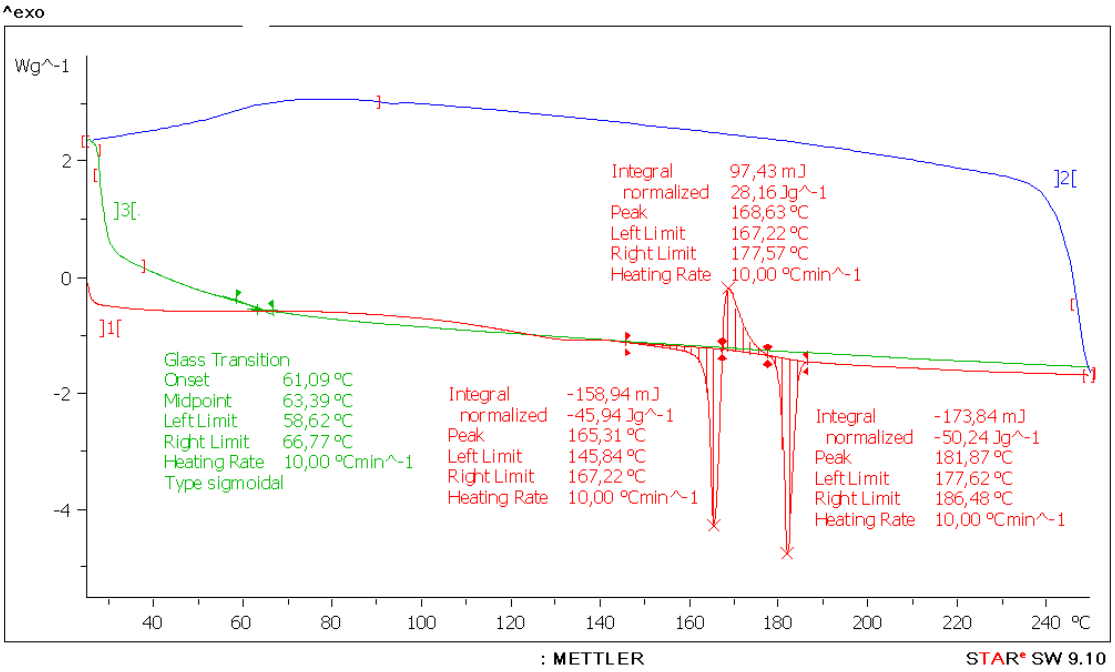
- **I-1** (cooling rate 50° C/min) **:**



I-1 (cooling rate 10° C/min), an additional crystallization peak during the cooling can be observed:

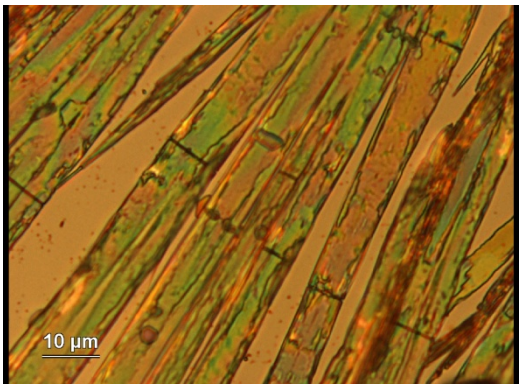


- **I-2:**

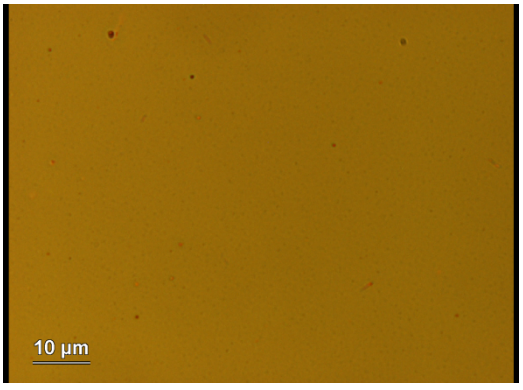


Microscope pictures of samples. All pictures are taken for poled samples after a month of storage (pictures for **I-1** and **I-2** are given in the paper).

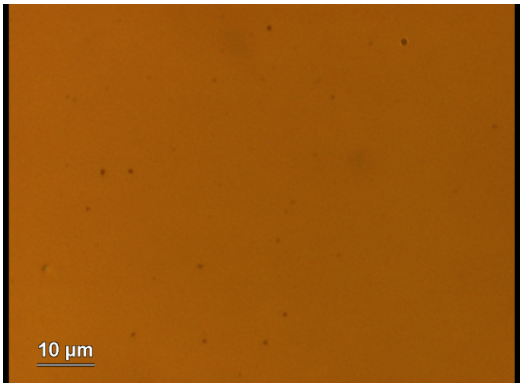
A-1 (samples underwent crystallization after being poled):



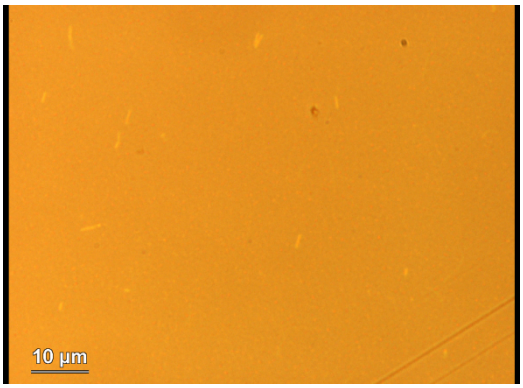
A-2:



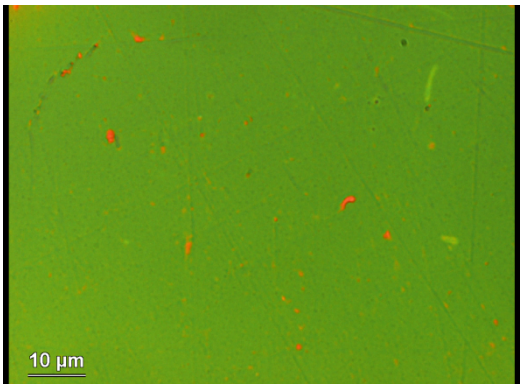
A-3:



A-4:



A-5:



Initial atomic coordinates for the quantum calculations.

Azo derivative A1

C	0.855979	1.041183	-0.559482
C	0.938273	2.268359	0.341526
C	1.267621	-1.007500	0.743773
C	1.743146	-2.123623	-0.179700
C	-1.553580	-1.588546	0.643164
C	-3.820438	-0.893059	0.200761
C	-1.982744	0.565809	-0.326753
C	-3.331850	0.312221	-0.299575
C	-2.911518	-1.827744	0.668880
N	0.306858	-0.121464	0.113536
C	-1.046548	-0.379422	0.143244
C	-9.615780	-0.166018	-0.487647
C	-9.126085	-2.317327	0.508389
C	-7.778416	-2.034627	0.465924
C	-8.261443	0.108416	-0.526014
C	-10.027270	-1.378052	0.030419
C	-7.342289	-0.816845	-0.053354
N	-5.178357	-1.246745	0.273816
N	-5.981538	-0.424308	-0.144565
C	4.531979	-3.255705	-0.898009

C	4.095741	-4.675364	1.084839
C	3.406585	-3.906124	-0.061871
C	2.447680	-4.816432	-0.858376
C	6.275155	-3.360648	-2.569736
C	6.686234	-2.077835	-2.251308
C	6.028719	-1.389586	-1.247395
C	4.968472	-1.975327	-0.575343
C	5.212440	-3.942724	-1.899459
C	5.422970	-6.546785	1.838380
C	5.427536	-6.042656	3.130392
C	4.765922	-4.859401	3.394205
C	4.104416	-4.179241	2.380284
C	4.765329	-5.869966	0.829448
C	0.733822	-6.522703	-0.823990
C	0.518236	-6.357860	-2.183144
C	1.253075	-5.413570	-2.874573
C	2.203579	-4.646439	-2.216257
C	1.683614	-5.758347	-0.171201
O	2.639230	-2.899199	0.571060
O	1.596550	3.260887	-0.399696
C	0.199556	5.221349	-0.167306
C	2.087637	4.615321	1.522466
C	1.596671	4.600044	0.058428
C	2.572595	5.350804	-0.871657
C	-1.478244	6.914254	0.235405
C	-2.275474	6.393389	-0.767871
C	-1.828688	5.294658	-1.481770
C	-0.603411	4.720994	-1.188152
C	-0.253832	6.336060	0.530478
C	1.688767	4.466399	3.904039
C	3.048535	4.413440	4.148278
C	3.930274	4.444651	3.080315
C	3.454063	4.540505	1.784745
C	1.214620	4.560090	2.604161
C	3.748018	7.378228	-1.454088
C	4.285691	6.761922	-2.574811
C	3.966179	5.444733	-2.837572
C	3.116201	4.741978	-1.992763
C	2.901623	6.680387	-0.615247
N	-11.451380	-1.679285	0.076333
O	-11.782170	-2.734075	0.528353
O	-12.207930	-0.854467	-0.340692
H	0.286148	1.268827	-1.450835
H	1.857588	0.800923	-0.895146
H	-0.052262	2.590014	0.643123
H	1.495026	2.027577	1.240429
H	2.122998	-0.418455	1.052450
H	0.855488	-1.435589	1.647724
H	0.904227	-2.718756	-0.517934
H	2.224476	-1.702213	-1.057005
H	-0.896017	-2.355226	0.999271
H	-1.656990	1.515366	-0.700146
H	-4.019434	1.053517	-0.659235
H	-3.281913	-2.761587	1.052013
H	-10.338360	0.537651	-0.848606
H	-9.484732	-3.246572	0.903029
H	-7.062145	-2.743997	0.829252
H	-7.901594	1.039568	-0.921218
H	6.780421	-3.913853	-3.341889
H	7.510043	-1.624778	-2.773802
H	6.342320	-0.395952	-0.978939
H	4.485659	-1.437254	0.217093
H	4.916945	-4.939014	-2.169144
H	5.929991	-7.469384	1.616388
H	5.938772	-6.568844	3.917132
H	4.758153	-4.456645	4.392061
H	3.593064	-3.264689	2.602353
H	4.766703	-6.285156	-0.161440
H	0.162346	-7.246753	-0.270379
H	-0.217496	-6.954454	-2.692947
H	1.088533	-5.264179	-3.927135
H	2.747923	-3.909471	-2.774835
H	1.832587	-5.896419	0.883060
H	-1.805641	7.773199	0.794425
H	-3.226997	6.840626	-0.994596
H	-2.429405	4.885977	-2.275476
H	-0.258389	3.886991	-1.768229
H	0.341679	6.763391	1.314889
H	0.990042	4.431176	4.721254
H	3.417689	4.343761	5.156282
H	4.990823	4.394667	3.253649
H	4.154056	4.558314	0.971206
H	0.153824	4.585151	2.443955
H	3.988991	8.403227	-1.233158
H	4.944362	7.304594	-3.229678
H	4.376507	4.952117	-3.701846
H	2.881422	3.719617	-2.208693
H	2.502017	7.176148	0.250097

Azo derivative A2

C	-3.970417	-0.879349	-0.135298
C	-2.152539	0.593809	0.420647
C	-1.694242	-1.535330	-0.589755
C	-3.048894	-1.792571	-0.620278
C	-3.497936	0.322655	0.388319
C	-1.202921	-0.329155	-0.067234
N	-5.323406	-1.249938	-0.215390
C	0.674406	1.119014	0.642507
C	0.732197	2.350549	-0.254015
C	2.019948	5.865049	1.586911
C	2.994660	4.947415	-1.221331
Si	1.565034	4.953795	0.007849
C	0.019651	5.687538	-0.790155
C	3.066769	7.741762	2.707902
C	2.655237	7.250377	3.936446
C	1.932786	6.070595	3.999643
C	1.620013	5.386399	2.835780
C	2.752702	7.053168	1.548530
C	4.218333	5.889269	-3.091238
C	5.205711	4.929970	-2.944444
C	5.098448	3.978410	-1.942380
C	4.006288	3.991301	-1.091916
C	3.124756	5.893932	-2.239187
C	-1.508349	5.855896	-2.669298
C	-2.332847	6.696125	-1.937831
C	-1.991093	7.036597	-0.640297
C	-0.828544	6.535960	-0.075283
C	-0.347154	5.361663	-2.100167
O	1.279858	3.399860	0.497110
N	0.146657	-0.053268	-0.031213
C	1.122232	-0.923202	-0.661427
C	1.604360	-2.045167	0.250955
C	4.690048	-4.437490	-1.212066
C	3.943885	-4.044969	1.784162

Si	3.291631	-4.193978	0.018943
C	2.023213	-5.584280	-0.095750
C	6.287011	-5.880674	-2.326213
C	6.806810	-4.793694	-3.010644
C	6.274275	-3.531802	-2.806005
C	5.226502	-3.357842	-1.915819
C	5.239024	-5.701223	-1.439377
C	3.551652	-3.960280	4.178541
C	4.898379	-3.720447	4.401844
C	5.770221	-3.642629	3.329506
C	5.295669	-3.802468	2.036894
C	3.084572	-4.121560	2.885408
C	1.120195	-7.727738	0.590394
C	0.156889	-7.653773	-0.400935
C	0.118639	-6.553978	-1.243924
C	1.043016	-5.535115	-1.091638
C	2.040710	-6.701730	0.740385
O	2.568154	-2.782841	-0.451201
H	-1.838752	1.538401	0.816265
H	-1.026977	-2.286082	-0.961229
H	-3.406677	-2.723972	-1.021018
H	-4.195248	1.047021	0.763369
H	0.099127	1.343798	1.530794
H	1.678665	0.897368	0.982884
H	1.347842	2.141288	-1.125508
H	-0.259662	2.610114	-0.608795
H	3.633859	8.654531	2.654169
H	2.900302	7.782140	4.839320
H	1.616406	5.682533	4.952134
H	1.067781	4.465894	2.898541
H	3.093249	7.444437	0.604809
H	4.296682	6.629676	-3.868015
H	6.053891	4.922917	-3.606557
H	5.863919	3.231540	-1.823894
H	3.939597	3.249029	-0.314986
H	2.363509	6.642254	-2.376648
H	-1.768040	5.589306	-3.678796
H	-3.234657	7.084073	-2.378349
H	-2.626127	7.690995	-0.069238
H	-0.579415	6.814562	0.933358
H	0.284253	4.719598	-2.690753
H	0.727422	-1.342025	-1.577708
H	1.980538	-0.327483	-0.947818
H	2.033564	-1.626764	1.156658
H	0.771246	-2.676788	0.545099
H	6.693080	-6.864006	-2.486738
H	7.619333	-4.930822	-3.702751
H	6.671136	-2.686157	-3.340187
H	4.814291	-2.374999	-1.773101
H	4.840012	-6.560545	-0.927461
H	2.869696	-4.024161	5.008315
H	5.264967	-3.597492	5.406009
H	6.817026	-3.459421	3.497514
H	5.989717	-3.740874	1.217448
H	2.036337	-4.318308	2.736377
H	1.153906	-8.579204	1.247317
H	-0.560115	-8.447622	-0.517037
H	-0.626909	-6.493474	-2.017449
H	1.005377	-4.690652	-1.758517
H	2.775543	-6.774759	1.523279
N	-6.137494	-0.445489	0.216612
C	-7.492957	-0.854148	0.118312
C	-8.424224	0.051835	0.604404
C	-9.774901	-0.239401	0.560589
C	-10.170390	-1.448516	0.023598
C	-9.256864	-2.368744	-0.467803
C	-7.912988	-2.069400	-0.419813
N	-11.590480	-1.767285	-0.028380
O	-12.357920	-0.958800	0.400507
O	-11.907300	-2.819144	-0.496986
H	-8.076646	0.981305	1.014282
H	-10.506670	0.449320	0.931714
H	-9.603233	-3.296427	-0.876816
H	-7.187391	-2.763932	-0.793158

Azo derivative A3

C	-3.250241	-1.396954	-0.323844
C	-1.636256	0.280493	0.275125
C	-0.902345	-1.785440	-0.709374
C	-2.215689	-2.199142	-0.777052
C	-2.938616	-0.144838	0.206211
C	-0.571182	-0.527833	-0.179939
N	-4.547740	-1.916874	-0.437439
C	1.101665	1.133094	0.572101
C	1.042185	2.358251	-0.332959
C	1.851655	6.005921	1.519827
C	2.990795	5.212878	-1.264259
Si	1.545729	5.044073	-0.065032
C	-0.061780	5.578576	-0.897187
C	2.641039	7.995916	2.656129
C	2.260753	7.461901	3.876896
C	1.681849	6.204898	3.928732
C	1.480924	5.485927	2.761191
C	2.439152	7.272443	1.493018
C	4.128974	6.298599	-3.110022
C	5.222703	5.466707	-2.941287
C	5.211514	4.508286	-1.940104
C	4.108533	4.387149	-1.112406
C	3.025583	6.169123	-2.280770
C	-1.557926	5.556814	-2.809022
C	-2.498741	6.281952	-2.095002
C	-2.231306	6.658905	-0.790118
C	-1.026651	6.309231	-0.200360
C	-0.355553	5.213090	-2.215130
O	1.444993	3.466865	0.423981
N	0.733767	-0.096600	-0.106770
C	1.823263	-0.849926	-0.700356
C	2.403932	-1.903764	0.235528
C	5.791084	-3.927343	-1.111670
C	4.905046	-3.616066	1.856124
Si	4.333990	-3.844117	0.071461
C	3.238828	-5.371844	-0.076488
C	7.578358	-5.179657	-2.166021
C	7.993479	-4.040887	-2.837595
C	7.314128	-2.847800	-2.656205
C	6.224241	-2.793942	-1.801969
C	6.487729	-5.120376	-1.315143
C	4.425543	-3.569990	4.235623
C	5.727623	-3.176381	4.501590
C	6.620282	-3.002092	3.458112
C	6.210859	-3.219170	2.151652
C	4.023717	-3.787649	2.928912
C	2.564872	-7.602776	0.593896
C	1.635276	-7.643893	-0.430934

C	1.500559	-6.558765	-1.283017
C	2.295404	-5.439528	-1.106259
C	3.355237	-6.476912	0.768109
O	3.468025	-2.527272	-0.431149
H	-1.445787	1.256245	0.673311
H	-0.141123	-2.453747	-1.056564
H	-2.450634	-3.167112	-1.182019
H	-3.729045	0.491942	0.555398
H	0.478537	1.293585	1.441732
H	2.114448	1.031120	0.942502
H	1.701619	2.216766	-1.185891
H	0.037210	2.499872	-0.716368
H	3.097051	8.969402	2.611386
H	2.418851	8.020976	4.782678
H	1.390346	5.784197	4.875277
H	1.040202	4.506606	2.815493
H	2.753782	7.699306	0.555773
H	4.132545	7.043752	-3.886199
H	6.078959	5.563746	-3.585699
H	6.059755	3.860265	-1.804565
H	4.116766	3.641686	-0.335714
H	2.181771	6.819151	-2.435142
H	-1.759759	5.262612	-3.824058
H	-3.433363	6.552350	-2.554480
H	-2.957203	7.224251	-0.232444
H	-0.837011	6.613868	0.813683
H	0.365283	4.658895	-2.792184
H	1.508549	-1.315839	-1.624803
H	2.614524	-0.159171	-0.965197
H	2.753199	-1.433996	1.150334
H	1.641041	-2.626628	0.509519
H	8.098972	-6.110354	-2.308699
H	8.838998	-4.084860	-3.501795
H	7.629715	-1.962719	-3.180595
H	5.698285	-1.864373	-1.677256
H	6.172382	-6.019282	-0.812927
H	3.727967	-3.709302	5.042861
H	6.043764	-3.009135	5.516438
H	7.632913	-2.699334	3.659333
H	6.920367	-3.080639	1.355166
H	3.010550	-4.103947	2.746752
H	2.673160	-8.442405	1.257946
H	1.019196	-8.515652	-0.566067
H	0.781139	-6.587490	-2.082693
H	2.184575	-4.607414	-1.780491
H	4.065469	-6.462032	1.576538
N	-5.452600	-1.200559	-0.029887
C	-6.751051	-1.746098	-0.154790
C	-7.820460	-0.965625	0.275375
C	-9.119618	-1.429826	0.187204
C	-9.336179	-2.686442	-0.336734
C	-8.296563	-3.489956	-0.773586
C	-7.009646	-3.012545	-0.678950
N	-10.703910	-3.179468	-0.431106
O	-11.579430	-2.464999	-0.047367
O	-10.866530	-4.270433	-0.887526
Br	-7.549183	0.761981	0.997770
H	-9.942470	-0.830590	0.517209
H	-8.501274	-4.461698	-1.175043
H	-6.183878	-3.610518	-1.008304

Azo derivative A4

C	-3.833061	-1.031277	-0.641130
C	-4.181603	-2.189979	0.286817
C	-3.640960	1.059509	0.644148
C	-3.865873	2.256750	-0.272689
C	-0.959484	-1.298740	-0.543302
C	1.217788	-0.347057	-0.129026
C	-0.770114	0.901546	0.393031
C	0.599855	0.801784	0.359310
C	0.418119	-1.383926	-0.576559
N	-2.972958	-0.043832	-0.018923
C	-1.595853	-0.148596	-0.056831
C	6.928882	1.053001	0.376749
C	6.655399	-1.207468	-0.302997
C	5.281019	-1.052698	-0.247982
C	5.559878	1.207779	0.423851
C	7.511607	-0.154928	-0.005351
C	4.703464	0.155968	0.105886
N	2.610664	-0.544890	-0.207977
N	3.307236	0.378229	0.187037
C	-6.309408	4.072012	-0.869188
C	-5.411837	5.333358	1.064149
C	-5.009628	4.406694	-0.102667
C	-3.890297	5.031379	-0.962072
C	-8.062375	4.640114	-2.434260
C	-8.765377	3.497178	-2.093342
C	-8.246590	2.649585	-1.131301
C	-7.035738	2.938174	-0.522780
C	-6.850899	4.924564	-1.827641
C	-6.134746	7.496094	1.858943
C	-6.234709	7.004547	3.151679
C	-5.921737	5.681414	3.395504
C	-5.513575	4.850511	2.360892
C	-5.728500	6.669235	0.829124
C	-1.774757	6.201227	-1.035964
C	-1.694889	6.004413	-2.405859
C	-2.701026	5.309250	-3.048848
C	-3.784641	4.821741	-2.331718
C	-2.857132	5.717231	-0.324810
O	-4.499803	3.236417	0.507508
O	-5.107582	-2.987687	-0.403669
C	-4.253666	-5.240547	-0.191280
C	-5.837013	-4.151336	1.567078
C	-5.430242	-4.276265	0.082586
C	-6.610652	-4.758201	-0.786919
C	-3.056441	-7.309238	0.169922
C	-2.197346	-7.019365	-0.874849
C	-2.375108	-5.846243	-1.587910
C	-3.395012	-4.971908	-1.253087
C	-4.074116	-6.430805	0.506082
C	-5.298611	-4.091778	3.924905
C	-6.584420	-3.684383	4.228291
C	-7.494526	-3.493532	3.201472
C	-7.122706	-3.720798	1.888289
C	-4.928458	-4.316536	2.607395
C	-8.299420	-6.415182	-1.270971
C	-8.709200	-5.694057	-2.383131
C	-8.070000	-4.509560	-2.690745
C	-7.028181	-4.042760	-1.899139
C	-7.262576	-5.952189	-0.485000
H	-3.383858	-1.404665	-1.552333
H	-4.756164	-0.546402	-0.936010
H	-3.292667	-2.752127	0.549575

H	-4.614397	-1.808123	1.204823
H	-4.600717	0.709944	1.006362
H	-3.086330	1.372477	1.518625
H	-2.922088	2.619979	-0.659187
H	-4.480740	1.968176	-1.119882
H	-1.527440	-2.141196	-0.882412
H	-1.199246	1.812501	0.758796
H	1.202896	1.619680	0.704705
H	0.889082	-2.275801	-0.949459
H	7.545693	1.886755	0.649954
H	7.043904	-2.168723	-0.569784
H	4.638763	-1.880286	-0.477594
H	-8.454935	5.315249	-3.174339
H	-9.705448	3.274875	-2.566467
H	-8.784817	1.762678	-0.845836
H	-6.659915	2.282759	0.238498
H	-6.329265	5.818561	-2.112848
H	-6.370097	8.525432	1.652319
H	-6.549668	7.647419	3.954664
H	-5.991239	5.285842	4.393856
H	-5.270556	3.827926	2.567225
H	-5.646735	7.075590	-0.162056
H	-0.992979	6.730012	-0.519838
H	-0.854498	6.382474	-2.960728
H	-2.646802	5.135948	-4.109206
H	-4.541998	4.269511	-2.853999
H	-2.898786	5.873042	0.736756
H	-2.938251	-8.220463	0.729620
H	-1.405501	-7.699810	-1.133442
H	-1.724672	-5.611775	-2.412405
H	-3.536535	-4.079486	-1.831451
H	-4.723902	-6.683669	1.322438
H	-4.575861	-4.232410	4.709226
H	-6.873508	-3.512185	5.250064
H	-8.495878	-3.167082	3.420742
H	-7.841485	-3.561791	1.107092
H	-3.919461	-4.617657	2.400501
H	-8.788714	-7.338659	-1.015320
H	-9.516150	-6.053902	-2.996810
H	-8.377346	-3.937707	-3.548981
H	-6.545254	-3.120116	-2.149069
H	-6.966596	-6.523998	0.375061
C	9.063831	-0.263268	0.001384
C	9.538686	-1.700797	-0.360715
C	10.250310	-2.522355	0.500169
C	10.683590	-3.782999	0.098917
C	10.416130	-4.246267	-1.170741
C	9.717997	-3.430027	-2.051684
C	9.297495	-2.178624	-1.653964
C	9.487404	0.142410	1.443169
C	10.340520	1.196578	1.731988
C	10.644710	1.536958	3.047071
C	10.100200	0.832812	4.098606
C	9.231004	-0.216367	3.827872
C	8.925995	-0.546484	2.524500
C	9.710906	0.658722	-1.072954
C	11.099330	0.608696	-1.243640
C	8.993629	1.486240	-1.923170
C	9.634664	2.255314	-2.890654
C	11.004480	2.210299	-3.028745
C	11.737730	1.374771	-2.195425
Cl	4.931548	2.762732	0.897262
H	10.490900	-2.195214	1.491280
H	11.235410	-4.392890	0.792641
H	10.750640	-5.220841	-1.479657
H	9.510526	-3.766622	-3.052305
H	8.779015	-1.556045	-2.359996
H	10.774100	1.778642	0.944309
H	11.308340	2.362840	3.234508
H	10.335250	1.097113	5.114432
H	8.783427	-0.770055	4.634458
H	8.235074	-1.348828	2.340358
H	11.684940	-0.045550	-0.624239
H	7.925862	1.542505	-1.860089
H	9.045561	2.885205	-3.533864
H	11.499190	2.805461	-3.775815
H	12.807360	1.314734	-2.295015

Azo derivative A5

C	-4.002289	-0.968965	-0.990454
C	-4.426676	-2.040184	0.007535
C	-3.737455	1.210816	0.126985
C	-3.845493	2.349911	-0.882289
C	-1.149063	-1.360750	-0.804319
C	1.059654	-0.499590	-0.359286
C	-0.877409	0.871119	0.032237
C	0.485528	0.701198	0.051629
C	0.222692	-1.516966	-0.783046
N	-3.111271	0.021737	-0.419082
C	-1.741022	-0.156404	-0.398513
C	6.818630	0.663257	0.190819
C	6.445886	-1.643830	-0.238656
C	5.080156	-1.417823	-0.241571
C	5.458694	0.887462	0.180948
C	7.347666	-0.606974	-0.036366
C	4.556919	-0.150477	-0.043035
N	2.442422	-0.768128	-0.380985
N	3.172301	0.144905	-0.023751
C	-4.176297	5.869548	-1.769695
C	-5.160698	5.719241	1.181042
Si	-4.006419	4.989377	-0.111841
C	-2.211307	5.033577	0.474732
C	-3.631584	7.664955	-3.306531
C	-4.562304	7.186503	-4.213950
C	-5.301960	6.055366	-3.909889
C	-5.110121	5.407977	-2.700583
C	-3.441480	7.010474	-2.100253
C	-6.105227	7.643541	2.312900
C	-6.845765	6.809058	3.135469
C	-6.753294	5.436046	2.985392
C	-5.919321	4.898734	2.016923
C	-5.275209	7.101422	1.347234
C	-0.602548	5.000855	2.292033
C	0.442593	4.947437	1.383873
C	0.173383	4.940463	0.024757
C	-1.138292	4.984185	-0.420515
C	-1.911439	5.044017	1.840411
O	-4.513438	3.425935	-0.277809
O	-5.318072	-2.906029	-0.644276
C	-4.586768	-5.624085	-0.051202
C	-6.641555	-4.077017	1.671822
Si	-5.949096	-4.320453	-0.067901
C	-7.306740	-4.762777	-1.289752
C	-3.559473	-7.643072	0.814269

C	-2.577211	-7.575707	-0.158876
C	-2.590807	-6.541061	-1.081192
C	-3.585862	-5.580392	-1.026338
C	-4.550776	-6.675151	0.866554
C	-6.297564	-3.774877	4.056027
C	-7.661345	-3.613888	4.243681
C	-8.517840	-3.683215	3.158465
C	-8.011048	-3.911251	1.888504
C	-5.798160	-4.004984	2.785562
C	-8.774558	-6.401909	-2.306267
C	-9.365081	-5.411428	-3.074587
C	-8.932038	-4.100939	-2.960564
C	-7.912938	-3.782279	-2.077158
C	-7.755761	-6.077923	-1.426382
H	-3.552888	-1.435909	-1.857241
H	-4.894153	-0.467289	-1.346671
H	-3.558478	-2.581013	0.372264
H	-4.908134	-1.577363	0.863961
H	-4.737349	0.953986	0.456540
H	-3.208307	1.554111	1.006394
H	-2.858944	2.634094	-1.231801
H	-4.413695	2.024612	-1.748080
H	-1.748421	-2.188137	-1.126326
H	-1.266334	1.818671	0.344130
H	1.114642	1.505864	0.380206
H	0.658966	-2.448678	-1.096027
H	7.470701	1.492033	0.386225
H	6.790827	-2.646905	-0.383579
H	4.401843	-2.234342	-0.394463
H	-3.053068	8.541987	-3.538712
H	-4.709270	7.691309	-5.152807
H	-6.025740	5.679669	-4.611877
H	-5.695093	4.532905	-2.476433
H	-2.704493	7.392419	-1.414558
H	-6.178009	8.711545	2.421401
H	-7.493672	7.227949	3.885685
H	-7.330630	4.784331	3.617828
H	-5.863935	3.831216	1.902827
H	-4.718013	7.768087	0.710903
H	-0.398626	5.010257	3.348357
H	1.460039	4.912446	1.731882
H	0.981011	4.899851	-0.684702
H	-1.323460	4.983785	-1.480768
H	-2.708478	5.091328	2.561772
H	-3.552841	-8.443849	1.532935
H	-1.805043	-8.324032	-0.199026
H	-1.830069	-6.485358	-1.840131
H	-3.587047	-4.786245	-1.753252
H	-5.299208	-6.740455	1.637226
H	-5.627094	-3.723979	4.896015
H	-8.052859	-3.437778	5.230417
H	-9.577621	-3.561542	3.298904
H	-8.693421	-3.963839	1.058692
H	-4.736362	-4.137964	2.664913
H	-9.103056	-7.422548	-2.396113
H	-10.155190	-5.660902	-3.761295
H	-9.383989	-3.329743	-3.559699
H	-7.577905	-2.763048	-2.005090
H	-7.300411	-6.863992	-0.848095
C	8.891695	-0.788430	0.028082
C	9.300948	-2.278831	-0.156940
C	9.949887	-3.030705	0.810560
C	10.327670	-4.347981	0.565575
C	10.066310	-4.938724	-0.651350
C	9.431059	-4.195027	-1.637789
C	9.065654	-2.887925	-1.394925
C	9.300977	-0.243053	1.427292
C	10.199080	0.795336	1.621401
C	10.488820	1.267275	2.898576
C	9.884759	0.713032	4.005816
C	8.970395	-0.317571	3.828648
C	8.680058	-0.777934	2.561932
C	9.610365	-0.026175	-1.123182
C	10.998200	-0.161108	-1.245809
C	8.956533	0.732282	-2.082031
C	9.658759	1.355049	-3.110361
C	11.027500	1.229758	-3.201674
C	11.697280	0.460613	-2.258272
Cl	4.899773	2.515642	0.457676
H	10.183910	-2.605321	1.765281
H	10.831650	-4.901103	1.338736
H	10.357870	-5.956913	-0.839481
H	9.229866	-4.632464	-2.599944
H	8.595932	-2.325210	-2.180814
H	10.680100	1.263365	0.786652
H	11.188750	2.076517	3.011927
H	10.108880	1.078796	4.992226
H	8.476615	-0.754875	4.678608
H	7.954177	-1.562310	2.448432
H	11.534880	-0.767779	-0.539714
H	7.891716	0.845694	-2.057604
H	9.117931	1.934762	-3.837657
H	11.569540	1.711896	-3.995905
H	12.764590	0.338939	-2.318676

Indandione derivative I1

C	9.107249	-1.831895	-0.852333
C	9.270088	-4.423417	0.249690
C	8.066990	-3.744786	0.181126
C	7.986405	-2.474869	-0.358709
C	10.316160	-2.504719	-0.787403
C	10.396860	-3.785927	-0.242591
C	3.292465	-2.371093	0.478388
C	0.891385	-2.218753	0.837795
C	2.072099	-0.376784	-0.148980
C	3.249281	-1.078857	-0.061311
C	2.078068	-2.905546	0.922382
C	0.850649	-0.921876	0.293744
C	6.711415	-4.178806	0.627324
C	4.473059	-3.198083	0.618651
C	6.576862	-1.975341	-0.309540
C	5.779355	-3.059785	0.315415
O	6.231741	-0.902291	-0.713537
O	6.441737	-5.226849	1.135359
C	-1.560621	-0.707484	0.785827
C	-2.344571	-1.616776	-0.153716
C	-5.486534	-3.177775	1.001952
C	-5.313122	-1.754105	-1.017967
C	-4.520027	-2.722936	-0.111872
C	-3.890141	-3.928047	-0.842179
C	-7.406916	-4.465130	1.699414
C	-7.305381	-3.949412	2.982840
C	-6.295419	-3.052383	3.270478
C	-5.391783	-2.668071	2.288657

C	-6.508261	-4.082528	0.722400
C	-6.902822	-1.310755	-2.784484
C	-6.866254	0.044519	-2.505341
C	-6.063509	0.498347	-1.474106
C	-5.301485	-0.392377	-0.735974
C	-6.137134	-2.198899	-2.048069
C	-2.871384	-4.955257	-2.780059
C	-2.535818	-6.070941	-2.036820
C	-2.861448	-6.111734	-0.690251
C	-3.526324	-5.051597	-0.101591
C	-3.536225	-3.892078	-2.185963
O	-3.488127	-2.018158	0.552889
N	-0.325709	-0.218860	0.199413
C	-0.411758	1.048984	-0.503790
C	-0.106826	2.246041	0.389485
C	-0.503355	5.674847	-0.926626
C	-0.483646	4.867906	1.493743
C	0.085125	4.657774	0.073530
C	1.623036	4.764716	-0.034109
C	-0.888608	7.967412	-1.580460
C	-1.495461	7.546109	-2.754725
C	-1.604604	6.193346	-3.008609
C	-1.113165	5.262617	-2.102009
C	-0.398477	7.042237	-0.679845
C	-0.341736	4.649957	3.898850
C	-1.657059	5.053856	4.032776
C	-2.393867	5.349648	2.897420
C	-1.814172	5.253499	1.644895
C	0.235838	4.552437	2.641601
C	3.734957	5.806546	0.510084
C	4.389414	5.011189	-0.413497
C	3.658377	4.103040	-1.159606
C	2.290807	3.988252	-0.976176
C	2.367271	5.685676	0.696288
O	-0.335756	3.388688	-0.391278
H	9.032915	-0.844705	-1.269808
H	9.319068	-5.410290	0.671772
H	11.208980	-2.035900	-1.161633
H	11.350380	-4.282343	-0.206342
H	-0.001582	-2.701272	1.179538
H	2.111569	0.614959	-0.551197
H	4.152694	-0.620718	-0.408364
H	2.061637	-3.897148	1.341266
H	4.268624	-4.155954	1.071994
H	-1.363223	-1.227310	1.713530
H	-2.175287	0.146428	1.043785
H	-2.608136	-1.079234	-1.059523
H	-1.745331	-2.471862	-0.440053
H	-8.185208	-5.168135	1.459402
H	-8.004051	-4.246892	3.744800
H	-6.201741	-2.645349	4.262215
H	-4.612067	-1.974229	2.529138
H	-6.600261	-4.503373	-0.261807
H	-7.527872	-1.682370	-3.577443
H	-7.458892	0.734689	-3.079256
H	-6.031535	1.547150	-1.235981
H	-4.703463	-0.026643	0.075930
H	-6.186569	-3.244050	-2.288617
H	-2.613707	-4.902285	-3.823158
H	-2.021592	-6.896250	-2.496749
H	-2.597394	-6.969037	-0.096448
H	-3.764889	-5.098823	0.944164
H	-3.769297	-3.031571	-2.783164
H	0.240866	1.049385	-1.366441
H	-1.419139	1.159428	-0.886489
H	-0.760083	2.234386	1.255001
H	0.916148	2.207285	0.746513
H	-0.797840	9.017752	-1.365731
H	-1.876903	8.265638	-3.457597
H	-2.074035	5.850525	-3.914233
H	-1.208848	4.216884	-2.312426
H	0.061637	7.391545	0.225971
H	0.240767	4.404730	4.769413
H	-2.105204	5.132714	5.007568
H	-3.421450	5.655958	2.984795
H	-2.403702	5.482116	0.777436
H	1.254164	4.222361	2.566890
H	4.286407	6.523668	1.092521
H	5.452051	5.100250	-0.553207
H	4.150093	3.484122	-1.889354
H	1.734005	3.298628	-1.580672
H	1.888702	6.315223	1.422475

Indandione derivative I2

C	8.701016	-3.668063	-0.938989
C	8.353695	-6.232443	0.183640
C	7.308536	-5.329345	0.114796
C	7.477963	-4.072569	-0.435100
C	9.752982	-4.566661	-0.873916
C	9.581470	-5.834484	-0.318892
C	2.903293	-3.033891	0.423030
C	0.586288	-2.399214	0.805294
C	2.096936	-0.845433	-0.225453
C	3.111214	-1.767210	-0.138528
C	1.612618	-3.308596	0.887933
C	0.797473	-1.127608	0.241044
C	5.896543	-5.482842	0.570602
C	3.897143	-4.077635	0.564805
C	6.195677	-3.303295	-0.383888
C	5.202668	-4.203816	0.252963
O	6.067973	-2.185640	-0.794296
O	5.427757	-6.452681	1.089083
C	-1.520085	-0.434846	0.742788
C	-2.474345	-1.180133	-0.183154
C	-6.192084	-2.130732	1.451628
C	-5.824030	-1.027172	-1.433514
Si	-5.069473	-2.067536	-0.054015
C	-4.666726	-3.799929	-0.686170
C	-8.402536	-2.345192	2.422438
C	-7.860928	-2.275549	3.696000
C	-6.493078	-2.129972	3.855913
C	-5.669181	-2.057932	2.743900
C	-7.574711	-2.271175	1.315119
C	-7.162601	-0.773151	-3.439665
C	-6.998076	0.600629	-3.390528
C	-6.251761	1.169221	-2.370345
C	-5.675188	0.362518	-1.404368
C	-6.578718	-1.575883	-2.471892
C	-3.740099	-5.263848	-2.386914
C	-3.969181	-6.366128	-1.578659
C	-4.544213	-6.196646	-0.330862
C	-4.887004	-4.927332	0.108071
C	-4.087481	-3.999100	-1.943807
O	-3.698294	-1.317223	0.486549

N	-0.215105	-0.204086	0.149455
C	-0.043551	1.057882	-0.548748
C	0.513511	2.162555	0.341484
C	0.786003	5.945973	-1.392860
C	0.452513	5.357587	1.644458
Si	1.231909	4.790576	0.020650
C	3.098434	4.621334	0.216959
C	1.158425	7.992260	-2.637282
C	0.091675	7.692431	-3.469223
C	-0.627359	6.525055	-3.273895
C	-0.281710	5.662037	-2.246195
C	1.500236	7.125467	-1.613094
C	0.256435	5.198711	4.059079
C	-0.777429	6.121638	4.047088
C	-1.199967	6.665546	2.846276
C	-0.590991	6.285485	1.660479
C	0.862250	4.825344	2.871505
C	5.220617	5.281367	1.186459
C	5.884422	4.365996	0.387466
C	5.168209	3.577264	-0.499036
C	3.792728	3.708849	-0.582772
C	3.842310	5.403291	1.102481
O	0.612112	3.326001	-0.434400
H	8.821256	-2.688812	-1.364385
H	8.208664	-7.206374	0.613630
H	10.718720	-4.286848	-1.256061
H	10.417910	-6.509770	-0.282819
H	-0.379506	-2.688014	1.166854
H	2.326420	0.110716	-0.649775
H	4.082722	-1.504583	-0.504121
H	1.403942	-4.270879	1.323222
H	3.510179	-4.971780	1.029132
H	-1.427436	-0.971999	1.677207
H	-1.960247	0.523874	0.988274
H	-2.603701	-0.619343	-1.105657
H	-2.068848	-2.151770	-0.444446
H	-9.465329	-2.451764	2.292968
H	-8.502311	-2.330129	4.558368
H	-6.069073	-2.069596	4.843084
H	-4.609857	-1.934219	2.880766
H	-8.016395	-2.313672	0.333900
H	-7.740362	-1.219408	-4.230099
H	-7.447955	1.225204	-4.142447
H	-6.121835	2.236502	-2.327664
H	-5.102661	0.819141	-0.615239
H	-6.710449	-2.642267	-2.534117
H	-3.294760	-5.389724	-3.358200
H	-3.702320	-7.350653	-1.921151
H	-4.726726	-7.049405	0.299293
H	-5.334947	-4.817078	1.079798
H	-3.910383	-3.158212	-2.592833
H	0.590306	0.934018	-1.416262
H	-1.008769	1.376575	-0.923197
H	-0.148324	2.324491	1.187485
H	1.484593	1.876675	0.734408
H	1.724473	8.894553	-2.789294
H	-0.174177	8.362815	-4.267951
H	-1.452406	6.285341	-3.921851
H	-0.840476	4.753259	-2.111322
H	2.341229	7.369373	-0.986313
H	0.590881	4.774511	4.989625
H	-1.248286	6.416062	4.968787
H	-2.000120	7.384722	2.831688
H	-0.932035	6.721759	0.738293
H	1.671403	4.115607	2.905668
H	5.772601	5.895120	1.876696
H	6.953530	4.265552	0.455527
H	5.679388	2.862894	-1.120121
H	3.250850	3.094035	-1.280886
H	3.344399	6.112204	1.741277