Electronic Supplementary Information

Effect of tailoring the π-linkers with extended conjugation on the SJ-IC molecule for achieving high Voc and improved charge mobility towards enhanced photovoltaic applications

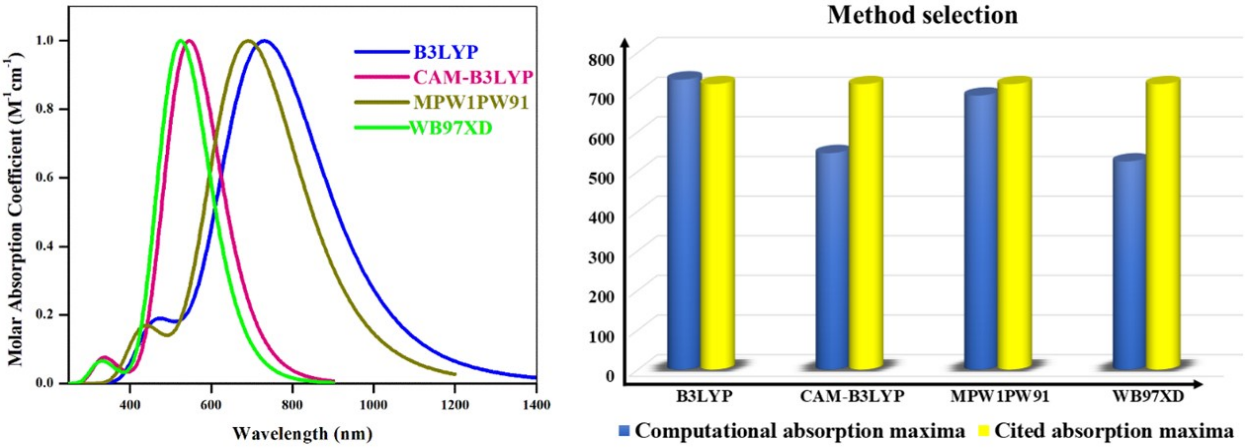


Figure S1. Origin graph (at left) for method selection through four basic levels of the DFT approach alongside a bar graph (at right) comparing λ_{max} from different functionals of DFT, revealing the selection of the best-suited functional.

Full width half maximum

Generally, a good absorption band is seen in absorption graphs of organic molecules with 50−150 nm FWHM. Broad absorption spectra indicate an efficient capability of the molecule for harvesting sunlight. In conceptualized molecules, the peaks with short wavelengths usually occur due to electronic transitions in lower frontier states. At the same time, an absorption band at a long wavelength appears due to ICT (of the donor to acceptor) from HOMO to LUMO. These long and short wavelength absorption bands co-exist, resulting in a wide spectrum. In the present research work, we calculated the full-width half maximum to look over the light-harvesting ability of our tailored molecules. The graphs were developed as provided in **Figure 11** and compared the resultant values of newly tailored molecules with those of R. The R molecule exhibited an FWHM at 306 nm. While all our modified molecules showed enough broader FWHM in contrast to R with values of 393 nm, 840 nm, 768 nm, 675 nm, 395 nm, 389 nm, and

382 nm for DL1−DL7, respectively. These higher values for FWHM of DL1−DL7 signify that all of these tailored molecules absorb in the wider area of the UV-Visible spectrum. The highest FWHM values for DL2 and DL3 depict high light harvesting capacity ensuring their remarkable potential to be used in manufacturing of improved OSCs in future.

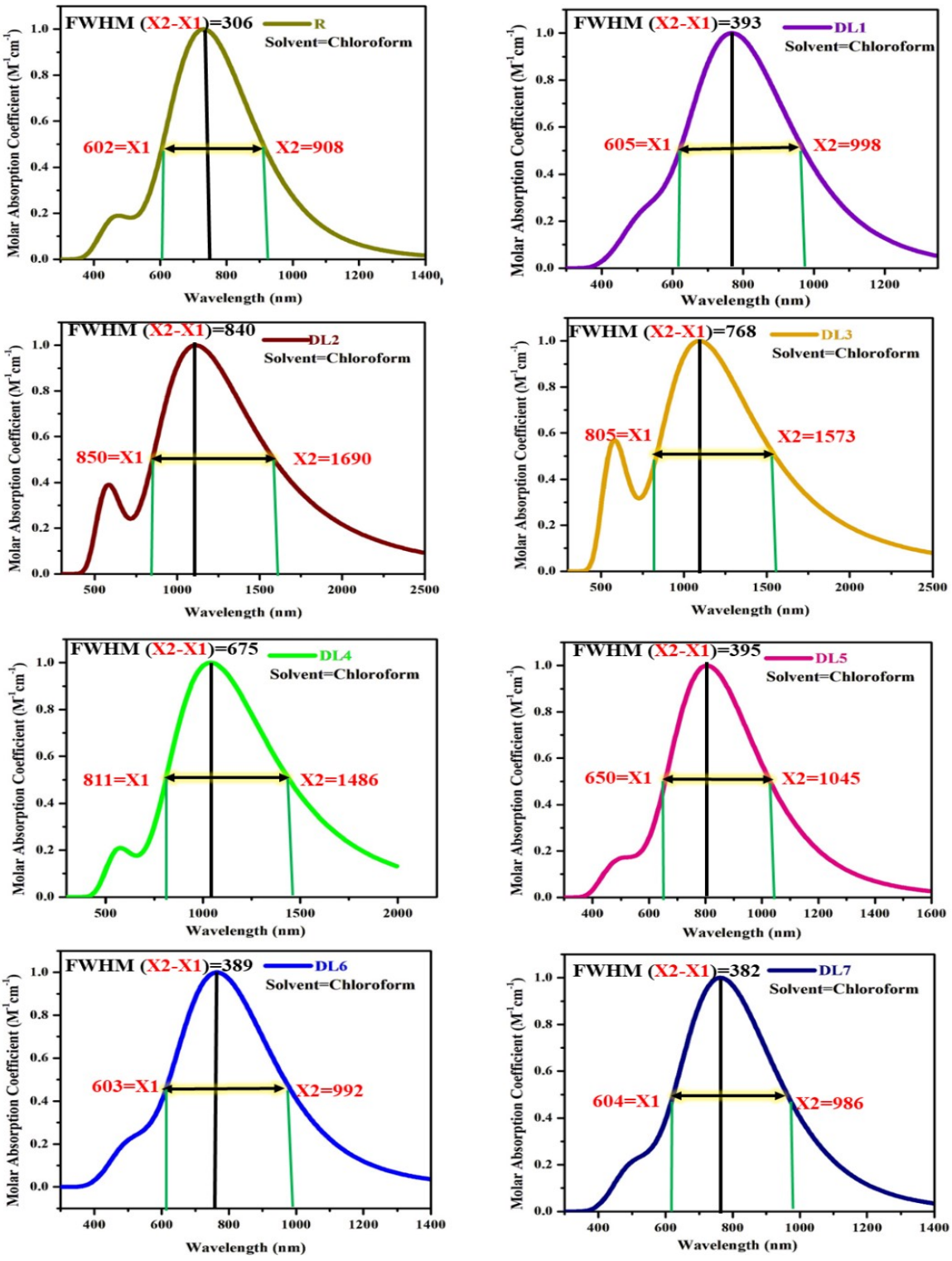
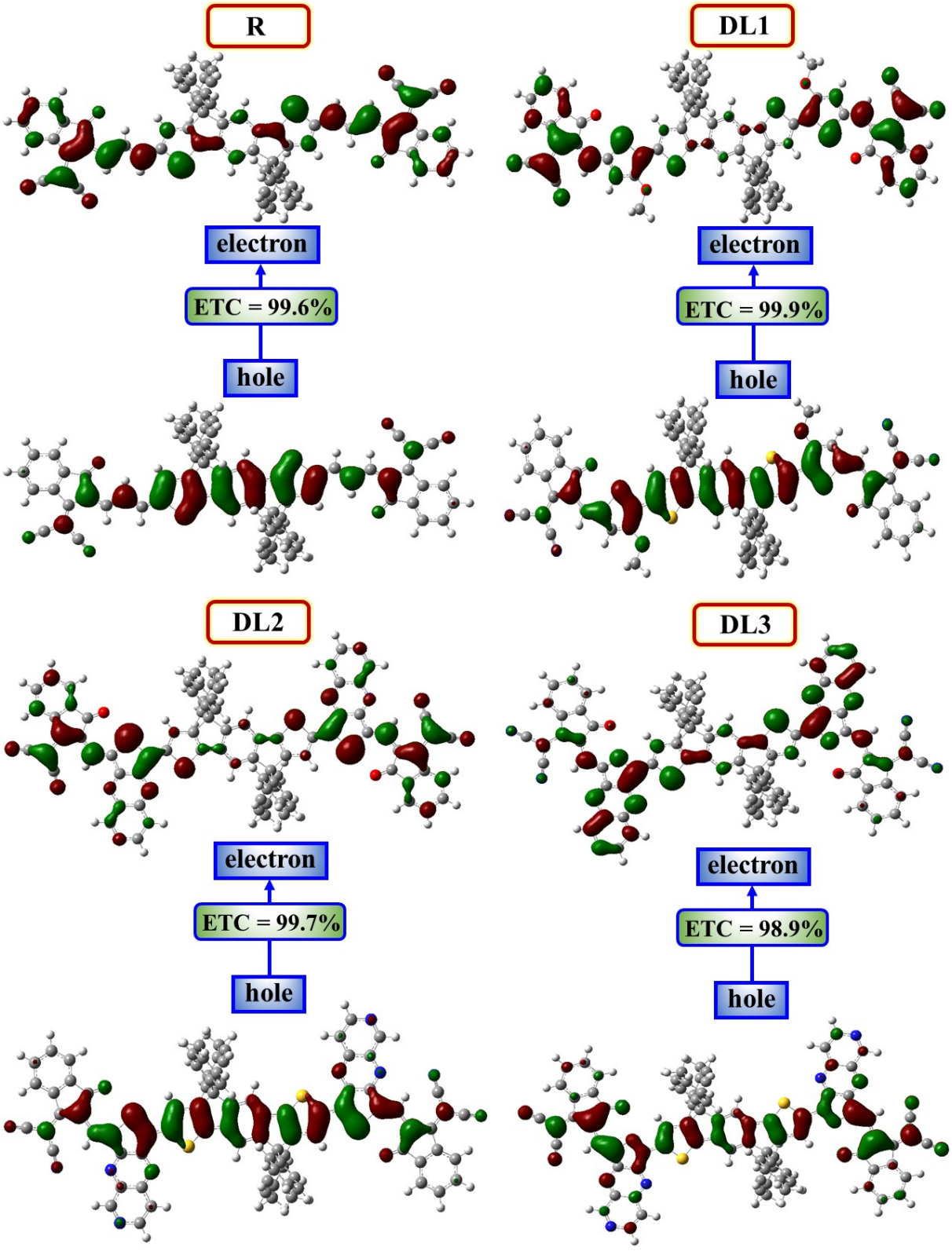


Figure S2. Pictorial representation of wide region absorption of studied molecules with their corresponding FWHM.


R
electron
ETC = 99.6%
hole
DL1
electron
ETC = 99.9%
hole
DL2
electron
ETC = 99.7%
hole
DL3
electron
ETC = 98.9%
hole

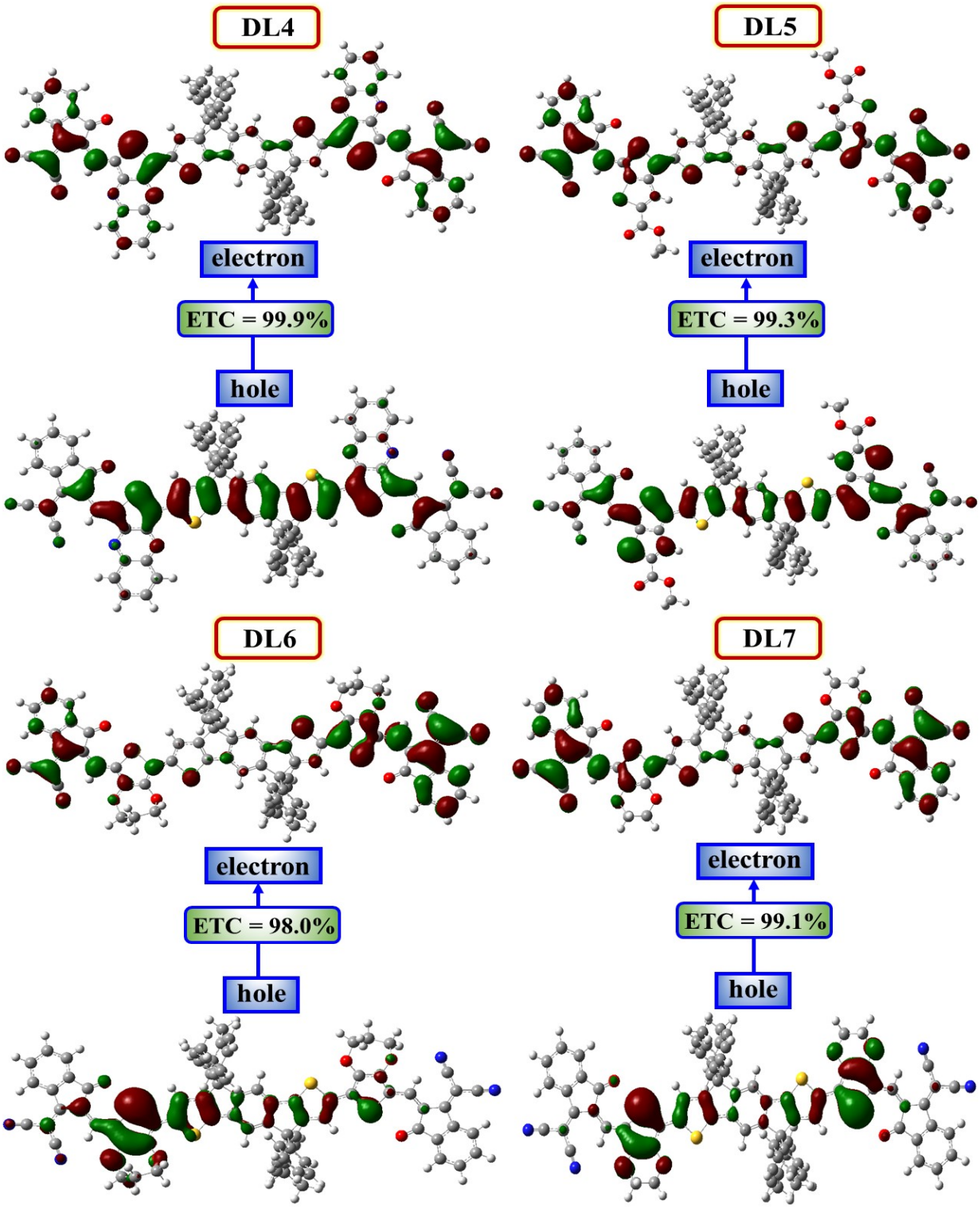
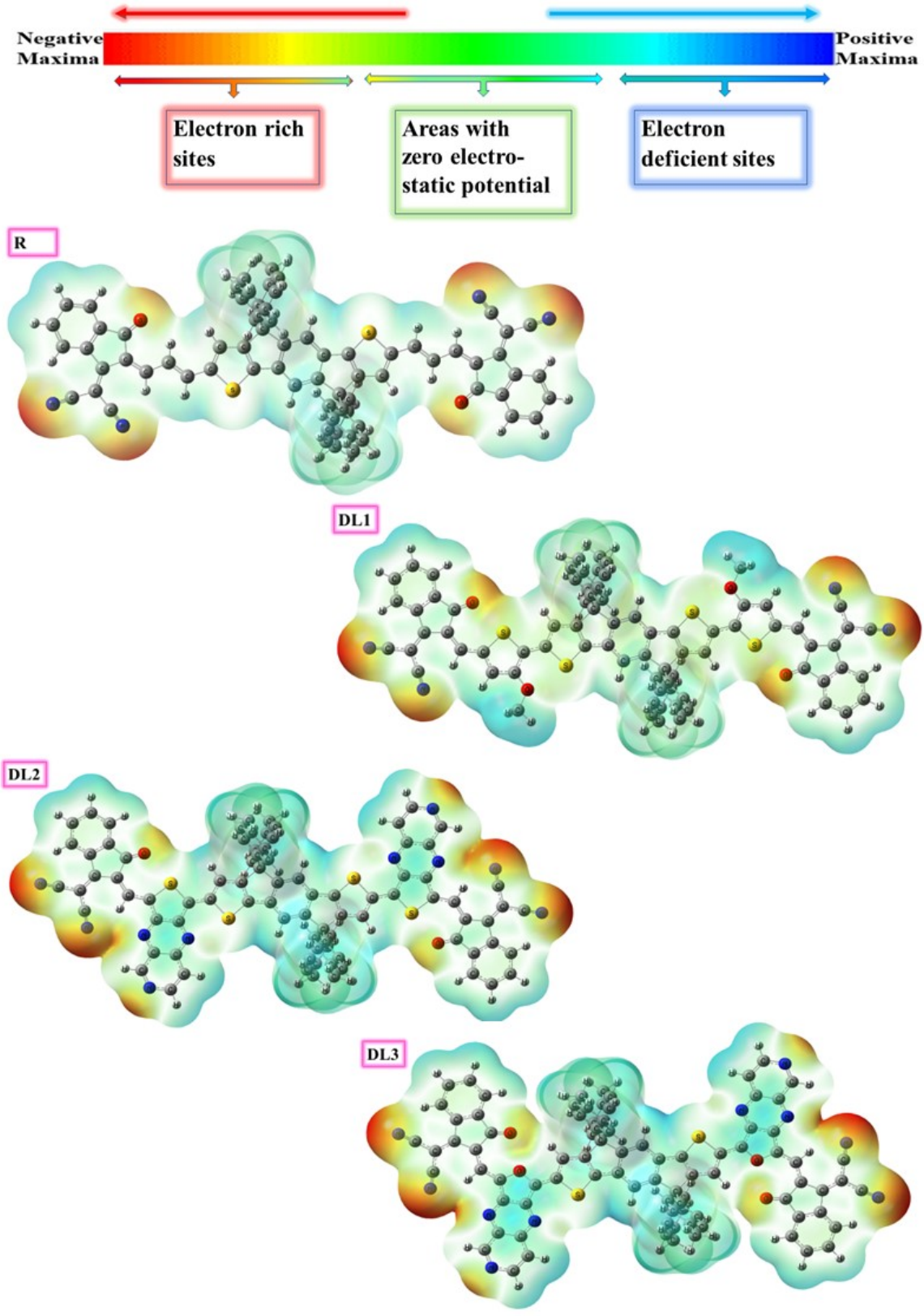


Figure S3. Visual representation of electronic transition contribution (ETC) from occupied-NTO to unoccupied-NTO.


Negative Maxima
Positive Maxima
Electron rich sites
Areas with zero electro-static potential
Electron deficient sites
R
DL1
DL2
DL3

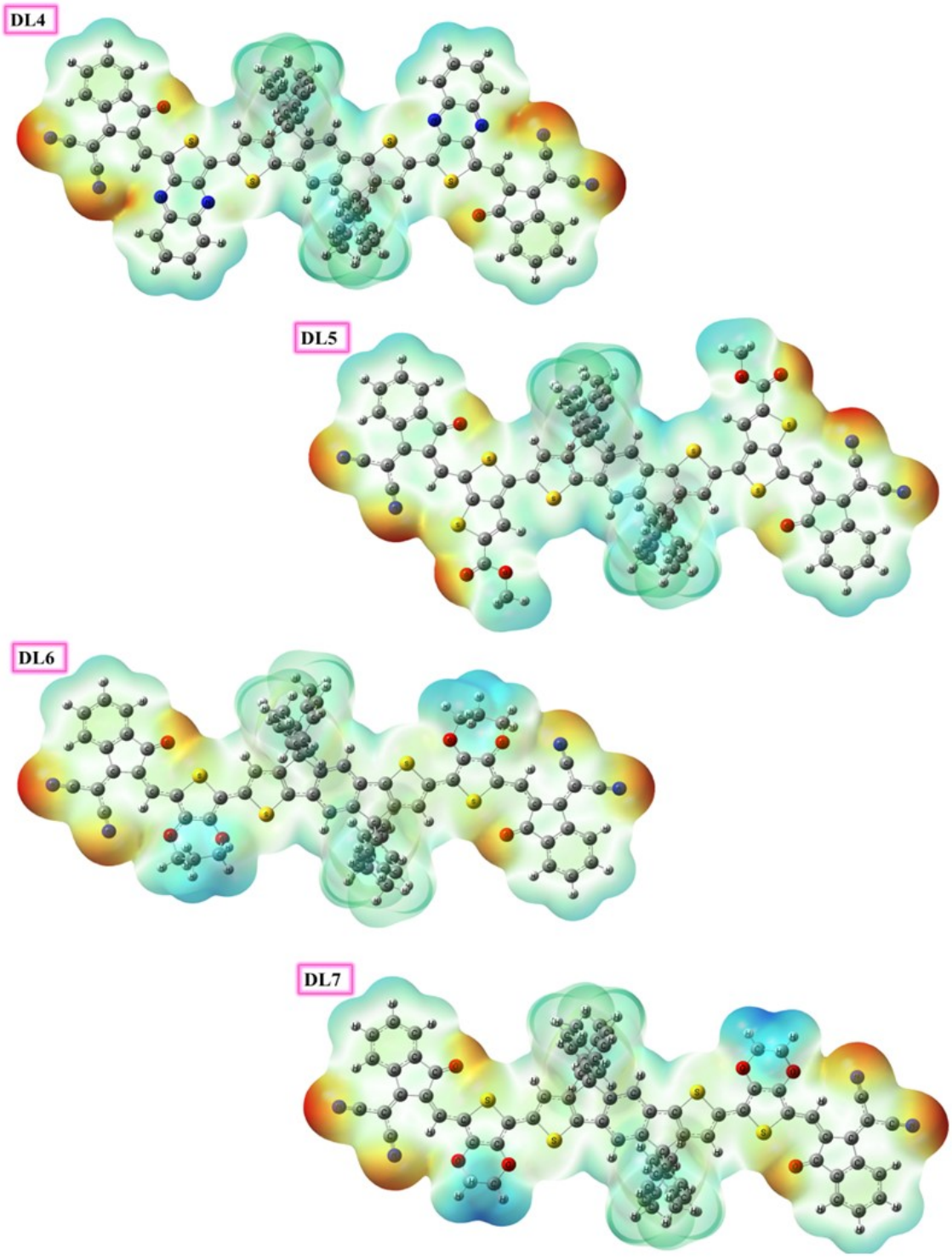


Figure S4. MEP map for studied molecules exposing electron density, reactive sites, nucleophilic and electrophilic regions.

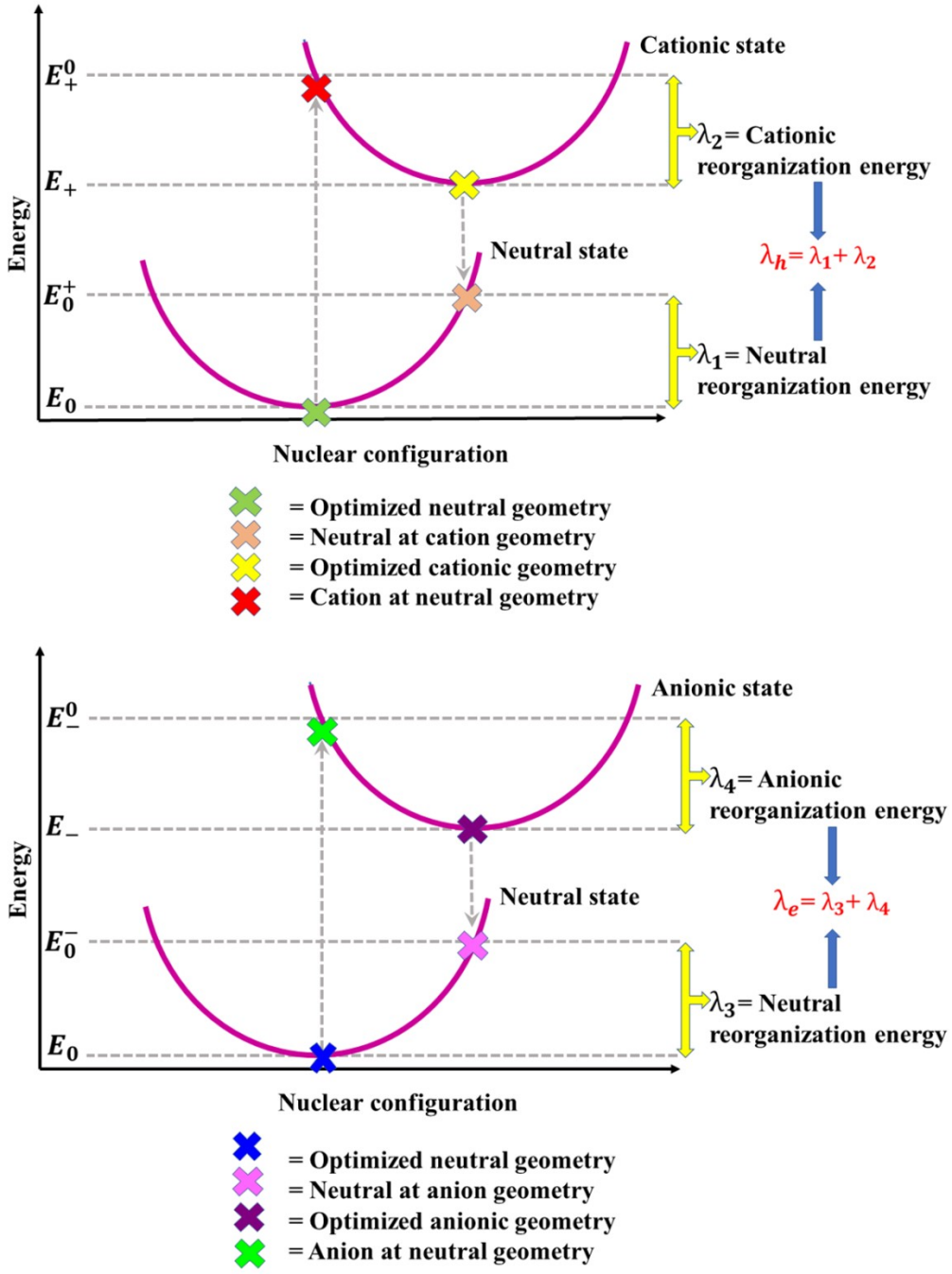


Figure S5. Reorganization energies for a hole (above) and electron (below).

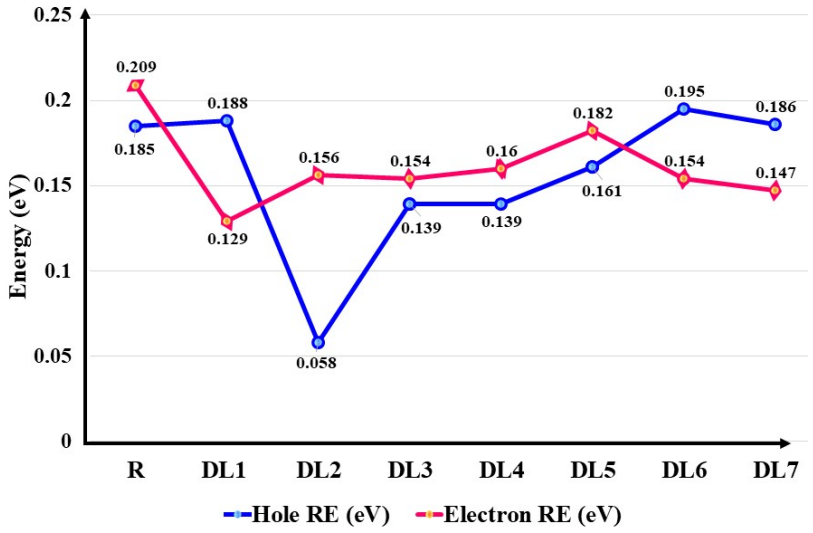


Figure S6. Comparison of electron and hole reorganization energies of designed molecules with those of reference.

Cartesian coordinates of internally optimized geometries of all molecules (reference **R**, and investigated molecules **DL1, DL2, DL3, DL4, DL5, DL6, and DL7** along X, Y and Z axis at B3LYP/6-31G (d, p) level of density functional theory (DFT).

Cartesian coordinates of Reference Molecule R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.049713	1.043082	-0.076291
2	6	0	1.327821	-0.287977	-0.087942
3	6	0	2.346259	1.900166	-0.030439
4	6	0	3.418281	0.843028	-0.023165
5	6	0	2.879077	-0.356787	-0.060950
6	6	0	5.360729	-0.590505	0.059851
7	6	0	4.952208	0.717570	-0.077272
8	16	0	4.100734	-1.685790	0.070978
9	1	0	5.613050	1.585686	-0.108857
10	6	0	8.965817	-1.772226	0.026759
11	6	0	7.799728	-0.820216	-0.046826
12	6	0	6.626446	-1.465765	0.000869
13	6	0	12.183361	0.111115	-0.047787
14	6	0	11.262071	1.084156	-0.051767
15	6	0	11.591771	2.445264	-0.087094

16	6	0	12.918540	2.723387	-0.117471
17	6	0	13.910855	1.675332	-0.113184
18	6	0	13.560575	0.365866	-0.078589
19	6	0	11.499718	-1.284788	-0.005203
20	6	0	10.050444	-0.985431	0.015011
21	6	0	9.830758	0.477923	-0.012412
22	1	0	10.830277	3.238516	-0.090147
23	1	0	13.279768	3.762315	-0.146451
24	1	0	14.968067	1.979179	-0.139158
25	1	0	14.311066	-0.437800	-0.075110
26	1	0	8.934508	-2.840576	0.077240
27	1	0	7.896951	0.242308	-0.127385
28	1	0	6.571811	-2.534366	-0.001885
29	8	0	8.735751	1.038095	-0.004321
30	6	0	12.043893	-2.509209	0.011117
31	6	0	10.599006	-3.033920	0.103737
32	7	0	10.548814	-4.190143	0.024813
33	6	0	13.423589	-3.180173	0.144702
34	7	0	13.526392	-4.332949	0.223059
35	6	0	2.562548	2.396239	2.885324
36	6	0	2.639112	3.589893	3.414437
37	6	0	2.665851	4.827994	2.499018
38	6	0	2.615298	4.701225	1.231974

39	6	0	2.525132	3.299247	0.587764
40	6	0	2.500592	2.241298	1.349261
41	1	0	2.542387	1.505663	3.530002
42	1	0	2.729616	5.830072	2.947425
43	1	0	2.635097	5.592151	0.587648
44	6	0	2.319685	2.299372	-1.325465
45	6	0	2.325382	2.473516	-2.860646
46	6	0	2.501643	3.656321	-3.380082
47	6	0	2.702226	4.875300	-2.451475
48	6	0	2.696931	4.730705	-1.185169
49	6	0	2.491336	3.341285	-0.553629
50	1	0	2.171723	1.302816	-0.884866
51	1	0	2.182133	1.599519	-3.512452
52	1	0	2.850550	5.871674	-2.892536
53	1	0	2.840500	5.604351	-0.532784
54	6	0	2.507986	3.828447	-4.910419
55	1	0	1.596640	4.295510	-5.220582
56	1	0	3.337791	4.440114	-5.197101
57	1	0	2.593934	2.869309	-5.376861
58	6	0	2.699825	3.745375	4.945364
59	1	0	1.890097	3.206263	5.391009
60	1	0	3.628880	3.356617	5.306783
61	1	0	2.622681	4.781275	5.201997

62	1	0	2.437639	1.267143	0.911131
63	6	0	-2.330209	-1.786579	-0.059231
64	6	0	-3.411957	-0.749456	-0.052653
65	6	0	-2.906381	0.464334	-0.105862
66	6	0	-5.392697	0.630729	0.029633
67	6	0	-4.949088	-0.666886	-0.097482
68	16	0	-4.163410	1.760396	0.021420
69	1	0	-5.585876	-1.553165	-0.116049
70	6	0	-9.029209	1.712209	0.009662
71	6	0	-7.837762	0.792028	-0.062588
72	6	0	-6.682482	1.470126	-0.029242
73	6	0	-12.193890	-0.259782	-0.024430
74	6	0	-11.246104	-1.207042	-0.025198
75	6	0	-11.538283	-2.577008	-0.044952
76	6	0	-12.857030	-2.891897	-0.063524
77	6	0	-13.877883	-1.871610	-0.062697
78	6	0	-13.563709	-0.552705	-0.043310
79	6	0	-11.548825	1.154795	-0.000183
80	6	0	-10.091729	0.895729	0.013036
81	6	0	-9.831866	-0.561211	-0.001575
82	1	0	-10.755192	-3.348952	-0.045458
83	1	0	-13.189587	-3.940627	-0.079867
84	1	0	-14.926441	-2.204736	-0.078459

85	1	0	-14.336088	0.229958	-0.042555
86	1	0	-9.027110	2.781466	0.049475
87	1	0	-7.906107	-0.273524	-0.132082
88	1	0	-6.657423	2.539746	-0.042822
89	8	0	-8.721765	-1.090869	0.004500
90	6	0	-12.126515	2.363848	0.007884
91	6	0	-10.696105	2.929096	0.085474
92	7	0	-10.678409	4.085419	-0.005098
93	6	0	-13.523321	2.997813	0.144342
94	7	0	-13.657430	4.148039	0.212120
95	6	0	-2.513535	-2.259342	2.862658
96	6	0	-2.553599	-3.449320	3.403932
97	6	0	-2.552124	-4.696750	2.500872
98	6	0	-2.513422	-4.581270	1.232332
99	6	0	-2.466277	-3.183830	0.573838
100	6	0	-2.465983	-2.118069	1.324764
101	1	0	-2.513759	-1.362167	3.498440
102	1	0	-2.585219	-5.695686	2.959486
103	1	0	-2.512824	-5.478781	0.596903
104	6	0	-2.301124	-2.197788	-1.350441
105	6	0	-2.312096	-2.387316	-2.883771
106	6	0	-2.459008	-3.579650	-3.390393
107	6	0	-2.619715	-4.794380	-2.448555

108	6	0	-2.610096	-4.637080	-1.183791
109	6	0	-2.438835	-3.236294	-0.567294
110	1	0	-2.177869	-1.193190	-0.920635
111	1	0	-2.197346	-1.516241	-3.545060
112	1	0	-2.743339	-5.798811	-2.878824
113	1	0	-2.725172	-5.507806	-0.521924
114	6	0	-2.470650	-3.767128	-4.918895
115	1	0	-1.548802	-4.211953	-5.230706
116	1	0	-3.285098	-4.404271	-5.193892
117	1	0	-2.586139	-2.815422	-5.394097
118	6	0	-2.599927	-3.591151	4.936687
119	1	0	-1.802497	-3.025502	5.371483
120	1	0	-3.536976	-3.224574	5.300637
121	1	0	-2.492495	-4.621920	5.202907
122	1	0	-2.432860	-1.146963	0.876705
123	6	0	0.291182	-1.414463	0.079415
124	6	0	-0.972894	-1.077944	0.105485
125	6	0	-1.369104	0.398079	-0.042692
126	6	0	-0.467015	1.287413	-0.183247
127	1	0	0.571717	-2.472736	0.182362
128	1	0	-0.746969	2.345910	-0.286610

Cartesian coordinates of Designed Molecule DL1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.051382	0.922841	0.077017
2	6	0	-1.297645	-0.476934	0.069642
3	6	0	-2.374270	1.724562	0.056189
4	6	0	-3.381841	0.572519	0.024891
5	6	0	-2.730908	-0.649681	0.049581
6	6	0	-5.209475	-0.875786	0.029011
7	6	0	-4.779298	0.451807	0.017380
8	16	0	-3.821607	-1.988370	0.059546
9	1	0	-5.470519	1.286363	0.008449
10	6	0	-10.491615	-1.492483	-0.033411
11	6	0	-13.449245	0.765344	-0.120930
12	6	0	-12.394806	1.697037	-0.123103
13	6	0	-12.607791	3.067904	-0.152620
14	6	0	-13.926181	3.527252	-0.180739
15	6	0	-14.986947	2.614310	-0.178538
16	6	0	-14.767869	1.232985	-0.148967
17	6	0	-12.875704	-0.607846	-0.087068
18	6	0	-11.418378	-0.468140	-0.067457
19	6	0	-11.102119	0.976158	-0.089799

20	1	0	-11.760722	3.746417	-0.153294
21	1	0	-14.132352	4.592944	-0.204278
22	1	0	-16.008306	2.981987	-0.200308
23	1	0	-15.615570	0.561994	-0.148405
24	1	0	-10.900426	-2.496255	-0.019290
25	8	0	-9.990788	1.496479	-0.084419
26	6	0	-13.626914	-1.772270	-0.078676
27	6	0	-13.067786	-3.086879	-0.047742
28	7	0	-12.644289	-4.172796	-0.022880
29	6	0	-15.055431	-1.788769	-0.100944
30	7	0	-16.219001	-1.850272	-0.118262
31	6	0	-2.829992	2.874670	-3.592516
32	6	0	-2.278954	4.161200	-3.587523
33	6	0	-1.782853	4.648346	-2.372216
34	6	0	-1.842267	3.884963	-1.207665
35	6	0	-2.399983	2.598628	-1.214968
36	6	0	-2.889530	2.106063	-2.430660
37	1	0	-3.220447	2.463483	-4.520235
38	1	0	-1.344998	5.642906	-2.333175
39	1	0	-1.461075	4.301623	-0.280818
40	6	0	-1.893232	2.338726	2.516131
41	6	0	-2.198912	3.043174	3.682600
42	6	0	-3.238705	3.976346	3.719296

43	6	0	-3.970783	4.177764	2.540596
44	6	0	-3.668956	3.479385	1.375447
45	6	0	-2.619707	2.546883	1.339661
46	1	0	-1.080911	1.620670	2.531400
47	1	0	-1.613980	2.859076	4.580397
48	1	0	-4.790594	4.892046	2.534646
49	1	0	-4.250432	3.668699	0.478251
50	6	0	-3.551991	4.758076	4.972546
51	1	0	-3.139857	5.773560	4.921716
52	1	0	-4.631864	4.856575	5.122879
53	1	0	-3.129621	4.277602	5.859508
54	6	0	-2.247725	5.004304	-4.839805
55	1	0	-2.158867	4.384798	-5.737220
56	1	0	-3.166016	5.595849	-4.943506
57	1	0	-1.409144	5.706911	-4.828423
58	1	0	-3.319208	1.110868	-2.475974
59	6	0	2.374240	-1.724258	0.054798
60	6	0	3.381807	-0.572219	0.023467
61	6	0	2.730900	0.649985	0.048714
62	6	0	5.209459	0.876056	0.026911
63	6	0	4.779258	-0.451530	0.015231
64	16	0	3.821624	1.988657	0.058260
65	1	0	5.470455	-1.286099	0.005646

66	6	0	10.491587	1.492616	-0.035339
67	6	0	13.448606	-0.766171	-0.120800
68	6	0	12.393857	-1.697484	-0.122521
69	6	0	12.606394	-3.068427	-0.151679
70	6	0	13.924638	-3.528200	-0.180049
71	6	0	14.985708	-2.615601	-0.178455
72	6	0	14.767072	-1.234203	-0.149145
73	6	0	12.875655	0.607222	-0.086889
74	6	0	11.418212	0.468091	-0.067666
75	6	0	11.101442	-0.976111	-0.089502
76	1	0	11.759109	-3.746671	-0.151951
77	1	0	14.130461	-4.593963	-0.203357
78	1	0	16.006941	-2.983612	-0.200498
79	1	0	15.614958	-0.563419	-0.149046
80	1	0	10.900420	2.496363	-0.022494
81	8	0	9.989929	-1.496035	-0.083342
82	6	0	13.627890	1.770993	-0.077316
83	6	0	13.070297	3.086222	-0.045109
84	7	0	12.649278	4.173077	-0.019215
85	6	0	15.056431	1.785864	-0.099264
86	7	0	16.220109	1.845409	-0.116348
87	6	0	2.829435	-2.873145	-3.594344
88	6	0	2.277360	-4.159234	-3.589998

89	6	0	1.780714	-4.646520	-2.374972
90	6	0	1.840627	-3.883720	-1.210062
91	6	0	2.399436	-2.597855	-1.216704
92	6	0	2.889468	-2.105119	-2.432132
93	1	0	3.220309	-2.461846	-4.521837
94	1	0	1.342021	-5.640731	-2.336436
95	1	0	1.458940	-4.300476	-0.283466
96	6	0	1.893485	-2.339706	2.514454
97	6	0	2.199597	-3.044340	3.680693
98	6	0	3.240042	-3.976802	3.717117
99	6	0	3.972331	-4.177279	2.538393
100	6	0	3.670068	-3.478712	1.373466
101	6	0	2.620141	-2.546963	1.337935
102	1	0	1.080678	-1.622203	2.529942
103	1	0	1.614502	-2.860946	4.578528
104	1	0	4.792668	-4.890954	2.532250
105	1	0	4.251758	-3.667271	0.476251
106	6	0	3.553770	-4.758766	4.970110
107	1	0	3.141351	-5.774141	4.919362
108	1	0	4.633690	-4.857543	5.119892
109	1	0	3.131947	-4.278309	5.857346
110	6	0	2.245578	-5.001742	-4.842668
111	1	0	2.157506	-4.381745	-5.739821

112	1	0	3.163317	-5.594130	-4.946443
113	1	0	1.406315	-5.703542	-4.831777
114	1	0	3.319932	-1.110240	-2.476952
115	6	0	-0.246663	-1.406974	0.065314
116	6	0	1.051375	-0.922530	0.076365
117	6	0	1.297640	0.477244	0.069242
118	6	0	0.246656	1.407284	0.065564
119	1	0	-0.446788	-2.473654	0.045077
120	1	0	0.446779	2.473968	0.045517
121	6	0	9.076960	1.539797	-0.014544
122	6	0	8.412036	2.775766	0.016683
123	6	0	7.019529	2.672921	0.033494
124	6	0	6.561387	1.342753	0.016159
125	16	0	7.905364	0.222487	-0.022541
126	1	0	8.960820	3.709108	0.026208
127	6	0	-6.561398	-1.342507	0.018475
128	6	0	-7.019539	-2.672650	0.037477
129	6	0	-8.412046	-2.775508	0.020754
130	6	0	-9.076984	-1.539583	-0.012113
131	16	0	-7.905374	-0.222297	-0.021922
132	1	0	-8.960821	-3.708840	0.031537
133	8	0	-6.118269	-3.685126	0.068321
134	8	0	6.118258	3.685432	0.063064

135	6	0	-6.624087	-5.017741	0.084478
136	6	0	6.624107	5.018044	0.078533
137	1	0	-7.214821	-5.227095	-0.815042
138	1	0	-5.751294	-5.670043	0.106875
139	1	0	-7.237829	-5.196699	0.975083
140	1	0	5.751324	5.670370	0.100544
141	1	0	7.237807	5.197454	0.969084
142	1	0	7.214894	5.226914	-0.821058

Cartesian coordinates of Designed Molecule DL2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.051382	0.922841	0.077017
2	6	0	-1.297645	-0.476934	0.069642
3	6	0	-2.374270	1.724562	0.056189
4	6	0	-3.381841	0.572519	0.024891
5	6	0	-2.730908	-0.649681	0.049581
6	6	0	-5.209475	-0.875786	0.029011
7	6	0	-4.779298	0.451807	0.017380
8	16	0	-3.821607	-1.988370	0.059546
9	1	0	-5.470519	1.286363	0.008449

10	6	0	-10.491615	-1.492483	-0.033411
11	6	0	-13.449245	0.765344	-0.120930
12	6	0	-12.394806	1.697037	-0.123103
13	6	0	-12.607791	3.067904	-0.152620
14	6	0	-13.926181	3.527252	-0.180739
15	6	0	-14.986947	2.614310	-0.178538
16	6	0	-14.767869	1.232985	-0.148967
17	6	0	-12.875704	-0.607846	-0.087068
18	6	0	-11.418378	-0.468140	-0.067457
19	6	0	-11.102119	0.976158	-0.089799
20	1	0	-11.760722	3.746417	-0.153294
21	1	0	-14.132352	4.592944	-0.204278
22	1	0	-16.008306	2.981987	-0.200308
23	1	0	-15.615570	0.561994	-0.148405
24	1	0	-10.900426	-2.496255	-0.019290
25	8	0	-9.990788	1.496479	-0.084419
26	6	0	-13.626914	-1.772270	-0.078676
27	6	0	-13.067786	-3.086879	-0.047742
28	7	0	-12.644289	-4.172796	-0.022880
29	6	0	-15.055431	-1.788769	-0.100944
30	7	0	-16.219001	-1.850272	-0.118262
31	6	0	-2.829992	2.874670	-3.592516
32	6	0	-2.278954	4.161200	-3.587523

33	6	0	-1.782853	4.648346	-2.372216
34	6	0	-1.842267	3.884963	-1.207665
35	6	0	-2.399983	2.598628	-1.214968
36	6	0	-2.889530	2.106063	-2.430660
37	1	0	-3.220447	2.463483	-4.520235
38	1	0	-1.344998	5.642906	-2.333175
39	1	0	-1.461075	4.301623	-0.280818
40	6	0	-1.893232	2.338726	2.516131
41	6	0	-2.198912	3.043174	3.682600
42	6	0	-3.238705	3.976346	3.719296
43	6	0	-3.970783	4.177764	2.540596
44	6	0	-3.668956	3.479385	1.375447
45	6	0	-2.619707	2.546883	1.339661
46	1	0	-1.080911	1.620670	2.531400
47	1	0	-1.613980	2.859076	4.580397
48	1	0	-4.790594	4.892046	2.534646
49	1	0	-4.250432	3.668699	0.478251
50	6	0	-3.551991	4.758076	4.972546
51	1	0	-3.139857	5.773560	4.921716
52	1	0	-4.631864	4.856575	5.122879
53	1	0	-3.129621	4.277602	5.859508
54	6	0	-2.247725	5.004304	-4.839805
55	1	0	-2.158867	4.384798	-5.737220

56	1	0	-3.166016	5.595849	-4.943506
57	1	0	-1.409144	5.706911	-4.828423
58	1	0	-3.319208	1.110868	-2.475974
59	6	0	2.374240	-1.724258	0.054798
60	6	0	3.381807	-0.572219	0.023467
61	6	0	2.730900	0.649985	0.048714
62	6	0	5.209459	0.876056	0.026911
63	6	0	4.779258	-0.451530	0.015231
64	16	0	3.821624	1.988657	0.058260
65	1	0	5.470455	-1.286099	0.005646
66	6	0	10.491587	1.492616	-0.035339
67	6	0	13.448606	-0.766171	-0.120800
68	6	0	12.393857	-1.697484	-0.122521
69	6	0	12.606394	-3.068427	-0.151679
70	6	0	13.924638	-3.528200	-0.180049
71	6	0	14.985708	-2.615601	-0.178455
72	6	0	14.767072	-1.234203	-0.149145
73	6	0	12.875655	0.607222	-0.086889
74	6	0	11.418212	0.468091	-0.067666
75	6	0	11.101442	-0.976111	-0.089502
76	1	0	11.759109	-3.746671	-0.151951
77	1	0	14.130461	-4.593963	-0.203357
78	1	0	16.006941	-2.983612	-0.200498

79	1	0	15.614958	-0.563419	-0.149046
80	1	0	10.900420	2.496363	-0.022494
81	8	0	9.989929	-1.496035	-0.083342
82	6	0	13.627890	1.770993	-0.077316
83	6	0	13.070297	3.086222	-0.045109
84	7	0	12.649278	4.173077	-0.019215
85	6	0	15.056431	1.785864	-0.099264
86	7	0	16.220109	1.845409	-0.116348
87	6	0	2.829435	-2.873145	-3.594344
88	6	0	2.277360	-4.159234	-3.589998
89	6	0	1.780714	-4.646520	-2.374972
90	6	0	1.840627	-3.883720	-1.210062
91	6	0	2.399436	-2.597855	-1.216704
92	6	0	2.889468	-2.105119	-2.432132
93	1	0	3.220309	-2.461846	-4.521837
94	1	0	1.342021	-5.640731	-2.336436
95	1	0	1.458940	-4.300476	-0.283466
96	6	0	1.893485	-2.339706	2.514454
97	6	0	2.199597	-3.044340	3.680693
98	6	0	3.240042	-3.976802	3.717117
99	6	0	3.972331	-4.177279	2.538393
100	6	0	3.670068	-3.478712	1.373466
101	6	0	2.620141	-2.546963	1.337935

102	1	0	1.080678	-1.622203	2.529942
103	1	0	1.614502	-2.860946	4.578528
104	1	0	4.792668	-4.890954	2.532250
105	1	0	4.251758	-3.667271	0.476251
106	6	0	3.553770	-4.758766	4.970110
107	1	0	3.141351	-5.774141	4.919362
108	1	0	4.633690	-4.857543	5.119892
109	1	0	3.131947	-4.278309	5.857346
110	6	0	2.245578	-5.001742	-4.842668
111	1	0	2.157506	-4.381745	-5.739821
112	1	0	3.163317	-5.594130	-4.946443
113	1	0	1.406315	-5.703542	-4.831777
114	1	0	3.319932	-1.110240	-2.476952
115	6	0	-0.246663	-1.406974	0.065314
116	6	0	1.051375	-0.922530	0.076365
117	6	0	1.297640	0.477244	0.069242
118	6	0	0.246656	1.407284	0.065564
119	1	0	-0.446788	-2.473654	0.045077
120	1	0	0.446779	2.473968	0.045517
121	6	0	9.076960	1.539797	-0.014544
122	6	0	8.412036	2.775766	0.016683
123	6	0	7.019529	2.672921	0.033494
124	6	0	6.561387	1.342753	0.016159

125	16	0	7.905364	0.222487	-0.022541
126	1	0	8.960820	3.709108	0.026208
127	6	0	-6.561398	-1.342507	0.018475
128	6	0	-7.019539	-2.672650	0.037477
129	6	0	-8.412046	-2.775508	0.020754
130	6	0	-9.076984	-1.539583	-0.012113
131	16	0	-7.905374	-0.222297	-0.021922
132	1	0	-8.960821	-3.708840	0.031537
133	8	0	-6.118269	-3.685126	0.068321
134	8	0	6.118258	3.685432	0.063064
135	6	0	-6.624087	-5.017741	0.084478
136	6	0	6.624107	5.018044	0.078533
137	1	0	-7.214821	-5.227095	-0.815042
138	1	0	-5.751294	-5.670043	0.106875
139	1	0	-7.237829	-5.196699	0.975083
140	1	0	5.751324	5.670370	0.100544
141	1	0	7.237807	5.197454	0.969084
142	1	0	7.214894	5.226914	-0.821058

Cartesian coordinates of Designed Molecule DL3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-1.089185	0.881190	0.137469
2	6	0	-1.274434	-0.530221	0.128326
3	6	0	-2.442732	1.627288	0.114749
4	6	0	-3.401142	0.434949	0.067972
5	6	0	-2.694536	-0.763202	0.099801
6	6	0	-5.137657	-1.098822	0.050288
7	6	0	-4.787827	0.256775	0.042187
8	16	0	-3.718762	-2.155950	0.098826
9	1	0	-5.542679	1.034371	0.018691
10	6	0	-9.926925	-0.726821	-0.092349
11	6	0	-11.615159	2.590637	-0.266707
12	6	0	-10.267617	2.986369	-0.249976
13	6	0	-9.877401	4.316935	-0.306126
14	6	0	-10.873382	5.291963	-0.382403
15	6	0	-12.221352	4.915340	-0.400479
16	6	0	-12.609786	3.573000	-0.343398
17	6	0	-11.676056	1.105101	-0.192245
18	6	0	-10.299471	0.609205	-0.141237
19	6	0	-9.390489	1.793132	-0.167461
20	1	0	-8.821852	4.569147	-0.290782
21	1	0	-10.606757	6.343531	-0.428421
22	1	0	-12.989467	5.680394	-0.460458

23	1	0	-13.661945	3.326159	-0.360371
24	1	0	-10.719624	-1.468266	-0.093087
25	8	0	-8.167318	1.829065	-0.133980
26	6	0	-12.855207	0.375984	-0.171714
27	6	0	-12.931823	-1.048078	-0.086665
28	7	0	-13.052941	-2.205433	-0.017332
29	6	0	-14.150664	0.976426	-0.229908
30	7	0	-15.228024	1.418535	-0.275536
31	6	0	-2.919405	2.797043	-3.524797
32	6	0	-2.427849	4.107250	-3.499509
33	6	0	-1.965714	4.602301	-2.273901
34	6	0	-2.001144	3.823727	-1.118495
35	6	0	-2.498657	2.513428	-1.147214
36	6	0	-2.953295	2.012496	-2.372768
37	1	0	-3.283189	2.380056	-4.460574
38	1	0	-1.574941	5.615438	-2.219148
39	1	0	-1.649819	4.246915	-0.182802
40	6	0	-1.973887	2.279545	2.570574
41	6	0	-2.315952	2.965477	3.738501
42	6	0	-3.424072	3.815320	3.786264
43	6	0	-4.186779	3.953113	2.617392
44	6	0	-3.849196	3.274744	1.450905
45	6	0	-2.731233	2.425983	1.404935

46	1	0	-1.109084	1.625462	2.579380
47	1	0	-1.705668	2.831803	4.628185
48	1	0	-5.060457	4.600106	2.620851
49	1	0	-4.459158	3.411429	0.563229
50	6	0	-3.780268	4.576212	5.040679
51	1	0	-3.464163	5.624479	4.972662
52	1	0	-4.861125	4.576977	5.214056
53	1	0	-3.296676	4.144617	5.921332
54	6	0	-2.423894	4.965616	-4.741564
55	1	0	-2.308047	4.360642	-5.645662
56	1	0	-3.364034	5.522237	-4.841634
57	1	0	-1.613220	5.699830	-4.718124
58	1	0	-3.337262	0.999595	-2.434959
59	6	0	2.442906	-1.627298	0.111788
60	6	0	3.401320	-0.434901	0.066477
61	6	0	2.694717	0.763203	0.100230
62	6	0	5.137815	1.098910	0.050292
63	6	0	4.787989	-0.256680	0.040420
64	16	0	3.718933	2.155957	0.100779
65	1	0	5.542843	-1.034227	0.015448
66	6	0	9.927044	0.727129	-0.093222
67	6	0	11.614554	-2.590823	-0.266002
68	6	0	10.266858	-2.986082	-0.251156

69	6	0	9.876278	-4.316544	-0.307242
70	6	0	10.872053	-5.291946	-0.381428
71	6	0	12.220180	-4.915789	-0.397568
72	6	0	12.608975	-3.573549	-0.340599
73	6	0	11.675901	-1.105295	-0.192106
74	6	0	10.299405	-0.608926	-0.142485
75	6	0	9.390030	-1.792490	-0.170651
76	1	0	8.820617	-4.568380	-0.293502
77	1	0	10.605151	-6.343449	-0.427314
78	1	0	12.988132	-5.681135	-0.455883
79	1	0	13.661249	-3.327056	-0.355979
80	1	0	10.719768	1.468530	-0.093584
81	8	0	8.166799	-1.827948	-0.138776
82	6	0	12.855446	-0.376826	-0.170789
83	6	0	12.933015	1.047232	-0.086512
84	7	0	13.055308	2.204500	-0.017787
85	6	0	14.150541	-0.978207	-0.227287
86	7	0	15.227541	-1.421334	-0.271536
87	6	0	2.918503	-2.791377	-3.529687
88	6	0	2.426890	-4.101608	-3.506346
89	6	0	1.965036	-4.598567	-2.281415
90	6	0	2.000823	-3.821829	-1.124772
91	6	0	2.498443	-2.511542	-1.151535

92	6	0	2.952750	-2.008671	-2.376428
93	1	0	3.282045	-2.372924	-4.464903
94	1	0	1.574198	-5.611759	-2.228167
95	1	0	1.649655	-4.246459	-0.189676
96	6	0	1.974355	-2.283617	2.566580
97	6	0	2.316770	-2.971162	3.733457
98	6	0	3.425327	-3.820508	3.779924
99	6	0	4.188094	-3.956114	2.610838
100	6	0	3.850164	-3.276131	1.445391
101	6	0	2.731765	-2.427871	1.400715
102	1	0	1.109218	-1.629988	2.576406
103	1	0	1.706414	-2.839143	4.623339
104	1	0	5.062112	-4.602653	2.613299
105	1	0	4.460215	-3.411152	0.557520
106	6	0	3.781899	-4.583133	5.033178
107	1	0	3.465628	-5.631268	4.963878
108	1	0	4.862819	-4.584266	5.206150
109	1	0	3.298684	-4.152668	5.914592
110	6	0	2.422563	-4.957998	-4.749764
111	1	0	2.306050	-4.351628	-5.652843
112	1	0	3.362834	-5.514149	-4.851214
113	1	0	1.612136	-5.692505	-4.727063
114	1	0	3.336726	-0.995679	-2.437116

115	6	0	-0.186262	-1.418265	0.124217
116	6	0	1.089377	-0.881233	0.135962
117	6	0	1.274625	0.530187	0.128788
118	6	0	0.186454	1.418235	0.126199
119	1	0	-0.342086	-2.492136	0.100750
120	1	0	0.342283	2.492135	0.104229
121	6	0	8.691652	1.372562	-0.044023
122	6	0	8.423959	2.767678	-0.008004
123	6	0	6.993068	2.927822	0.035270
124	6	0	6.450177	1.613459	0.023830
125	6	0	8.651049	5.000124	0.030618
126	6	0	7.209525	5.160494	0.075292
127	7	0	6.371913	4.103945	0.076642
128	7	0	9.262287	3.806100	-0.011528
129	7	0	8.952885	7.402712	0.072450
130	6	0	7.585274	7.538040	0.115075
131	6	0	6.703715	6.490806	0.118221
132	1	0	5.630384	6.642677	0.152636
133	6	0	9.450332	6.194359	0.032481
134	1	0	7.225655	8.562747	0.147462
135	1	0	10.532045	6.074921	-0.000937
136	6	0	-8.691528	-1.372282	-0.043318
137	6	0	-8.423889	-2.767421	-0.007707

138	6	0	-6.992987	-2.927659	0.034895
139	6	0	-6.450032	-1.613327	0.023509
140	6	0	-8.651090	-4.999865	0.030563
141	6	0	-7.209555	-5.160327	0.074559
142	7	0	-6.371882	-4.103828	0.075748
143	7	0	-9.262278	-3.805795	-0.011041
144	7	0	-8.953046	-7.402444	0.072008
145	6	0	-7.585424	-7.537860	0.114000
146	6	0	-6.703803	-6.490678	0.116978
147	1	0	-5.630466	-6.642619	0.150881
148	6	0	-9.450440	-6.194054	0.032518
149	1	0	-7.225849	-8.562595	0.146011
150	1	0	-10.532160	-6.074548	-0.000409
151	8	0	7.470328	0.737332	-0.022120
152	8	0	-7.470152	-0.737140	-0.021965

Cartesian coordinates of Designed Molecule DL4

Center Number	Atomic Number	Atomic Type	Atomic Coordinates (Angstroms) X	Y	Z
1	6	0	-1.031723	1.020318	0.103613
2	6	0	-1.327945	-0.369842	0.080865

3	6	0	-2.322438	1.871968	0.092930
4	6	0	-3.373951	0.760092	0.050354
5	6	0	-2.765662	-0.488480	0.061278
6	6	0	-5.251242	-0.616906	0.040458
7	6	0	-4.773835	0.695338	0.042913
8	16	0	-3.910038	-1.776833	0.057376
9	1	0	-5.433547	1.554412	0.042942
10	6	0	-10.710722	-1.050889	-0.059648
11	6	0	-12.754826	2.064220	-0.127868
12	6	0	-11.449732	2.584580	-0.053092
13	6	0	-11.189715	3.947792	-0.020907
14	6	0	-12.274435	4.824998	-0.064904
15	6	0	-13.579763	4.323677	-0.139355
16	6	0	-13.838114	2.949969	-0.171800
17	6	0	-12.680676	0.578939	-0.144779
18	6	0	-11.265084	0.211307	-0.074869
19	6	0	-10.469752	1.473586	-0.017491
20	1	0	-10.164611	4.299542	0.036859
21	1	0	-12.110237	5.897980	-0.041630
22	1	0	-14.416230	5.015062	-0.173030
23	1	0	-14.860694	2.603552	-0.229535
24	1	0	-11.374010	-1.908596	-0.103533
25	8	0	-9.252604	1.599060	0.046671

26	6	0	-13.774744	-0.265641	-0.215607
27	6	0	-13.680509	-1.691321	-0.232894
28	7	0	-13.639685	-2.855907	-0.249417
29	6	0	-15.125078	0.197411	-0.280337
30	7	0	-16.239829	0.532184	-0.334432
31	6	0	-2.731798	3.076210	-3.544025
32	6	0	-2.131884	4.340598	-3.525029
33	6	0	-1.618585	4.795659	-2.304325
34	6	0	-1.708397	4.023190	-1.147798
35	6	0	-2.315248	2.759490	-1.169436
36	6	0	-2.821705	2.298222	-2.390400
37	1	0	-3.136834	2.690066	-4.476147
38	1	0	-1.143047	5.772140	-2.254479
39	1	0	-1.312930	4.415713	-0.216440
40	6	0	-1.817326	2.439070	2.559452
41	6	0	-2.096003	3.141065	3.734109
42	6	0	-3.100595	4.111583	3.782245
43	6	0	-3.825477	4.353393	2.606583
44	6	0	-3.550383	3.657971	1.433142
45	6	0	-2.536152	2.688067	1.386312
46	1	0	-1.032211	1.691155	2.566767
47	1	0	-1.517711	2.925447	4.629071
48	1	0	-4.618068	5.097635	2.609443

49	1	0	-4.124543	3.879577	0.538664
50	6	0	-3.383897	4.890234	5.044333
51	1	0	-2.932980	5.889485	5.004187
52	1	0	-4.459176	5.028385	5.195811
53	1	0	-2.980213	4.384112	5.925625
54	6	0	-2.067124	5.195052	-4.768119
55	1	0	-2.005321	4.582199	-5.672254
56	1	0	-2.960415	5.824942	-4.863193
57	1	0	-1.200336	5.862260	-4.750411
58	1	0	-3.288896	1.320629	-2.447829
59	6	0	2.291485	-1.756513	0.039002
60	6	0	3.342839	-0.643881	0.017450
61	6	0	2.734682	0.604056	0.060646
62	6	0	5.220141	0.733073	0.030785
63	6	0	4.742675	-0.578893	0.004732
64	16	0	3.879103	1.892207	0.081459
65	1	0	5.402327	-1.437694	-0.018623
66	6	0	10.682758	0.921386	-0.044737
67	6	0	12.618270	-2.263006	-0.063532
68	6	0	11.294249	-2.737196	-0.105317
69	6	0	10.986034	-4.090289	-0.139016
70	6	0	12.040276	-5.004918	-0.130493
71	6	0	13.363855	-4.549761	-0.089007

72	6	0	13.670788	-3.186117	-0.055339
73	6	0	12.596505	-0.776197	-0.035758
74	6	0	11.193136	-0.359218	-0.060702
75	6	0	10.353020	-1.592633	-0.106372
76	1	0	9.948087	-4.405810	-0.170874
77	1	0	11.838157	-6.071355	-0.156007
78	1	0	14.176289	-5.269995	-0.082686
79	1	0	14.706036	-2.875831	-0.023818
80	1	0	11.376418	1.755123	-0.009279
81	8	0	9.130961	-1.675292	-0.138730
82	6	0	13.721041	0.029458	0.004944
83	6	0	13.677249	1.457484	0.028794
84	7	0	13.677689	2.622733	0.048614
85	6	0	15.055720	-0.480597	0.026884
86	7	0	16.159225	-0.854207	0.045946
87	6	0	2.682964	-2.874770	-3.627265
88	6	0	2.083024	-4.139273	-3.635118
89	6	0	1.575664	-4.622963	-2.422978
90	6	0	1.671214	-3.877941	-1.249026
91	6	0	2.278065	-2.614075	-1.243864
92	6	0	2.778584	-2.124169	-2.456098
93	1	0	3.083470	-2.466770	-4.552005
94	1	0	1.100289	-5.600358	-2.393815

95	1	0	1.280276	-4.292307	-0.325248
96	6	0	1.798430	-2.381483	2.493945
97	6	0	2.082796	-3.110900	3.650382
98	6	0	3.087512	-4.082278	3.670748
99	6	0	3.806600	-4.296348	2.486190
100	6	0	3.525818	-3.573528	1.330786
101	6	0	2.511464	-2.602815	1.311750
102	1	0	1.013451	-1.633942	2.522700
103	1	0	1.508932	-2.916389	4.553000
104	1	0	4.599129	-5.040429	2.467660
105	1	0	4.095569	-3.774026	0.428543
106	6	0	3.376880	-4.890407	4.912769
107	1	0	2.924803	-5.888077	4.851751
108	1	0	4.452825	-5.032931	5.055170
109	1	0	2.978410	-4.404675	5.807804
110	6	0	2.012101	-4.964170	-4.897684
111	1	0	1.944310	-4.330179	-5.786694
112	1	0	2.905608	-5.590397	-5.012805
113	1	0	1.146249	-5.632782	-4.890774
114	1	0	3.245566	-1.145478	-2.492776
115	6	0	-0.314445	-1.340081	0.063153
116	6	0	1.000884	-0.905422	0.076002
117	6	0	1.297072	0.484906	0.084445

118	6	0	0.283556	1.455234	0.094501
119	1	0	-0.555223	-2.397940	0.030634
120	1	0	0.524231	2.513579	0.085642
121	6	0	9.147994	0.905379	-0.170607
122	6	0	8.781240	2.193797	-0.137887
123	6	0	7.206636	2.127529	-0.108536
124	6	0	6.744832	0.869943	-0.137090
125	16	0	7.945002	-0.317393	-0.184379
126	6	0	8.780773	4.769621	-0.049896
127	6	0	7.208093	4.701223	0.042985
128	7	0	6.688710	3.534466	-0.003200
129	7	0	9.355847	3.626992	-0.151778
130	6	0	7.255990	7.277836	-0.047045
131	6	0	6.593382	6.110334	-0.036867
132	1	0	5.496078	6.110274	-0.040593
133	6	0	9.366875	6.231330	-0.027410
134	1	0	6.702107	8.193248	-0.058632
135	1	0	10.433459	6.310571	0.004517
136	6	0	-9.176848	-0.990796	0.063713
137	6	0	-8.708154	-2.246139	0.057225
138	6	0	-7.143585	-2.054836	0.069715
139	6	0	-6.783921	-0.764006	0.069724
140	16	0	-8.075445	0.324285	0.068782

141	6	0	-8.501172	-4.815075	0.075496
142	6	0	-6.937803	-4.623457	0.151569
143	7	0	-6.513756	-3.418066	0.130816
144	7	0	-9.166848	-3.719879	0.011375
145	6	0	-6.781447	-7.192419	-0.007552
146	6	0	-6.213918	-5.976289	0.026358
147	1	0	-5.120268	-5.888302	0.009645
148	6	0	-8.968542	-6.319095	0.065371
149	1	0	-6.156586	-8.059948	-0.050453
150	1	0	-10.024868	-6.484256	0.107767
151	6	0	8.725151	7.327280	-0.042635
152	6	0	-8.241790	-7.359396	0.012911
153	1	0	9.241657	8.264315	-0.052028
154	1	0	-8.682053	-8.334204	-0.015711

Cartesian coordinates of Designed Molecule DL5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.985329	1.094957	0.148227
2	6	0	-1.299041	-0.291524	0.156284
3	6	0	-2.264960	1.962221	0.106194

4	6	0	-3.330169	0.862915	0.081356
5	6	0	-2.737944	-0.392562	0.127353
6	6	0	-5.224705	-0.490275	0.088537
7	6	0	-4.730656	0.815559	0.063596
8	16	0	-3.898570	-1.666185	0.144618
9	1	0	-5.379349	1.682589	0.037445
10	6	0	-9.818485	-0.614636	-0.068786
11	6	0	-11.536999	2.691593	-0.118540
12	6	0	-10.187230	3.076504	-0.020564
13	6	0	-9.791562	4.405972	0.033807
14	6	0	-10.781619	5.388724	-0.011210
15	6	0	-12.129707	5.022772	-0.108599
16	6	0	-12.524773	3.682699	-0.163355
17	6	0	-11.612748	1.206750	-0.155257
18	6	0	-10.242512	0.697183	-0.073179
19	6	0	-9.324825	1.871861	0.011518
20	1	0	-8.737097	4.651639	0.109002
21	1	0	-10.510413	6.439258	0.029033
22	1	0	-12.891675	5.795467	-0.142852
23	1	0	-13.576189	3.442081	-0.238413
24	1	0	-10.564209	-1.400349	-0.132735
25	8	0	-8.102211	1.872953	0.092299
26	6	0	-12.785328	0.477941	-0.251227

27	6	0	-12.835081	-0.949634	-0.287242
28	7	0	-12.911656	-2.112086	-0.319506
29	6	0	-14.081094	1.075777	-0.325997
30	7	0	-15.155578	1.522074	-0.389042
31	6	0	-2.629190	3.083622	-3.561913
32	6	0	-2.013394	4.340480	-3.568132
33	6	0	-1.504339	4.818315	-2.354373
34	6	0	-1.613439	4.075091	-1.180472
35	6	0	-2.236142	2.818944	-1.176970
36	6	0	-2.738432	2.334812	-2.390782
37	1	0	-3.031477	2.680266	-4.487916
38	1	0	-1.016824	5.789673	-2.323908
39	1	0	-1.220633	4.484925	-0.255466
40	6	0	-1.772851	2.582142	2.562615
41	6	0	-2.052160	3.315643	3.717708
42	6	0	-3.044666	4.299559	3.734053
43	6	0	-3.756772	4.522074	2.546829
44	6	0	-3.480971	3.795218	1.392763
45	6	0	-2.478830	2.811827	1.377791
46	1	0	-0.997414	1.824834	2.594507
47	1	0	-1.483999	3.114391	4.622451
48	1	0	-4.539814	5.276049	2.525132
49	1	0	-4.044928	4.002414	0.488395

50	6	0	-3.328338	5.111849	4.974673
51	1	0	-2.864414	6.104112	4.914421
52	1	0	-4.402973	5.267079	5.113671
53	1	0	-2.938355	4.622062	5.871231
54	6	0	-1.927591	5.163890	-4.830745
55	1	0	-1.866209	4.528727	-5.719379
56	1	0	-2.811977	5.802460	-4.948458
57	1	0	-1.052547	5.820409	-4.821679
58	1	0	-3.217554	1.362055	-2.428730
59	6	0	2.302652	-1.724075	0.178359
60	6	0	3.368236	-0.625555	0.139070
61	6	0	2.775693	0.630588	0.147192
62	6	0	5.262754	0.727674	0.135328
63	6	0	4.768843	-0.578449	0.136671
64	16	0	3.936222	1.904415	0.146838
65	1	0	5.417671	-1.445768	0.139496
66	6	0	9.903911	0.404316	-0.039517
67	6	0	10.938723	-3.174419	-0.132920
68	6	0	9.538483	-3.287439	-0.054246
69	6	0	8.888296	-4.513623	-0.027385
70	6	0	9.666098	-5.671291	-0.080964
71	6	0	11.060953	-5.576534	-0.159404
72	6	0	11.712640	-4.339830	-0.186466

73	6	0	11.305625	-1.733191	-0.142274
74	6	0	10.061532	-0.965085	-0.063609
75	6	0	8.929651	-1.937194	-0.008440
76	1	0	7.805248	-4.547948	0.033719
77	1	0	9.192994	-6.648331	-0.062078
78	1	0	11.656342	-6.483531	-0.200539
79	1	0	12.791704	-4.309857	-0.247549
80	1	0	10.790408	1.028670	-0.082492
81	8	0	7.729814	-1.698735	0.061099
82	6	0	12.599798	-1.248187	-0.214417
83	6	0	12.929935	0.142013	-0.224351
84	7	0	13.234152	1.266973	-0.235048
85	6	0	13.753422	-2.088269	-0.288047
86	7	0	14.719781	-2.736400	-0.349260
87	6	0	2.709822	-2.935065	-3.456608
88	6	0	2.093906	-4.191769	-3.439247
89	6	0	1.570530	-4.639747	-2.220212
90	6	0	1.665960	-3.867944	-1.063681
91	6	0	2.288800	-2.612028	-1.083658
92	6	0	2.805415	-2.157753	-2.302994
93	1	0	3.123042	-2.554493	-4.387430
94	1	0	1.082520	-5.610119	-2.171671
95	1	0	1.262234	-4.255023	-0.133588

96	6	0	1.781616	-2.283550	2.643302
97	6	0	2.047201	-2.988433	3.819256
98	6	0	3.039261	-3.971560	3.871412
99	6	0	3.765226	-4.223077	2.698465
100	6	0	3.503133	-3.524810	1.523733
101	6	0	2.501416	-2.542193	1.472840
102	1	0	1.006016	-1.525750	2.647479
103	1	0	1.468499	-2.765074	4.712053
104	1	0	4.548337	-4.977268	2.704492
105	1	0	4.077643	-3.754092	0.631417
106	6	0	3.308144	-4.753129	5.134850
107	1	0	2.843909	-5.746232	5.093923
108	1	0	4.380986	-4.905664	5.289745
109	1	0	2.908589	-4.241039	6.014577
110	6	0	2.022808	-5.045858	-4.682241
111	1	0	1.970371	-4.432647	-5.586731
112	1	0	2.909176	-5.685829	-4.774742
113	1	0	1.148481	-5.703201	-4.666656
114	1	0	3.285112	-1.186161	-2.359151
115	6	0	-0.297872	-1.274540	0.170422
116	6	0	1.022739	-0.856224	0.184008
117	6	0	1.336535	0.530080	0.161645
118	6	0	0.335414	1.513002	0.139852

119	1	0	-0.551832	-2.329773	0.161220
120	1	0	0.589616	2.567726	0.107677
121	6	0	8.910365	1.579693	0.014841
122	6	0	8.458453	2.880339	0.043960
123	6	0	6.994987	3.074613	0.046340
124	6	0	6.470024	1.679916	0.049690
125	16	0	7.643096	0.488743	0.012980
126	6	0	-6.267456	-1.623054	0.055633
127	6	0	-6.743017	-2.917222	0.085627
128	6	0	-8.151455	-2.891563	0.030496
129	6	0	-8.707723	-1.680794	-0.035400
130	16	0	-7.512919	-0.510848	-0.033626
131	6	0	-7.317070	-5.272463	0.016702
132	6	0	-6.284927	-4.381993	0.212908
133	16	0	-8.827759	-4.569227	0.094951
134	1	0	-5.223188	-4.635043	0.209808
135	6	0	-7.163340	-6.782699	-0.242436
136	8	0	-8.020320	-7.645866	-0.427077
137	8	0	-5.863595	-7.172245	-0.260488
138	6	0	-5.762760	-8.577867	-0.503302
139	1	0	-4.862465	-8.952261	-0.062622
140	1	0	-6.605372	-9.075850	-0.070960
141	1	0	-5.744994	-8.757250	-1.558008

142	6	0	6.636729	4.559926	-0.146268
143	6	0	7.738010	5.476307	-0.196263
144	16	0	9.126048	4.543806	-0.207624
145	1	0	5.611784	4.934972	-0.132765
146	6	0	7.768258	7.015827	-0.219997
147	8	0	8.724545	7.788627	-0.263072
148	8	0	6.523757	7.555752	-0.186695
149	6	0	6.593894	8.983840	-0.210096
150	1	0	5.735921	9.391196	0.282694
151	1	0	7.481093	9.305673	0.294088
152	1	0	6.617149	9.323218	-1.224582

Cartesian coordinates of Designed Molecule DL6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.028379	0.946889	0.113072
2	6	0	-1.315201	-0.444690	0.085411
3	6	0	-2.326716	1.787414	0.091061
4	6	0	-3.366408	0.664884	0.037629
5	6	0	-2.753528	-0.575866	0.053779
6	6	0	-5.235643	-0.729010	0.012082

7	6	0	-4.766437	0.585001	0.016535
8	16	0	-3.883872	-1.883025	0.040323
9	1	0	-5.431788	1.440271	0.011799
10	6	0	-10.506995	-1.047757	-0.108095
11	6	0	-13.317931	1.388031	-0.304597
12	6	0	-12.208062	2.248600	-0.384835
13	6	0	-12.335582	3.623107	-0.518810
14	6	0	-13.623215	4.161421	-0.575281
15	6	0	-14.738189	3.320158	-0.495927
16	6	0	-14.604763	1.933923	-0.359775
17	6	0	-12.825741	-0.012037	-0.166447
18	6	0	-11.367133	0.037880	-0.181314
19	6	0	-10.961818	1.450524	-0.305320
20	1	0	-11.447582	4.244393	-0.576967
21	1	0	-13.762697	5.233016	-0.680517
22	1	0	-15.735050	3.748146	-0.540505
23	1	0	-15.492416	1.319539	-0.301927
24	1	0	-10.974596	-2.023052	-0.051830
25	8	0	-9.820435	1.901766	-0.346748
26	6	0	-13.648023	-1.121857	-0.039533
27	6	0	-13.175904	-2.460349	0.122543
28	7	0	-12.843493	-3.569327	0.262259
29	6	0	-15.074566	-1.049563	-0.040762

30	7	0	-16.240112	-1.036026	-0.037443
31	6	0	-2.721856	2.990265	-3.547593
32	6	0	-2.139115	4.262517	-3.523304
33	6	0	-1.640036	4.722847	-2.298817
34	6	0	-1.727260	3.947703	-1.143774
35	6	0	-2.317331	2.676147	-1.170185
36	6	0	-2.809750	2.210268	-2.395237
37	1	0	-3.115913	2.599947	-4.482768
38	1	0	-1.178295	5.705904	-2.244922
39	1	0	-1.343071	4.343716	-0.209111
40	6	0	-1.843914	2.367794	2.559207
41	6	0	-2.140687	3.067233	3.731063
42	6	0	-3.160853	4.021644	3.771821
43	6	0	-3.882245	4.250179	2.591450
44	6	0	-3.589038	3.556993	1.421052
45	6	0	-2.559963	2.602440	1.381308
46	1	0	-1.047149	1.632477	2.571150
47	1	0	-1.564636	2.861894	4.630063
48	1	0	-4.687062	4.981325	2.588435
49	1	0	-4.161917	3.766884	0.522914
50	6	0	-3.464728	4.797034	5.031354
51	1	0	-3.030884	5.804043	4.993651
52	1	0	-4.543111	4.917004	5.176581

53	1	0	-3.057984	4.298491	5.915694
54	6	0	-2.078919	5.119505	-4.765060
55	1	0	-2.001494	4.508747	-5.669499
56	1	0	-2.980855	5.736095	-4.866240
57	1	0	-1.222339	5.799826	-4.741034
58	1	0	-3.264931	1.227283	-2.454877
59	6	0	2.319302	-1.797604	0.064230
60	6	0	3.359497	-0.674313	0.056682
61	6	0	2.746101	0.565226	0.102094
62	6	0	5.231058	0.718265	0.096327
63	6	0	4.760179	-0.594719	0.056224
64	16	0	3.877716	1.870601	0.147116
65	1	0	5.424965	-1.449985	0.033682
66	6	0	10.502862	1.033250	-0.018885
67	6	0	13.340601	-1.364394	-0.299203
68	6	0	12.244227	-2.244916	-0.318324
69	6	0	12.392382	-3.620037	-0.419658
70	6	0	13.687197	-4.137142	-0.504857
71	6	0	14.788959	-3.275074	-0.486004
72	6	0	14.634754	-1.888257	-0.383753
73	6	0	12.829607	0.030081	-0.186481
74	6	0	11.372236	-0.043015	-0.133425
75	6	0	10.987638	-1.465576	-0.216967

76	1	0	11.514455	-4.257960	-0.431078
77	1	0	13.842726	-5.208610	-0.585596
78	1	0	15.791383	-3.686940	-0.552064
79	1	0	15.512110	-1.256255	-0.372162
80	1	0	10.966456	2.009629	0.043723
81	8	0	9.855107	-1.940666	-0.204802
82	6	0	13.641246	1.154136	-0.150621
83	6	0	13.160253	2.495403	-0.051876
84	7	0	12.821472	3.608428	0.026746
85	6	0	15.066882	1.093635	-0.212721
86	7	0	16.231478	1.082545	-0.260868
87	6	0	2.756322	-2.891919	-3.603745
88	6	0	2.170415	-4.162782	-3.624686
89	6	0	1.655910	-4.658471	-2.420570
90	6	0	1.731202	-3.918627	-1.241797
91	6	0	2.324219	-2.648314	-1.222922
92	6	0	2.832306	-2.147118	-2.427482
93	1	0	3.162232	-2.474701	-4.522090
94	1	0	1.191165	-5.641391	-2.401776
95	1	0	1.334900	-4.341523	-0.324126
96	6	0	1.811242	-2.447524	2.509686
97	6	0	2.095253	-3.180743	3.663898
98	6	0	3.112612	-4.138756	3.687061

99	6	0	3.844395	-4.335816	2.507441
100	6	0	3.563946	-3.608830	1.354528
101	6	0	2.537782	-2.650593	1.332362
102	1	0	1.016456	-1.710397	2.535091
103	1	0	1.511397	-2.999322	4.563007
104	1	0	4.647324	-5.068863	2.491168
105	1	0	4.144570	-3.794745	0.456099
106	6	0	3.402810	-4.950247	4.926928
107	1	0	2.965850	-5.954212	4.857328
108	1	0	4.479466	-5.078172	5.078011
109	1	0	2.990100	-4.475151	5.821356
110	6	0	2.122474	-4.981780	-4.892353
111	1	0	2.055239	-4.343917	-5.778719
112	1	0	3.024741	-5.596328	-5.002606
113	1	0	1.264904	-5.661228	-4.897839
114	1	0	3.290340	-1.163949	-2.452082
115	6	0	-0.291274	-1.404074	0.072125
116	6	0	1.020533	-0.958048	0.096474
117	6	0	1.307464	0.433654	0.113106
118	6	0	0.283601	1.393167	0.116831
119	1	0	-0.522082	-2.464047	0.033184
120	1	0	0.514636	2.453798	0.112359
121	6	0	9.105802	1.163864	0.033706

122	6	0	8.516094	2.458786	0.152244
123	6	0	7.109081	2.430735	0.177037
124	6	0	6.604639	1.125360	0.087124
125	16	0	7.863480	-0.079305	-0.044372
126	6	0	-6.608396	-1.136507	-0.014621
127	6	0	-7.112438	-2.445108	0.023215
128	6	0	-8.517476	-2.474994	-0.026913
129	6	0	-9.109153	-1.180238	-0.090214
130	16	0	-7.869255	0.069053	-0.120927
131	6	0	-9.156494	-4.891588	0.265048
132	6	0	-7.768055	-5.508579	0.586189
133	6	0	-6.384278	-4.817934	0.437625
134	1	0	-9.809919	-5.045021	1.127913
135	1	0	-7.820852	-5.856853	1.620717
136	1	0	-5.798938	-5.377798	-0.295324
137	8	0	-6.215812	-3.458900	0.030606
138	8	0	-9.347891	-3.520454	-0.090114
139	6	0	6.367746	4.840422	0.401738
140	6	0	7.745693	5.559546	0.414559
141	6	0	9.147967	4.900328	0.337632
142	1	0	5.778646	5.254777	-0.421076
143	1	0	7.712926	6.279254	-0.407368
144	1	0	9.714721	5.183131	1.227753

145	8	0	9.361039	3.492023	0.225841
146	8	0	6.200018	3.428213	0.274074
147	1	0	9.682610	5.317044	-0.518986
148	1	0	7.754127	6.161083	1.327129
149	1	0	5.842858	5.094018	1.327206
150	1	0	-5.860788	-4.901811	1.395561
151	1	0	-7.707006	-6.414649	-0.022571
152	1	0	-9.604632	-5.436188	-0.568270

Cartesian coordinates of Designed Molecule DL7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.021705	0.949290	0.089792
2	6	0	-1.311281	-0.441507	0.064626
3	6	0	-2.316069	1.793175	0.077890
4	6	0	-3.358686	0.671667	0.035618
5	6	0	-2.751242	-0.571081	0.046404
6	6	0	-5.228686	-0.703094	0.016271
7	6	0	-4.759587	0.602991	0.025871
8	16	0	-3.889478	-1.871181	0.041487
9	1	0	-5.423416	1.460109	0.019906

10	6	0	-10.511901	-1.159781	0.014176
11	6	0	-13.493489	1.048293	-0.230315
12	6	0	-12.457784	1.993169	-0.356741
13	6	0	-12.708745	3.345770	-0.535143
14	6	0	-14.039835	3.767393	-0.590874
15	6	0	-15.078779	2.838707	-0.466421
16	6	0	-14.824452	1.474490	-0.284135
17	6	0	-12.890873	-0.297553	-0.049209
18	6	0	-11.442630	-0.144706	-0.081832
19	6	0	-11.152984	1.294417	-0.268509
20	1	0	-11.883311	4.044333	-0.629264
21	1	0	-14.271402	4.818986	-0.730606
22	1	0	-16.108437	3.180229	-0.510637
23	1	0	-15.650257	0.782332	-0.189957
24	1	0	-10.904264	-2.169684	0.122441
25	8	0	-10.052984	1.834210	-0.324623
26	6	0	-13.606282	-1.467409	0.124743
27	6	0	-12.966825	-2.728906	0.318593
28	7	0	-12.476863	-3.773245	0.484913
29	6	0	-15.031829	-1.507342	0.136417
30	7	0	-16.194768	-1.579000	0.150555
31	6	0	-2.737830	2.990626	-3.559729
32	6	0	-2.152636	4.261770	-3.542416

33	6	0	-1.644096	4.723898	-2.322465
34	6	0	-1.724046	3.950938	-1.165444
35	6	0	-2.315193	2.679681	-1.185158
36	6	0	-2.818283	2.212677	-2.405315
37	1	0	-3.139454	2.599184	-4.491293
38	1	0	-1.180738	5.706472	-2.273583
39	1	0	-1.333293	4.348672	-0.234250
40	6	0	-1.808915	2.381372	2.539924
41	6	0	-2.093063	3.085921	3.711919
42	6	0	-3.110283	4.043062	3.758512
43	6	0	-3.842240	4.268704	2.584152
44	6	0	-3.562200	3.569936	1.413911
45	6	0	-2.535551	2.612941	1.367886
46	1	0	-1.013327	1.644795	2.547163
47	1	0	-1.508957	2.882669	4.606202
48	1	0	-4.645403	5.001758	2.586047
49	1	0	-4.143815	3.776999	0.520746
50	6	0	-3.400292	4.824064	5.017935
51	1	0	-2.964710	5.830037	4.972313
52	1	0	-4.477024	4.946899	5.173169
53	1	0	-2.986040	4.327977	5.900178
54	6	0	-2.099870	5.116218	-4.786381
55	1	0	-2.027741	4.503556	-5.690021

56	1	0	-3.002310	5.732795	-4.883763
57	1	0	-1.243033	5.796399	-4.768625
58	1	0	-3.275389	1.230256	-2.459616
59	6	0	2.320614	-1.796430	0.028500
60	6	0	3.362546	-0.673759	0.010409
61	6	0	2.752974	0.566655	0.059158
62	6	0	5.231983	0.707342	0.026887
63	6	0	4.765501	-0.600492	-0.001178
64	16	0	3.888939	1.869039	0.092401
65	1	0	5.432792	-1.454261	-0.034789
66	6	0	10.516364	1.241160	-0.013617
67	6	0	13.420313	-1.087225	-0.178936
68	6	0	12.329438	-1.975869	-0.271454
69	6	0	12.504227	-3.345265	-0.389949
70	6	0	13.809636	-3.845500	-0.415778
71	6	0	14.899978	-2.975291	-0.322566
72	6	0	14.723047	-1.591662	-0.202978
73	6	0	12.905894	0.306102	-0.068628
74	6	0	11.450441	0.225592	-0.089683
75	6	0	11.077967	-1.188976	-0.222086
76	1	0	11.642024	-4.000962	-0.461004
77	1	0	13.979230	-4.913834	-0.507892
78	1	0	15.908556	-3.376757	-0.342644

79	1	0	15.587333	-0.945019	-0.132518
80	1	0	10.884489	2.255417	0.060715
81	8	0	9.936955	-1.645242	-0.279695
82	6	0	13.719425	1.427343	0.026525
83	6	0	13.206977	2.755090	0.126551
84	7	0	12.863209	3.865745	0.208355
85	6	0	15.141894	1.344053	0.029070
86	7	0	16.305955	1.287602	0.031959
87	6	0	2.726878	-2.915500	-3.635888
88	6	0	2.154220	-4.192430	-3.639647
89	6	0	1.659669	-4.683973	-2.425413
90	6	0	1.740715	-3.933480	-1.253838
91	6	0	2.318540	-2.656013	-1.252664
92	6	0	2.808469	-2.159956	-2.466746
93	1	0	3.117877	-2.501760	-4.562324
94	1	0	1.206787	-5.672080	-2.392693
95	1	0	1.361790	-4.353853	-0.327633
96	6	0	1.830517	-2.431271	2.482855
97	6	0	2.119085	-3.162971	3.636976
98	6	0	3.127609	-4.130277	3.653577
99	6	0	3.845798	-4.338339	2.467564
100	6	0	3.561441	-3.612385	1.315024
101	6	0	2.544198	-2.644506	1.299402

102	1	0	1.042222	-1.687535	2.513331
103	1	0	1.545625	-2.973066	4.541022
104	1	0	4.641794	-5.078877	2.446183
105	1	0	4.132268	-3.806306	0.411976
106	6	0	3.422599	-4.939855	4.893656
107	1	0	2.976013	-5.940149	4.832308
108	1	0	4.499563	-5.076855	5.034833
109	1	0	3.022935	-4.457654	5.790217
110	6	0	2.100415	-5.022440	-4.899992
111	1	0	2.014016	-4.392728	-5.790569
112	1	0	3.008697	-5.626904	-5.017071
113	1	0	1.251251	-5.712316	-4.888894
114	1	0	3.256049	-1.172426	-2.504534
115	6	0	-0.288296	-1.400832	0.046616
116	6	0	1.024203	-0.954808	0.062953
117	6	0	1.313372	0.435955	0.075828
118	6	0	0.290710	1.395529	0.085071
119	1	0	-0.518164	-2.460963	0.011282
120	1	0	0.520944	2.456173	0.078849
121	6	0	9.137937	1.235584	-0.020881
122	6	0	8.474284	2.470560	0.077128
123	6	0	7.089466	2.403049	0.119337
124	6	0	6.591820	1.098833	0.059439

125	16	0	7.897646	-0.080900	-0.062278
126	6	0	-6.582517	-1.082711	0.038696
127	6	0	-7.083786	-2.378731	0.022411
128	6	0	-8.473740	-2.436024	0.014948
129	6	0	-9.123090	-1.185238	0.011056
130	16	0	-7.886967	0.107558	-0.030197
131	8	0	-6.290006	-3.482395	-0.026087
132	8	0	-9.152039	-3.598937	0.081646
133	8	0	9.159087	3.630168	0.157628
134	8	0	6.287442	3.497516	0.167308
135	6	0	-6.964896	-4.742669	-0.149594
136	6	0	-8.366094	-4.726108	0.489380
137	1	0	-6.344507	-5.488509	0.349517
138	1	0	-7.014247	-4.998345	-1.211475
139	1	0	-8.306438	-4.715642	1.580733
140	1	0	-8.915181	-5.615272	0.177370
141	6	0	6.920691	4.768564	-0.020727
142	6	0	8.397333	4.818036	0.419170
143	1	0	6.824859	5.044635	-1.075795
144	1	0	6.343750	5.482490	0.566958
145	1	0	8.890821	5.625104	-0.126096
146	1	0	8.484913	5.021449	1.488583
