Electronic Supplementary Information to

Tobias Risthaus, Andreas Hansen and Stefan Grimme: "Excited States using the simplified Tamm–Dancoff–Approach for Range–Separated Hybrid Density Functionals: Development and Application"

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SCS-CC2/def2-TZVP(-f) singlet-singlet excitation energies in eV, supplemented by consistent, back-corrected experimental values for the DYE12 subset marked DYE12-2010 taken from L. Goerigk and S. Grimme, *J. Chem. Phys.*, 2010, **132**, 184103.

System	State symmetry	SCS-CC2	DYE12-2010
Acetamid	$1A$	5.8867	
Anthracene	$1B_{2u}$	3.8142	
t-Azobenzene	$1B_g$	3.0334	
t-Azobenzene	$1B_u$	4.2624	
Azulene	$1B_1$	2.4521	
Benzene	$1B_{1u}$	5.0964	
CH_2O	$1A_2$	4.2317	
CH_2S	$1A_2$	2.4194	
DMABN	$1B_2$	4.3922	
DMABN	$2A_1$	4.8231	
Glyoxal	$1A_u$	3.1172	
Hexatriene	$1B_u$	5.4286	
Norbornadiene	$1A_2$	5.7988	
Norbornadiene	$1B_2$	6.6699	
Octatetraene	$1B_u$	4.7369	
P_4	$1T_1$	5.4770	
1,4-diethynylbenzene	$1B_{3u}$	4.6492	
Perylene	$1B_{2u}$	3.2531	
Porphyrine	$1B_{2u}$	2.1355	
Porphyrine	$1B_{3u}$	2.5105	
Porphyrine	$2B_{2u}$	3.5500	
Porphyrine	$2B_{3u}$	3.6515	
Pyridine	$1B_2$	5.2680	
Tetrazine	$1B_{1u}$	2.6614	
Uracil	$1A''$	5.1435	
Uracil	$2A'$	5.5212	
1 Coumarine-153	$2A$	3.4366	3.51
2 Oxazine9	$2A'$	2.4664	2.41
3 6,6'-Difluoroindigo	$1B_u$	2.5541	2.48
4 Azoborane	$2A$	3.2023	3.11
5 Perylene	$1B_{1u}$	2.7440	2.68
6 Nile Red	$2A$	2.8565	2.66
7 Bithiophene	$2A$	4.0150	3.66
8 Acridine Red	$1B_2$	2.7630	2.52
9 Benzcarbazole	$2A$	3.4858	3.37
10 Anthanthrene	$1B_u$	3.1990	3.15
11 Rubicene	$1B_u$	2.7765	2.60
12 DBQ	$2A$	3.3596	3.60

Zincbacteriochlorin-bacteriochlorin: lowest 10 excited state transition energies in eV for sTDA-B3LYP/def2-TZVP(-f)

state number	transition energy
1	1.497
2	1.637
3	2.029
4	2.052
5	2.199
6	2.255
7	2.275
8	2.319
9	2.861
10	3.139

glyoxal (part of the fit set): Cartesian coordinates in ångström

O	-0.576491	1.638753	0.000000
C	-0.631431	0.428566	0.000000
C	0.631431	-0.428566	0.000000
O	0.576491	-1.638753	0.000000
H	-1.584290	-0.141523	0.000000
H	1.584290	0.141523	0.000000

pyridine (part of the fit set): Cartesian coordinates in ångström

N	0.000000	0.000000	1.611338
C	-1.143765	0.000000	0.911064
H	-2.060283	0.000000	1.498722
C	-1.197827	0.000000	-0.483002
H	-2.156184	0.000000	-0.994042
C	0.000000	0.000000	-1.195190
H	0.000000	0.000000	-2.281631
C	1.197827	0.000000	-0.483002
H	2.156184	0.000000	-0.994042
C	1.143765	0.000000	0.911064
H	2.060283	0.000000	1.498722

1,4-diethynylbenzene (part of the fit set): Cartesian coordinates in ångström

C	0.000000	1.410603	0.000000
C	-1.212234	0.693267	0.000000
C	-1.212234	-0.693267	0.000000
C	0.000000	-1.410603	0.000000
C	1.212234	-0.693267	0.000000
C	1.212234	0.693267	0.000000
C	0.000000	2.832968	0.000000
C	0.000000	-2.832968	0.000000
C	0.000000	4.043371	0.000000
C	0.000000	-4.043371	0.000000
H	-2.149898	1.239413	0.000000
H	-2.149898	-1.239413	0.000000
H	2.149898	-1.239413	0.000000
H	2.149898	1.239413	0.000000
H	0.000000	5.108799	0.000000
H	0.000000	-5.108799	0.000000

coumarin-152 (part of the CT test set): Cartesian coordinates in ångström

C	-3.558714	-0.762996	0.349325
C	-3.550910	0.683210	0.288106
C	-2.409629	-1.489510	0.282792
O	-2.287052	1.287268	0.150528
C	-1.133309	-0.849809	0.148538
C	-1.127274	0.562554	0.086713
C	0.120049	-1.494642	0.068031
C	0.040771	1.298044	-0.044352
C	1.293212	-0.783612	-0.061265
C	1.284587	0.638646	-0.116597
H	-4.529332	-1.229549	0.450766
O	-4.513940	1.414935	0.339536
H	0.167323	-2.576906	0.106451
H	-0.042140	2.376397	-0.088663
H	2.229523	-1.324617	-0.120848
C	-2.489131	-2.998739	0.354417
F	-1.791757	-3.486017	1.418623
F	-3.757792	-3.450965	0.474751
F	-1.964877	-3.581468	-0.759871
N	2.452326	1.346369	-0.234332
C	2.415266	2.799557	-0.334979
H	1.916256	3.239044	0.537166
H	3.438454	3.174301	-0.369876
H	1.887831	3.130402	-1.240386
C	3.723210	0.649551	-0.391321
H	4.518557	1.391303	-0.467254
H	3.932586	0.006674	0.472476
H	3.735907	0.030577	-1.298476

DCS (part of the CT test set): Cartesian coordinates in ångström

C	-4.200851	1.259280	-0.084769
C	-5.575202	1.095969	-0.013828
C	-6.119043	-0.177880	0.226114
C	-5.249365	-1.274167	0.392009
C	-3.879231	-1.097769	0.319245
C	-3.313324	0.174011	0.078164
C	-1.884060	0.416826	-0.008229
C	1.121068	0.969568	-0.191223
C	0.527807	-0.290588	0.030913
C	1.404918	-1.383002	0.178033
C	2.781509	-1.244295	0.110326
C	3.367239	0.023726	-0.112910
C	2.492249	1.130016	-0.261854
C	-0.902061	-0.509632	0.113204
N	4.732193	0.180710	-0.182299
C	5.307630	1.496558	-0.414545
C	5.606481	-0.971103	-0.024793
H	-3.790104	2.248255	-0.271931
H	-6.238979	1.944745	-0.142741
C	-7.530437	-0.359624	0.302033
H	-5.666286	-2.258551	0.579172
H	-3.234345	-1.960410	0.454030
H	-1.609837	1.454931	-0.190686
H	0.493443	1.848025	-0.311181
H	0.985239	-2.371582	0.351636
H	3.406340	-2.121602	0.231470
H	2.895485	2.121475	-0.433624
H	-1.186260	-1.546339	0.293265
H	4.975389	1.917541	-1.373261
H	5.036924	2.201350	0.383406
H	6.394036	1.404253	-0.437615
H	5.420670	-1.726356	-0.800671
H	5.471960	-1.445973	0.956644
H	6.642026	-0.639347	-0.107879
N	-8.683222	-0.509021	0.364372

DANS (part of the CT test set): Cartesian coordinates in ångström

C	-3.974568	1.320954	-0.064733
C	-5.351139	1.170235	-0.006628
C	-5.878704	-0.106793	0.180694
C	-5.050226	-1.224963	0.309260
C	-3.677899	-1.058646	0.250898
C	-3.099785	0.218355	0.062540
C	-1.669558	0.450243	-0.005080
C	1.342231	0.974845	-0.145232
C	0.733345	-0.285521	0.031853
C	1.596957	-1.392905	0.149525
C	2.974718	-1.268465	0.092773
C	3.576247	-0.001005	-0.091915
C	2.714933	1.120721	-0.206495
C	-0.697812	-0.491385	0.094110
N	4.941758	0.139783	-0.165465
C	5.534269	1.453714	-0.366859
C	5.802270	-1.028009	-0.050614
H	-3.550921	2.311135	-0.211702
H	-6.024314	2.013873	-0.102195
N	-7.331407	-0.281057	0.243099
H	-5.500078	-2.201002	0.447872
H	-3.041181	-1.931706	0.352005
H	-1.382865	1.490639	-0.151118
H	0.725287	1.864156	-0.237136
H	1.164365	-2.380731	0.292685
H	3.589050	-2.155601	0.193637
H	3.131116	2.111925	-0.345326
H	-0.995173	-1.530039	0.237063
H	5.197922	1.905771	-1.309752
H	5.282070	2.138676	0.453747
H	6.618865	1.346287	-0.404412
H	5.604132	-1.753658	-0.851041
H	5.664299	-1.533368	0.914794
H	6.841610	-0.706487	-0.125962
O	-8.040414	0.727813	0.126443
O	-7.769400	-1.427783	0.408666

TCNE-benzene (part of the CT test set): Cartesian coordinates in ångström

C	-2.274205	-1.398789	-0.000000
C	-2.274206	1.398791	-0.000000
C	-2.274506	-0.699551	1.213150
C	-2.274505	-0.699551	-1.213150
C	-2.274506	0.699551	1.213150
C	-2.274505	0.699551	-1.213150
H	-2.278385	-2.491323	-0.000000
H	-2.278386	2.491321	-0.000000
C	1.368996	-0.686302	0.000000
C	1.368996	0.686301	0.000000
C	1.379968	-1.434052	-1.220900
C	1.379968	-1.434052	1.220895
C	1.379968	1.434051	-1.220900
C	1.379967	1.434051	1.220895
N	1.400955	-2.054479	-2.204820
N	1.400955	-2.054479	2.204824
N	1.400955	2.054481	-2.204820
N	1.400954	2.054481	2.204824
H	-2.276046	-1.246672	2.158733
H	-2.276045	-1.246672	-2.158730
H	-2.276045	1.246671	-2.158730
H	-2.276046	1.246671	2.158733

TCNE-*o*-xylene (part of the CT test set): Cartesian coordinates in ångström

C	0.689433	-0.436131	-2.332517
C	2.237632	0.706521	-0.269215
C	0.753531	0.952311	-2.199731
C	1.398214	-1.247821	-1.438598
C	1.523805	1.509468	-1.173946
C	2.173147	-0.701782	-0.405082
H	0.096668	-0.889164	-3.130461
C	-1.729097	-0.639017	0.321888
C	-1.363038	0.546726	0.909769
C	-1.271942	-1.897265	0.829790
C	-2.608713	-0.675063	-0.806999
C	-0.496756	0.580170	2.048545
C	-1.843532	1.803601	0.421102
N	-0.925432	-2.928994	1.241117
N	-3.336303	-0.727199	-1.713495
N	0.204252	0.624705	2.976540
N	-2.233669	2.833174	0.045046
H	0.211164	1.600952	-2.890884
H	1.353327	-2.335001	-1.545685
H	1.582588	2.596852	-1.074686
C	3.059213	1.339021	0.825853
H	3.062667	2.435306	0.741085
H	2.664976	1.081215	1.824174
H	4.106352	0.994186	0.799923
C	2.928551	-1.605669	0.539382
H	2.604254	-1.467239	1.584410
H	2.781378	-2.663415	0.279460
H	4.012039	-1.399039	0.516680

TCNE-hexamethylbenzene (part of the CT test set): Cartesian coordinates in ångström

C	-1.526348	2.528794	1.460000
C	-1.526348	1.221096	0.705000
C	-1.526348	0.000000	1.410000
C	-1.526348	-1.221096	0.705000
C	-1.526348	-1.221096	-0.705000
C	-1.526348	0.000000	-1.410000
C	-1.526348	1.221096	-0.705000
C	-1.526348	0.000000	2.920000
C	-1.526348	-2.528794	1.460000
C	-1.526348	-2.528794	-1.460000
C	-1.526348	0.000000	-2.920000
C	-1.526348	2.528794	-1.460000
H	-1.526348	1.027663	3.283329
H	-2.416330	-0.513832	3.283329
H	-0.636366	-0.513832	3.283329
H	-1.526348	3.357278	0.751682
H	-2.416330	2.586531	2.086656
H	-0.636366	2.586531	2.086656
H	-1.526348	2.329615	-2.531647
H	-2.416330	3.100362	-1.196673
H	-0.636366	3.100362	-1.196673
H	-1.526348	-1.027663	-3.283329
H	-2.416330	0.513832	-3.283329
H	-0.636366	0.513832	-3.283329
H	-1.526348	-3.357278	-0.751682
H	-2.416330	-2.586531	-2.086656
H	-0.636366	-2.586531	-2.086656
H	-1.526348	-2.329615	2.531647
H	-2.416330	-3.100362	1.196673
H	-0.636366	-3.100362	1.196673
C	1.933652	0.000000	0.685000
C	1.933652	0.000000	-0.685000
C	1.933652	-1.219275	1.432173
N	1.933652	-2.208338	2.038271
C	1.933652	1.219275	1.432173
N	1.933652	2.208338	2.038271
C	1.933652	1.219275	-1.432173
N	1.933652	2.208338	-2.038271
C	1.933652	-1.219275	-1.432173
N	1.933652	-2.208338	-2.038271

TCNE-diphenylene (part of the CT test set): Cartesian coordinates in ångström

C	-0.750110	1.667780	0.710680
C	0.749890	1.668049	0.710397
C	0.749621	1.668351	-0.709603
C	-0.750378	1.668082	-0.709320
C	-1.912342	1.668028	-1.435089
C	-1.911799	1.667417	1.436889
C	1.911853	1.668103	1.436167
C	1.911310	1.668713	-1.435812
C	-3.116169	1.667361	0.684632
C	-3.116428	1.667652	-0.685368
C	3.114338	1.668769	-0.684393
C	3.115939	1.668479	0.683454
H	-1.912548	1.668259	-2.525089
H	-4.068917	1.667594	-1.215335
H	-4.069405	1.667078	1.213254
H	-1.911593	1.667186	2.526889
H	1.912059	1.667872	2.526167
H	4.069374	1.668538	1.211716
H	4.067574	1.669053	-1.213015
H	1.911104	1.668945	-2.525812
C	0.685419	-1.981812	-0.000366
C	-0.684581	-1.982057	-0.000108
C	-1.431984	-1.981932	-1.219243
C	1.432822	-1.981937	1.218768
C	1.432362	-1.981419	-1.219783
C	-1.431524	-1.982451	1.219308
N	-2.037435	-1.982769	2.208485
N	2.039107	-1.982038	2.207716
N	2.038274	-1.981100	-2.208960
N	-2.038268	-1.981831	-2.208191

CA-hexamethylbenzene (part of the CT test set): Cartesian coordinates in ångström

C	-1.270434	1.455159	-0.674994
C	-0.704990	-2.204838	-1.221110
C	-1.459980	-2.204832	-2.528814
C	0.705010	-2.204838	-1.221099
C	1.410000	-2.204843	0.000002
C	0.704991	-2.204849	1.221092
C	-0.705009	-2.204849	1.221082
C	-1.410000	-2.204844	-0.000019
C	-1.270434	1.455153	0.675006
C	-0.000000	1.455150	1.453529
C	1.270434	1.455154	0.675006
C	1.270434	1.455160	-0.674994
C	-0.000000	1.455163	-1.453517
C	2.920000	-2.204843	0.000013
C	1.459981	-2.204855	2.528796
C	-1.460019	-2.204855	2.528774
C	-2.920000	-2.204844	-0.000031
C	1.460020	-2.204832	-2.528792
O	-0.000000	1.455144	2.663529
Cl	2.688039	1.455150	1.613299
Cl	2.688039	1.455164	-1.613287
O	-0.000000	1.455169	-2.663517
Cl	-2.688040	1.455163	-1.613287
Cl	-2.688040	1.455149	1.613299
H	-0.751656	-2.204828	-3.357293
H	-2.086636	-3.094814	-2.586559
H	-2.086636	-1.314850	-2.586551
H	2.531665	-2.204832	-2.329605
H	1.196697	-1.314847	-3.100358
H	1.196697	-3.094812	-3.100366
H	3.283322	-2.204848	1.027679
H	3.283334	-1.314858	-0.513812
H	3.283334	-3.094823	-0.513820
H	0.751657	-2.204859	3.357275
H	2.086637	-3.094838	2.586534
H	2.086637	-1.314873	2.586542
H	-2.531664	-2.204855	2.329587
H	-1.196696	-3.094840	3.100341
H	-1.196697	-1.314875	3.100349
H	-3.283321	-2.204839	-1.027697
H	-3.283333	-3.094829	0.513794
H	-3.283333	-1.314864	0.513802

CA-diphenylene (part of the CT test set): Cartesian coordinates in ångström

C	0.000000	1.453523	0.000000
C	-1.270434	0.675000	0.000000
C	-1.270434	-0.675000	0.000000
C	0.000000	-1.453523	0.000000
C	1.270434	-0.675000	0.000000
C	1.270434	0.675000	0.000000
Cl	-2.688040	1.613293	0.000000
Cl	-2.688040	-1.613293	0.000000
O	0.000000	-2.663523	0.000000
Cl	2.688040	-1.613293	0.000000
Cl	2.688040	1.613293	0.000000
O	0.000000	2.663523	0.000000
C	-0.683256	-3.116292	3.520000
C	-1.435968	-1.912205	3.520000
C	-0.710198	-0.750242	3.520000
C	0.709802	-0.749975	3.520000
C	1.436010	-1.911664	3.520000
C	0.684590	-3.114692	3.520000
C	-0.710480	0.749758	3.520000
C	0.709520	0.750025	3.520000
C	1.435290	1.911988	3.520000
C	0.685570	3.116075	3.520000
C	-0.684430	3.115817	3.520000
C	-1.436688	1.911447	3.520000
H	2.525290	1.912193	3.520000
H	1.215538	4.068563	3.520000
H	-1.213052	4.069053	3.520000
H	-2.526688	1.911242	3.520000
H	-2.525968	-1.912410	3.520000
H	-1.211519	-4.069726	3.520000
H	1.213212	-4.067927	3.520000
H	2.526010	-1.911459	3.520000

NKX2553 (part of the dye test set): Cartesian coordinates in ångström

C	-2.771318	-0.012133	-0.000394
C	-2.315404	-1.354540	0.000100
C	-0.963089	-1.636407	0.000078
C	0.018214	-0.620625	-0.000281
C	-0.445619	0.715464	-0.000654
C	-1.790937	1.016743	-0.000726
N	-4.108160	0.285273	-0.000555
C	-5.096951	-0.785560	0.001490
C	-4.554742	1.673248	-0.000351
C	1.408453	-0.979261	-0.000251
C	2.487977	-0.137018	-0.000221
C	3.814383	-0.628347	-0.000487
C	4.958088	0.134778	-0.000310
C	4.917727	1.551517	0.000646
N	4.948378	2.718681	0.001494
C	6.287579	-0.540361	-0.000982
O	6.426181	-1.744480	-0.002181
O	7.377232	0.278683	-0.000188
H	-3.026098	-2.172394	0.000474
H	-0.640795	-2.675068	0.000417
H	0.268212	1.533738	-0.000944
H	-2.096217	2.056500	-0.000924
H	-6.092695	-0.342131	0.001246
H	-4.997791	-1.418351	0.892963
H	-4.998554	-1.420888	-0.888233
H	-5.644693	1.688936	-0.001626
H	-4.198456	2.207419	-0.890442
H	-4.200424	2.206831	0.890929
H	1.616169	-2.050227	-0.000173
H	2.345914	0.941919	0.000126
H	3.976721	-1.705339	-0.000808
H	7.090718	1.213399	0.000770

TC1 (part of the dye test set): Cartesian coordinates in ångström

C	-0.021152	-0.199307	-0.074116
C	0.849890	0.822136	0.368302
C	2.218546	0.655429	0.321280
C	2.796175	-0.539675	-0.171776
C	1.910548	-1.554277	-0.607298
C	0.539604	-1.397766	-0.563437
C	-3.609867	2.883448	0.686135
C	-3.146143	3.815357	-0.244202
C	-2.100797	3.470216	-1.102840
C	-1.524313	2.204219	-1.038556
C	-1.982340	1.276772	-0.094714
C	-3.029944	1.620054	0.768088
C	-4.298444	-2.295100	-0.571855
C	-3.430270	-1.214000	-0.701817
C	-2.279881	-1.144576	0.092643
C	-2.008228	-2.161402	1.016175
C	-2.875034	-3.245319	1.128923
C	-4.023848	-3.316957	0.338692
N	-1.403741	-0.025083	-0.023914
C	4.202390	-0.800397	-0.261996
C	5.288344	-0.028632	0.056879
C	5.236075	1.286461	0.579344
N	5.300072	2.370302	1.009731
C	6.651064	-0.617562	-0.165004
O	6.831718	-1.730199	-0.607686
O	7.707393	0.174318	0.161760
H	7.390001	1.034420	0.502628
H	0.432314	1.741754	0.763259
H	2.851156	1.455735	0.687845
H	2.327914	-2.476982	-1.002402
H	-0.112058	-2.188928	-0.917339
H	-4.419847	3.143906	1.361161
H	-3.596958	4.801296	-0.301436
H	-1.740510	4.183932	-1.837912
H	-0.721591	1.927440	-1.714916
H	-3.383152	0.894202	1.493801
H	-5.187732	-2.343518	-1.193517
H	-3.637111	-0.419197	-1.411624
H	-1.122238	-2.094446	1.639909
H	-2.659085	-4.028841	1.849421
H	-4.700824	-4.160291	0.434320
H	4.481903	-1.778942	-0.651934

TA-St-CA (part of the dye test set): Cartesian coordinates in ångström

C	-3.791508	-0.120047	0.015705
C	-4.694348	0.893779	0.409240
C	-6.065841	0.733049	0.341466
C	-6.621438	-0.479091	-0.131627
C	-5.713246	-1.500526	-0.522912
C	-4.346997	-1.332290	-0.454566
C	2.865321	-0.128041	-0.053534
C	1.990067	0.858782	0.445283
C	0.620514	0.681871	0.387550
C	0.049145	-0.486839	-0.162321
C	0.939236	-1.468006	-0.646259
C	2.313560	-1.299228	-0.601613
C	6.448996	3.001061	0.598440
C	5.937236	3.918423	-0.321331
C	4.864146	3.548322	-1.134280
C	4.309607	2.274875	-1.036611
C	4.816834	1.359296	-0.104600
C	5.891190	1.730689	0.714945
C	7.172307	-2.211017	-0.431252
C	6.311769	-1.128240	-0.592477
C	5.128171	-1.056969	0.153945
C	4.817848	-2.081897	1.057883
C	5.677265	-3.167871	1.200604
C	6.859477	-3.238193	0.460896
N	4.256546	0.056778	0.003029
C	-1.376526	-0.720986	-0.250787
C	-2.369484	0.131071	0.111846
C	-8.015319	-0.813084	-0.264328
C	-9.226309	-0.191333	-0.040102
C	-10.381823	-0.981596	-0.337484
N	-11.295947	-1.656005	-0.590434
C	-9.487944	1.175742	0.458873
O	-8.671072	2.026015	0.768583
O	-10.828430	1.411603	0.543207
H	-10.916611	2.325399	0.875220
H	-4.290057	1.834372	0.776170
H	-6.727465	1.531761	0.647807
H	-6.116382	-2.442724	-0.886821
H	-3.698145	-2.145535	-0.764421
H	2.403224	1.760273	0.885630
H	-0.020979	1.456762	0.796557
H	0.531421	-2.375788	-1.084873
H	2.971150	-2.067319	-0.994798
H	7.280095	3.279059	1.240276
H	6.371156	4.910047	-0.405195
H	4.464510	4.249158	-1.861704
H	3.484667	1.981486	-1.678262
H	6.282811	1.019092	1.435011
H	8.086137	-2.257351	-1.016720
H	6.550084	-0.332174	-1.290876
H	3.905225	-2.019405	1.642332
H	5.428316	-3.955493	1.906109
H	7.530481	-4.083315	0.580180
H	-1.649460	-1.691729	-0.663379
H	-2.104807	1.109546	0.509770
H	-8.148375	-1.826217	-0.642991

Bimane (part of the dye test set): Cartesian coordinates in ångström

C	1.331698	-1.879605	-0.108603
C	2.132097	-0.654088	-0.003948
C	1.302873	0.426430	-0.104903
C	-1.300787	0.433951	-0.101824
C	-2.136017	-0.641707	0.001280
C	-1.342993	-1.871870	-0.104659
N	-0.000534	-0.021248	-0.324354
N	-0.004568	-1.403598	-0.331622
O	-1.679176	-3.039253	-0.043168
O	1.661467	-3.048960	-0.049039
C	-1.615093	1.891323	-0.058117
C	-3.618641	-0.678771	0.170347
C	1.626055	1.881942	-0.064754
C	3.614962	-0.700043	0.160744
H	-4.049414	0.325596	0.200326
H	-3.887430	-1.197656	1.097229
H	-4.086348	-1.233771	-0.650635
H	-1.173280	2.374317	0.820379
H	-2.696603	2.026980	-0.008719
H	-1.243008	2.407629	-0.949030
H	2.707594	2.010775	-0.000483
H	1.174301	2.373283	0.803861
H	1.270709	2.395192	-0.964373
H	4.079173	-1.241294	-0.671464
H	3.883147	-1.237421	1.077108
H	4.049818	0.301869	0.208419

Solvent Blue 59 (part of the dye test set): Cartesian coordinates in ångström

C	0.188652	5.218636	0.701274
C	0.188652	5.218636	-0.701274
C	0.063249	4.024357	1.397669
C	0.063249	4.024357	-1.397669
C	-0.062407	2.811834	0.702897
C	-0.062407	2.811834	-0.702897
C	-0.195687	1.552897	1.461636
C	-0.195687	1.552897	-1.461636
C	-0.313137	0.304604	0.719243
C	-0.313137	0.304604	-0.719243
C	-0.417143	-0.926421	1.433536
C	-0.417143	-0.926421	-1.433536
C	-0.499583	-2.134379	0.683736
C	-0.499583	-2.134379	-0.683736
H	0.058838	3.995564	2.482327
H	0.058838	3.995564	-2.482327
H	0.286507	6.155232	1.243302
H	0.286507	6.155232	-1.243302
H	-0.564867	-3.081306	1.208261
H	-0.564867	-3.081306	-1.208261
O	-0.198677	1.602110	2.719463
O	-0.198677	1.602110	-2.719463
N	-0.449548	-0.953163	2.790562
N	-0.449548	-0.953163	-2.790562
H	-0.344538	-0.018001	3.208813
H	-0.344538	-0.018001	-3.208813
C	-0.438012	-2.151788	3.611665
H	-0.795251	-1.855247	4.602360
H	-1.163816	-2.875835	3.220608
C	-0.438012	-2.151788	-3.611665
H	-1.163816	-2.875835	-3.220608
H	-0.795251	-1.855247	-4.602360
C	0.949922	-2.796962	3.729897
H	0.903797	-3.688854	4.364618
H	1.330693	-3.091513	2.746907
H	1.661007	-2.091766	4.170533
C	0.949922	-2.796962	-3.729897
H	1.330693	-3.091513	-2.746907
H	0.903797	-3.688854	-4.364618
H	1.661007	-2.091766	-4.170533

Squaraine (part of the dye test set): Cartesian coordinates in ångström

C	0.000000	0.000000	-1.038401
C	0.000000	0.000000	1.038401
C	1.053630	0.000000	0.000000
C	-1.053630	0.000000	0.000000
O	-2.285873	0.000000	0.000000
O	2.285873	0.000000	0.000000
C	0.000000	0.000000	2.447303
C	0.000000	0.000000	-2.447303
C	1.217381	0.000127	3.177367
C	-1.217381	-0.000127	3.177367
C	1.217381	-0.000127	-3.177367
C	-1.217381	0.000127	-3.177367
C	1.220386	0.000162	4.555139
C	-1.220386	-0.000162	4.555139
C	1.220386	-0.000162	-4.555139
C	-1.220386	0.000162	-4.555139
C	0.000000	0.000000	-5.284803
C	0.000000	0.000000	5.284803
H	-2.151197	-0.000200	2.622665
H	2.151197	0.000200	2.622665
H	-2.151197	0.000200	-2.622665
H	2.151197	-0.000200	-2.622665
H	-2.167241	-0.000341	5.082590
H	2.167241	0.000341	5.082590
H	-2.167241	0.000341	-5.082590
H	2.167241	-0.000341	-5.082590
N	0.000000	0.000000	6.654692
N	0.000000	0.000000	-6.654692
C	-1.257889	0.000198	-7.391578
H	-1.856288	-0.889935	-7.159238
H	-1.855992	0.890537	-7.159265
H	-1.037086	0.000146	-8.459182
C	1.257889	-0.000198	-7.391578
H	1.855992	-0.890537	-7.159265
H	1.856288	0.889935	-7.159238
H	1.037086	-0.000146	-8.459182
C	1.257889	0.000198	7.391578
H	1.856288	-0.889935	7.159238
H	1.855992	0.890537	7.159265
H	1.037086	0.000146	8.459182
C	-1.257889	-0.000198	7.391578
H	-1.855992	-0.890537	7.159265
H	-1.856288	0.889935	7.159238
H	-1.037086	-0.000146	8.459182

Benzofurazan (part of the dye test set): Cartesian coordinates in ångström

C	-2.078593	1.090221	-0.042965
C	-3.512241	0.999940	-0.033195
C	-4.108577	-0.294407	0.004159
C	-3.269368	-1.391194	0.028101
C	-1.863290	-1.299232	0.018145
C	-1.217158	-0.062085	-0.016606
H	-3.739247	-2.368602	0.055262
H	-1.282690	-2.214338	0.037593
N	-1.712226	2.356983	-0.078708
N	-4.010503	2.230958	-0.062990
O	-2.891412	3.054425	-0.091148
N	-5.545245	-0.482339	0.016782
O	-5.979460	-1.644825	0.052108
O	-6.247291	0.535271	-0.008616
N	0.121922	0.115535	-0.025738
H	0.476330	1.063726	-0.057576
C	1.095788	-0.978405	-0.001460
H	0.920499	-1.592168	0.892021
H	0.943266	-1.617433	-0.881345
C	2.496020	-0.418832	0.008281
C	3.178812	-0.198687	-1.192371
C	3.110948	-0.076065	1.217466
C	4.458744	0.354838	-1.185391
H	2.706681	-0.465687	-2.134854
C	4.390214	0.477989	1.226329
H	2.586096	-0.247993	2.154233
C	5.065376	0.694229	0.024284
H	4.982524	0.518062	-2.122636
H	4.860992	0.736938	2.170108
H	6.063088	1.123178	0.030729

Amine-Aurone (part of the dye test set): Cartesian coordinates in ångström

C	-3.140331	0.651371	-0.011296
C	-2.494084	-0.587613	-0.014862
C	-3.178931	-1.794601	-0.018587
C	-4.573733	-1.716837	-0.018690
C	-5.248063	-0.484022	-0.015143
C	-4.535451	0.712289	-0.011485
C	-2.089065	1.684681	-0.008120
C	-0.827599	0.898307	-0.010823
H	-2.656869	-2.745682	-0.021534
H	-5.151205	-2.637043	-0.021765
H	-6.333657	-0.471219	-0.015384
H	-5.037397	1.675267	-0.009059
O	-1.116464	-0.470328	-0.014304
O	-2.195675	2.909565	-0.004082
C	0.426403	1.405045	-0.010864
H	0.430067	2.494592	-0.008991
C	1.710057	0.752315	-0.013995
C	1.890613	-0.650272	-0.013061
C	2.873591	1.553416	-0.016106
C	3.155910	-1.208923	-0.014424
H	1.023200	-1.299095	-0.009051
C	4.141875	1.001267	-0.017340
H	2.764448	2.635089	-0.014679
C	4.307379	-0.396571	-0.015264
H	3.268259	-2.290820	-0.016348
H	5.017493	1.646026	-0.021444
N	5.570714	-0.961540	-0.074418
H	6.344908	-0.379710	0.218160
H	5.653611	-1.924952	0.222957

Diaryl-cyclopentanone (part of the dye test set): Cartesian coordinates in ångström

C	-0.137909	-0.766008	-0.831269
C	0.137909	0.766008	-0.831269
C	0.034479	1.193543	0.611161
C	0.000000	0.000000	1.488657
C	-0.034479	-1.193543	0.611161
O	0.000000	0.000000	2.722099
C	-0.011564	2.452650	1.117394
C	0.020514	3.661087	0.353200
H	-0.079116	2.535786	2.202986
H	0.090073	3.569184	-0.729401
C	-0.029384	4.894343	0.922932
H	-0.095824	4.941766	2.010481
C	0.011564	-2.452650	1.117394
C	-0.020514	-3.661087	0.353200
H	0.079116	-2.535786	2.202986
H	-0.090073	-3.569184	-0.729401
C	0.029384	-4.894343	0.922932
H	0.095824	-4.941766	2.010481
C	-0.003248	6.180317	0.246248
C	0.079879	6.316748	-1.154951
C	-0.064265	7.355769	1.020534
C	0.100147	7.572308	-1.747701
H	0.128922	5.431413	-1.781904
C	-0.044002	8.613589	0.425786
H	-0.128307	7.268000	2.102517
C	0.038279	8.728232	-0.962206
H	0.164575	7.655463	-2.829069
H	-0.092364	9.505041	1.044674
H	0.054371	9.707841	-1.430837
C	0.003248	-6.180317	0.246248
C	-0.079879	-6.316748	-1.154951
C	0.064265	-7.355769	1.020534
C	-0.100147	-7.572308	-1.747701
H	-0.128922	-5.431413	-1.781904
C	0.044002	-8.613589	0.425786
H	0.128307	-7.268000	2.102517
C	-0.038279	-8.728232	-0.962206
H	-0.164575	-7.655463	-2.829069
H	0.092364	-9.505041	1.044674
H	-0.054371	-9.707841	-1.430837
H	1.146956	0.966693	-1.214716
H	-0.560273	1.303799	-1.481238
H	0.560273	-1.303799	-1.481238
H	-1.146956	-0.966693	-1.214716

Al-Q_3 (part of the dye test set): Cartesian coordinates in ångström

Al	0.011095	-0.010681	-0.981150
C	1.977702	-1.911742	-0.248913
C	0.289607	-2.113960	1.335897
C	2.759291	-2.945328	0.344957
C	2.397496	-1.207781	-1.428246
C	0.985667	-3.152206	1.983366
H	-0.672058	-1.766499	1.698046
C	2.210483	-3.561862	1.495782
C	4.000681	-3.271756	-0.248679
C	3.633845	-1.563661	-1.971894
H	0.547185	-3.617309	2.860124
H	2.761202	-4.360045	1.987634
C	4.406853	-2.581016	-1.379265
H	4.615691	-4.056149	0.181632
H	3.983225	-1.051638	-2.862841
H	5.360703	-2.833326	-1.835949
C	0.658815	2.645225	-0.243517
C	1.700587	1.287454	1.328871
C	1.149182	3.841412	0.357057
C	-0.166131	2.654382	-1.419132
C	2.238858	2.412161	1.982447
H	1.894139	0.281083	1.684583
C	1.963129	3.677431	1.504259
C	0.792376	5.079355	-0.226252
C	-0.494588	3.902707	-1.952777
H	2.864521	2.267375	2.857034
H	2.368155	4.555624	2.001314
C	-0.013354	5.083181	-1.353733
H	1.152587	6.005978	0.210029
H	-1.117467	3.947601	-2.840511
H	-0.287152	6.035160	-1.801856
N	0.774749	-1.511609	0.254442
N	0.931934	1.403404	0.250275
O	-0.550318	1.497545	-1.903021
O	1.595296	-0.287045	-1.906312
C	-2.624487	-0.743267	-0.244544
C	-1.946291	0.818315	1.337360
C	-3.914749	-0.887323	0.344181
C	-2.227832	-1.467799	-1.419447
C	-3.197022	0.750068	1.979922
H	-1.159562	1.470324	1.701644
C	-4.171217	-0.096903	1.490958
C	-4.825867	-1.791012	-0.250131
C	-3.162024	-2.351882	-1.964140
H	-3.377844	1.367494	2.853646
H	-5.141151	-0.162107	1.978131
C	-4.433995	-2.496337	-1.376782
H	-5.815985	-1.918819	0.176559
H	-2.895965	-2.916119	-2.852328
H	-5.135400	-3.189734	-1.834269
O	-1.024790	-1.249326	-1.893604
N	-1.669803	0.090966	0.259147

Amino-Benzoate (part of the dye test set): Cartesian coordinates in ångström

C	-0.799252	0.639025	-0.000197
C	-0.304795	-0.674066	-0.000153
C	1.057496	-0.926414	0.000124
C	1.992496	0.137875	0.000171
C	1.486656	1.461681	0.000203
C	0.122828	1.696207	-0.000078
H	-1.001938	-1.504967	-0.000364
H	1.402118	-1.954007	0.000389
H	2.166937	2.305376	0.000536
H	-0.257719	2.713011	-0.000234
N	3.345961	-0.105262	0.000039
C	-2.238322	0.958806	-0.000188
C	4.288039	1.003612	0.000012
C	3.843659	-1.472283	-0.000059
O	-3.019278	-0.162883	-0.000204
O	-2.708839	2.085494	-0.000124
H	4.165737	1.635642	0.890052
H	4.165555	1.635750	-0.889926
H	5.301826	0.601649	-0.000118
H	3.509329	-2.022499	0.890009
H	3.509137	-2.022437	-0.890093
H	4.933993	-1.448078	-0.000177
C	-4.449506	0.090376	-0.000034
C	-5.143428	-1.257505	0.000087
H	-4.697239	0.685196	0.884722
H	-4.697464	0.685154	-0.884755
H	-4.872613	-1.836141	-0.888333
H	-6.229028	-1.112196	0.000249
H	-4.872346	-1.836116	0.888442

Zincbacteriochlorin-bacteriochlorin, linked by a phenyl ring: Cartesian coordinates in ångström

H	1.160636	0.024630	2.150397
C	0.612757	0.020866	1.211841
C	-0.789615	0.016209	-1.189312
C	-0.781201	0.042684	1.216313
C	1.324361	-0.006385	0.006516
C	0.604366	-0.006589	-1.194014
C	-1.501123	0.040622	0.015805
H	-1.322642	0.058005	2.158486
C	2.820618	-0.038970	0.002043
H	1.145432	-0.023757	-2.136438
C	-2.997868	0.072258	0.020434
H	-1.337149	0.011322	-2.128115
C	3.438214	-1.289826	-0.047552
C	3.467727	1.209832	0.050955
N	4.776545	-1.508320	-0.057727
C	2.634533	-2.585500	-0.092020
H	3.750605	4.520610	0.167076
H	-9.038756	-4.434662	-0.505081
C	5.013581	-2.840530	-0.100272
C	3.729808	-3.662295	-0.116757
C	6.263061	-3.447583	-0.125406
H	7.124991	-0.771307	-0.056319
C	7.532759	-2.862176	-0.112873
H	6.266606	-4.534097	-0.158556
C	8.791182	-3.536383	-0.136562
N	4.830378	1.421160	0.060612
H	10.858369	-2.749423	-0.117799
H	8.903730	-4.611584	-0.167975
C	9.789388	-2.585527	-0.111110

C	9.800193	-0.049090	-0.032121
C	9.173726	-1.298914	-0.070523
N	7.813841	-1.515339	-0.072694
C	9.200611	1.202762	0.018840
H	10.886490	-0.073845	-0.041239
C	10.011841	2.493177	0.054220
C	6.383395	3.360221	0.129118
H	1.789339	2.663977	0.097247
C	2.856956	2.498523	0.095259
C	8.921774	3.575758	0.129668
C	7.633383	2.759254	0.098261
N	7.865885	1.426834	0.040907
C	5.114642	2.767970	0.109174
H	6.371972	4.446366	0.172069
C	3.859693	3.445144	0.130987
H	10.634893	2.585357	-0.842173
H	10.685791	2.509925	0.917319
H	1.988797	-2.614792	-0.975618
H	1.974050	-2.665997	0.777419
H	8.982865	4.170224	1.047797
H	8.962827	4.276695	-0.710756
H	3.680800	-4.294011	-1.010212
H	3.683717	-4.329344	0.751022
C	-3.661700	-1.171002	0.075808
C	-3.599222	1.321170	-0.025596
N	-5.032984	-1.364895	0.079072
C	-2.997807	-2.440383	0.139508
N	-4.941461	1.554013	-0.025790
C	-2.810915	2.620692	-0.096483
C	-9.250904	1.251458	-0.107774
C	-6.445126	3.466685	-0.078920
H	-3.847516	-4.478418	0.239653
C	-3.973562	-3.404676	0.184272
H	-1.925361	-2.575819	0.149079
C	-5.235861	-2.731186	0.145445
C	-5.190589	2.891696	-0.046012
C	-6.478426	-3.380792	0.175232
Zn	-6.459248	0.041151	0.003195
C	-3.904255	3.699139	-0.011443
C	-7.732532	-2.810680	0.127759
H	-6.438578	-4.464729	0.244941
C	-9.026429	-3.604661	0.207149
N	-7.976343	-1.474698	0.032924
C	-9.896605	0.008322	-0.101704
H	-9.084359	4.562720	-0.179321
H	-10.996451	2.645170	-0.196876
C	-10.101527	-2.541311	-0.079386
C	-9.314381	-1.241349	-0.040535
H	-6.479702	4.552873	-0.097809
C	-7.686811	2.819704	-0.096481
N	-7.883771	1.452214	-0.069388
C	-8.953602	3.488566	-0.150393
H	-10.981783	0.039276	-0.152294
C	-9.922241	2.517098	-0.158710
H	-10.551527	-2.673983	-1.070798
H	-3.843678	4.274914	0.919403
H	-3.861681	4.416821	-0.836458
H	-2.246234	2.670738	-1.034155
H	-2.077071	2.685160	0.711846
H	-10.917531	-2.544222	0.648953
H	-9.137658	-4.035833	1.209478
H	5.516659	0.674921	0.042048

2H bacteriochlorin monomer: Cartesian coordinates in ångström

H	-3.139859	3.264949	-0.000255
C	-2.399924	2.468853	-0.000293
C	-2.887321	1.168542	-0.000584
C	-1.069191	2.901644	0.000065
N	-2.130567	0.046069	-0.000160
C	-4.382311	0.865734	-0.001954
H	1.461437	5.060420	0.001039
C	-2.936902	-1.041404	0.000305
C	-4.416799	-0.671955	0.001590
C	-2.507885	-2.362147	0.000201
H	-0.026535	-1.082428	0.000566
C	-1.197432	-2.852870	-0.000068
H	-3.282299	-3.124717	0.000330
C	-0.782799	-4.218248	-0.000194
N	0.047312	2.096068	-0.000070
H	1.237893	-5.118364	-0.000425
H	-1.461464	-5.060334	-0.000242
C	0.596040	-4.247911	-0.000209
C	2.399910	-2.468861	0.000378
C	1.069196	-2.901649	0.000029
N	-0.047286	-2.096049	-0.000058
C	2.887299	-1.168561	0.000565
H	3.139849	-3.264931	0.000414
C	4.382282	-0.865754	0.001975
C	2.507904	2.362145	-0.000254
H	-1.237945	5.118372	0.000764
C	-0.596052	4.247928	0.000522
C	4.416792	0.671932	-0.002038
C	2.936894	1.041385	-0.000464
N	2.130560	-0.046090	0.000124
C	1.197458	2.852910	0.000103
H	3.282358	3.124684	-0.000302
C	0.782806	4.218292	0.000601
H	4.870254	-1.301172	-0.876680
H	4.866765	-1.295965	0.885185
H	-4.866925	1.296246	-0.884949
H	-4.870163	1.300849	0.876930
H	4.923876	1.085034	0.876573
H	4.919960	1.079992	-0.885315
H	-4.923599	-1.084767	-0.877326
H	-4.920257	-1.080311	0.884562
H	0.026674	1.082437	-0.000982

Zincbacteriochlorin monomer: Cartesian coordinates in ångström

H	3.175099	3.214853	0.104028
C	2.435151	2.419689	0.065788
H	-4.998235	1.308687	0.583048
C	1.097173	2.836141	0.029908
C	2.916804	1.126767	0.052620
N	-0.007280	2.005484	-0.002165
C	0.670624	4.204201	0.017376
N	2.144662	0.007664	-0.001254
C	4.393850	0.774320	0.128106
C	-1.097487	-2.836065	0.036769
C	2.452259	-2.402245	-0.067044
H	-1.371699	5.048566	-0.048542
C	-0.700929	4.199241	-0.026009
H	1.335285	5.058359	0.038230
C	-1.117652	2.828145	-0.036172
C	2.924744	-1.105944	-0.054523
C	-2.452598	2.402040	-0.072820
Zn	-0.000443	0.000000	-0.000020
C	4.399258	-0.743018	-0.129903
C	-2.924866	1.105724	-0.057519
H	-3.198212	3.191770	-0.113287
C	-4.398959	0.741756	-0.134913
N	-2.144619	-0.007675	-0.000429
C	-2.435420	-2.419496	0.073458
H	1.371340	-5.048637	-0.038065
H	-1.335569	-5.058258	0.049738
C	-4.393436	-0.773080	0.136553
C	-2.916866	-1.126560	0.057888
H	3.197822	-3.192151	-0.105061
C	1.117305	-2.828192	-0.030173
N	0.006936	-2.005478	0.002360
C	0.700578	-4.199271	-0.017144
H	-3.175380	-3.214472	0.114695
C	-0.670944	-4.204140	0.026773
H	-4.777609	-1.006721	1.137255
H	4.790566	-0.983887	-1.126020
H	4.994883	-1.303507	0.596203
H	4.783315	1.017947	1.124275
H	4.985553	1.339079	-0.597907
H	-4.989310	-1.344309	-0.580836
H	-4.785694	0.972675	-1.135264

(P)-[11]helicene: Cartesian coordinates in ångström

C	0.60363329	-1.63643305	-3.51606602
C	-2.41121975	-2.54945022	1.20257846
C	-1.99701813	-2.01859476	2.39300968
C	-0.96909630	-1.02967917	2.42552453
C	1.75559553	-1.08678306	-0.99701068
C	-0.38127435	-0.60963789	1.20673582
C	0.36202987	-1.45746597	-1.07494954
C	-0.55765424	-1.43517935	0.03932401
C	-0.14226479	-1.89423016	-2.33114018
C	-1.69223069	-2.28711889	-0.00223380
C	-1.38613604	-2.58871045	-2.38629893
C	-2.08510181	-2.86388422	-1.24431012
C	2.08510181	2.86388422	-1.24431012
C	0.50848320	0.45814664	3.64849714
C	1.38613604	2.58871045	-2.38629893
C	-0.50848320	-0.45814664	3.64849714
C	0.14226479	1.89423016	-2.33114018
C	-0.36202987	1.45746597	-1.07494954
C	0.55765424	1.43517935	0.03932401
C	0.38127435	0.60963789	1.20673582
C	1.69223069	2.28711889	-0.00223380
C	0.96909630	1.02967917	2.42552453
C	2.41121975	2.54945022	1.20257846
C	1.99701813	2.01859476	2.39300968
C	-0.60363329	1.63643305	-3.51606602
C	-1.79991950	0.97905695	-3.45381906
C	-2.41737794	0.71925272	-2.19717175
C	-1.75559553	1.08678306	-0.99701068
C	2.41737794	-0.71925272	-2.19717175
C	1.79991950	-0.97905695	-3.45381906
C	3.71579774	-0.12615918	-2.14056598
C	4.37062985	0.02797706	-0.95503399
C	3.83715272	-0.54001571	0.24122242
C	2.55458659	-1.16811713	0.21057180
C	-3.71579774	0.12615918	-2.14056598
C	-4.37062985	-0.02797706	-0.95503399
C	-3.83715272	0.54001571	0.24122242
C	-2.55458659	1.16811713	0.21057180
C	4.59671157	-0.56261623	1.43474461
C	4.15655090	-1.25142244	2.54534377
C	2.95364150	-1.98044022	2.47582096
C	2.17744889	-1.94108974	1.33527543
C	-2.17744889	1.94108974	1.33527543
C	-2.95364150	1.98044022	2.47582096
C	-4.15655090	1.25142244	2.54534377
C	-4.59671157	0.56261623	1.43474461
H	0.17769299	-1.93213412	-4.47130452
H	-3.26462233	-3.22127652	1.16035046
H	-2.48126380	-2.29679680	3.32535800
H	-1.73993074	-2.93800326	-3.35301064
H	-2.98283481	-3.47569445	-1.27303636
H	2.98283481	3.47569445	-1.27303636
H	0.94023269	0.81022244	4.58189478
H	1.73993074	2.93800326	-3.35301064
H	-0.94023269	-0.81022244	4.58189478
H	3.26462233	3.22127652	1.16035046
H	2.48126380	2.29679680	3.32535800
H	-0.17769299	1.93213412	-4.47130452
H	-2.33208396	0.70231016	-4.36049250
H	2.33208396	-0.70231016	-4.36049250
H	4.16316066	0.21445019	-3.07106155

H	5.34088509	0.51684461	-0.91285517
H	-4.16316066	-0.21445019	-3.07106155
H	-5.34088509	-0.51684461	-0.91285517
H	5.55437246	-0.04743205	1.44792713
H	4.75181713	-1.26637527	3.45400804
H	2.63329839	-2.58223638	3.32124236
H	1.26996971	-2.52987631	1.29093137
H	-1.26996971	2.52987631	1.29093137
H	-2.63329839	2.58223638	3.32124236
H	-4.75181713	1.26637527	3.45400804
H	-5.55437246	0.04743205	1.44792713