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Supporting information for:

Effect of exchange–correlation functionals on ground state geometries, optoelectronic and charge transfer of Triphenylamine-based dyes

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Computational details

All calculations were study by using the Gaussian 09 (Revision A.02) program package. The geometric and electronic properties of all systems (neutral and doped) were studied by Density Functional Theory method using the B3LYP correlation exchange functional (Becke's three-parameter hybrid functional, and Lee-Yang- Parr's correlation functional) combined with the 6-31G (d, p) basis set for all atoms, without any geometrical constraints.

The absorption spectra have been performed by using BHandHLYP hybrid functional (Becke-Half-and-Half-LYP) which include 50% fraction of Hartree-Fock (HF) exchange and 50% of Becke 88 exchange.

Molecular orbitals have been visualized with the GaussView 3.0 program. Cartesian coordinates for the neutral, cationic and anionic states optimized structures are presented below.

Optimized Cartesian coordinates for compound D1 in the neutral state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3,647556	-2,030563	1,067419
2	6	4,604478	-3,030734	1,159236
3	6	5,686535	-3,062103	0,266191
4	6	5,789231	-2,078007	-0,723755
5	6	4,811155	-1,086449	-0,821527
6	6	3,733600	-1,046786	0,067589
7	1	2,821809	-2,005911	1,771077
8	1	4,544490	-3,794176	1,927714
9	1	6,612542	-2,076832	-1,427891
10	1	4,890265	-0,329356	-1,594913
11	7	2,755462	-0,008977	-0,022910
12	6	2,750819	2,215379	-1,084469
13	6	3,210612	1,344659	-0,081788
14	6	4,144719	1,819510	0,842704
15	6	4,620762	3,130287	0,776712
16	6	4,145578	3,994500	-0,216508
17	6	3,203284	3,525286	-1,144662
18	1	2,032265	1,857658	-1,814780
19	1	4,509405	1,155398	1,619570
20	1	5,347020	3,464423	1,507839
21	1	2,850994	4,204092	-1,914083
22	6	-1,393948	-0,928892	-0,081296
23	6	-0,429467	-1,848186	-0,542838
24	6	0,923332	-1,552164	-0,528607
25	6	1,387450	-0,310577	-0,043593
26	6	0,428866	0,616187	0,417689
27	6	-0,922105	0,310995	0,394501
28	1	-0,749010	-2,800036	-0,955161
29	1	1,633862	-2,275585	-0,910918
30	1	0,754445	1,572119	0,810570
31	1	-1,625335	1,040190	0,786478
32	16	-4,038614	-0,018893	-0,025868
33	6	-2,811826	-1,262236	-0,099359
34	6	-5,335704	-1,208633	-0,077750
35	6	-4,796088	-2,490291	-0,164890
36	6	-3,394750	-2,522737	-0,176528
37	1	-5,423893	-3,374072	-0,203870
38	1	-2,817083	-3,438229	-0,206774
39	6	-6,729397	-0,937477	-0,039787
40	6	-7,422279	0,241704	0,055264
41	6	-8,903295	0,159789	0,068887
42	8	-9,542224	-0,873601	0,002774
43	8	-9,486961	1,375905	0,164264
44	1	-10,444755	1,214114	0,165100
45	8	4,532738	5,293689	-0,369669
46	8	6,575951	-4,081018	0,447957
47	6	5,474899	5,826238	0,548509
48	6	7,686338	-4,167354	-0,431625
49	1	5,094367	5,804500	1,577648
50	1	6,429895	5,286714	0,507977
51	1	8,324976	-3,277053	-0,367191
52	1	7,368434	-4,305524	-1,472936
53	1	8,256275	-5,040768	-0,112085
54	1	5,635649	6,862288	0,247705
55	1	-7,366405	-1,818463	-0,095915
56	6	-6,795672	1,518027	0,141574
57	7	-6,267820	2,554799	0,211820

Optimized Cartesian coordinates for compound D2 in the neutral state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.445268	-1.955188	1.095353
2	6	4.475260	-2.876574	1.215304
3	6	5.573415	-2.833459	0.342074
4	6	5.615842	-1.854682	-0.658017
5	6	4.564649	-0.944319	-0.784915
6	6	3.471475	-0.978781	0.085069
7	1	2.607420	-1.987202	1.784297
8	1	4.460935	-3.633834	1.992096
9	1	6.449425	-1.795471	-1.347361
10	1	4.598250	-0.191541	-1.565787
11	7	2.417069	-0.021930	-0.032721
12	6	2.259329	2.178140	-1.133620
13	6	2.766037	1.361972	-0.108166
14	6	3.641108	1.923919	0.825146
15	6	4.014577	3.266816	0.745368
16	6	3.493691	4.076011	-0.271510
17	6	2.609054	3.518476	-1.208076
18	1	1.584125	1.753734	-1.869597
19	1	4.040754	1.302803	1.620232
20	1	4.697270	3.667829	1.484620
21	1	2.219003	4.155264	-1.995013
22	6	-1.646119	-1.260676	-0.155828
23	6	-0.607831	-2.107837	-0.587887
24	6	0.718392	-1.708480	-0.554029
25	6	1.076353	-0.430487	-0.075311
26	6	0.041550	0.422480	0.361880
27	6	-1.282666	0.014937	0.319236
28	1	-0.847073	-3.088736	-0.986599
29	1	1.489476	-2.380698	-0.911752
30	1	0.285545	1.403949	0.750978
31	1	-2.038706	0.697473	0.697675
32	6	-3.032045	-1.702152	-0.201920
33	6	-5.289908	-1.529331	-0.152218
34	6	-3.569541	-2.996329	-0.353884
35	1	-2.994213	-3.905649	-0.444081
36	8	3.780698	5.399070	-0.441417
37	8	6.536973	-3.776306	0.555189
38	6	4.661933	6.022250	0.484298
39	6	7.663382	-3.797162	-0.312291
40	1	4.261839	5.989231	1.505818
41	1	5.655667	5.556033	0.470818
42	1	8.236204	-2.862766	-0.251216
43	1	7.365967	-3.970377	-1.354505
44	6	-6.581441	-0.964480	-0.065051
45	6	-6.958664	0.349430	0.124649
46	6	-5.987343	1.380897	0.275862
47	6	-8.366940	0.772697	0.189279
48	7	-5.110743	2.142629	0.388181
49	8	-8.741979	1.916773	0.357335
50	8	-9.240070	-0.262235	0.037805
51	1	-7.393780	-1.677570	-0.162076
52	1	-10.122215	0.138440	0.098692
53	6	-4.958691	-2.887392	-0.323370
54	1	-5.678812	-3.690529	-0.400450
55	7	-4.084343	-0.843885	-0.079989
56	1	-4.011985	0.162555	-0.011867
57	1	8.288112	-4.625267	0.026681
58	1	4.747185	7.062047	0.164252

Optimized Cartesian coordinates for compound D3 in the neutral state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.600693	-2.060562	1.069509
2	6	4.533381	-3.082907	1.164788
3	6	5.615817	-3.141695	0.273022
4	6	5.742634	-2.161847	-0.719173
5	6	4.788565	-1.147849	-0.820188
6	6	3.711355	-1.081262	0.067373
7	1	2.775392	-2.014892	1.772623
8	1	4.454596	-3.843125	1.934725
9	1	6.566989	-2.181283	-1.421883
10	1	4.886612	-0.394369	-1.594982
11	7	2.760855	-0.017730	-0.026671
12	6	2.831816	2.199422	-1.099928
13	6	3.254135	1.323228	-0.085627
14	6	4.188404	1.777513	0.848688
15	6	4.700631	3.074408	0.781464
16	6	4.262312	3.945554	-0.223720
17	6	3.320311	3.496042	-1.162273
18	1	2.114190	1.856245	-1.838130
19	1	4.524771	1.108010	1.633702
20	1	5.426591	3.393013	1.519852
21	1	2.997751	4.179202	-1.940779
22	6	-1.412980	-0.810908	-0.085337
23	6	-0.475971	-1.765238	-0.534316
24	6	0.884769	-1.511294	-0.517519
25	6	1.386296	-0.278825	-0.044538
26	6	0.454810	0.682399	0.403488
27	6	-0.904380	0.418832	0.379077
28	1	-0.822294	-2.711234	-0.938206
29	1	1.573492	-2.260406	-0.889896
30	1	0.808317	1.632783	0.785225
31	1	-1.586346	1.174999	0.757462
32	6	-2.838001	-1.099727	-0.104983
33	6	-5.309669	-1.110766	-0.088760
34	6	-3.470830	-2.336570	-0.204448
35	1	-2.944661	-3.281990	-0.262187
36	8	4.685411	5.229465	-0.380100
37	8	6.478760	-4.177974	0.457610
38	6	5.627782	5.736545	0.559916
39	6	7.587521	-4.281636	-0.430509
40	1	5.227007	5.729358	1.580064
41	1	6.569809	5.176616	0.532910
42	1	8.246218	-3.408189	-0.361011
43	1	7.264128	-4.414050	-1.469408
44	6	-6.724474	-0.903642	-0.053464
45	6	-7.450665	0.249068	0.062053
46	6	-6.851166	1.539484	0.177210
47	6	-8.935057	0.239264	0.077504
48	7	-6.332810	2.578190	0.269364
49	8	-9.625994	1.230985	0.180065
50	8	-9.455784	-1.009038	-0.036982
51	1	-7.283004	-1.830506	-0.134038
52	1	-10.419583	-0.892681	-0.015062
53	16	-4.059642	0.137521	-0.001350
54	7	-4.818089	-2.338051	-0.196404
55	1	5.809305	6.764971	0.249876
56	1	8.127914	-5.169346	-0.103868

Optimized Cartesian coordinates for compound D4 in the neutral state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.288369	-2.083438	-0.982567
2	6	-4.273418	-3.049316	-1.153563
3	6	-5.490414	-2.963108	-0.463454
4	6	-5.693142	-1.883334	0.402306
5	6	-4.695740	-0.918059	0.573097
6	6	-3.480322	-0.996933	-0.112597
7	1	-2.362847	-2.154888	-1.543102
8	1	-4.131741	-3.881083	-1.835946
9	1	-6.617129	-1.793917	0.962551
10	1	-4.857230	-0.100074	1.266083
11	7	-2.463379	-0.006359	0.061139
12	6	-2.171326	2.231120	1.061264
13	6	-2.810745	1.379019	0.145235
14	6	-3.796213	1.930864	-0.677886
15	6	-4.139351	3.284325	-0.598418
16	6	-3.491728	4.125256	0.312268
17	6	-2.503577	3.578377	1.142423
18	1	-1.419241	1.823023	1.727204
19	1	-4.288840	1.297552	-1.406936
20	1	-4.899404	3.676879	-1.264474
21	1	-2.018497	4.234071	1.858132
22	6	1.605987	-1.197343	0.332735
23	6	0.579825	-1.963510	0.928311
24	6	-0.746745	-1.577413	0.835040
25	6	-1.112313	-0.400267	0.147821
26	6	-0.090224	0.369091	-0.444540
27	6	1.235945	-0.024440	-0.353459
28	1	0.829021	-2.851453	1.500596
29	1	-1.514676	-2.167124	1.321665
30	1	-0.351140	1.262919	-0.998471
31	1	2.008140	0.561431	-0.841984
32	6	2.978733	-1.592780	0.420550
33	6	5.248097	-1.480660	0.293318
34	6	3.604601	-2.747833	0.733195
35	1	3.110052	-3.676488	0.989816
36	8	-3.742775	5.452580	0.466539
37	8	-6.389840	-3.955202	-0.700061
38	6	-4.740885	6.029010	-0.363499
39	6	-7.630978	-3.888012	-0.012642
40	1	-4.479338	5.934131	-1.431133
41	1	-5.727593	5.569333	-0.181692
42	1	-8.185641	-2.970860	-0.275216
43	1	-7.487294	-3.933502	1.080379
44	6	6.565050	-0.991231	0.125860
45	6	6.961891	0.263974	-0.248201
46	6	6.029130	1.312430	-0.513422
47	6	8.395604	0.635086	-0.388083
48	7	5.243304	2.148299	-0.712405
49	8	8.791273	1.735158	-0.712345
50	8	9.233672	-0.393559	-0.113122
51	1	7.328477	-1.733477	0.334002
52	1	10.132843	-0.048369	-0.234537
53	7	4.959361	-2.678896	0.653855
54	7	4.020782	-0.675854	0.047031
55	1	4.119020	0.129436	0.681534
56	1	-4.760315	7.085130	-0.075903
57	1	-8.181981	-4.770059	-0.354549

Optimized Cartesian coordinates for compound D1 in the cationic state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.405326	-2.202885	-1.009290
2	6	-4.219963	-3.317313	-1.066711
3	6	-5.318800	-3.438333	-0.193525
4	6	-5.590170	-2.421292	0.737427
5	6	-4.770843	-1.300175	0.788196
6	6	-3.672037	-1.181593	-0.075111
7	1	-2.568928	-2.106346	-1.694024
8	1	-4.038025	-4.106339	-1.787868
9	1	-6.423611	-2.495219	1.424075
10	1	-4.975648	-0.517334	1.511234
11	7	-2.852704	-0.020483	-0.022256
12	6	-3.063317	2.208888	0.990322
13	6	-3.494422	1.246522	0.054837
14	6	-4.579409	1.532679	-0.786395
15	6	-5.223548	2.761935	-0.713022
16	6	-4.787595	3.719623	0.218564
17	6	-3.703204	3.430524	1.070012
18	1	-2.237741	1.984127	1.657778
19	1	-4.909486	0.794742	-1.510284
20	1	-6.049649	2.964692	-1.382522
21	1	-3.394205	4.177966	1.792170
22	6	1.364376	-0.305793	-0.020847
23	6	0.558257	-1.372360	0.446627
24	6	-0.818786	-1.287919	0.444463
25	6	-1.463178	-0.118699	-0.026517
26	6	-0.668425	0.953142	-0.498914
27	6	0.707590	0.855246	-0.494007
28	1	1.023178	-2.262484	0.855488
29	1	-1.407638	-2.107507	0.839419
30	1	-1.142343	1.843956	-0.894082
31	1	1.287884	1.679893	-0.895740
32	16	3.832921	0.992037	-0.124837
33	6	2.809115	-0.411750	-0.005617
34	6	5.298813	0.011019	-0.032429
35	6	4.961095	-1.339718	0.080318
36	6	3.580805	-1.568484	0.099388
37	1	5.713593	-2.111587	0.140255
38	1	3.149693	-2.560869	0.158258
39	6	6.530752	0.737637	-0.086314
40	6	7.858849	0.385236	-0.027452
41	6	6.390701	1.811314	-0.196778
42	8	8.799592	1.461198	-0.120746
43	8	8.414966	-0.982415	0.121952
44	1	9.529794	2.364038	-0.200428
45	8	7.773217	-2.013273	0.206213
46	8	9.762939	-0.961939	0.156751
47	6	10.051959	-1.885118	0.254668
48	6	-5.338541	4.942886	0.382134
49	1	-6.047976	-4.567533	-0.335561
50	1	-6.443004	5.322826	-0.435619
51	1	-7.181905	-4.772544	0.504383
52	1	-6.171361	5.330066	-1.497741
53	1	-7.302604	4.660056	-0.281826
54	1	-7.935450	-3.989640	0.359312
55	1	-6.895271	-4.813655	1.561785
56	6	-7.601351	-5.733691	0.208344
57	7	-6.708864	6.333147	-0.125890

Optimized Cartesian coordinates for compound D2 in the cationic state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.260437	-2.039442	-1.044782
2	6	-4.264243	-2.967059	-1.237575
3	6	-5.475720	-2.869459	-0.520344
4	6	-5.658193	-1.815090	0.393749
5	6	-4.647666	-0.881873	0.582048
6	6	-3.438416	-0.981552	-0.127398
7	1	-2.342294	-2.108087	-1.617759
8	1	-4.151867	-3.775219	-1.951548
9	1	-6.572925	-1.727028	0.966141
10	1	-4.782288	-0.081926	1.301702
11	7	-2.414500	-0.020770	0.070563
12	6	-2.150366	2.177573	1.134209
13	6	-2.762880	1.349537	0.168388
14	6	-3.730695	1.895999	-0.692876
15	6	-4.078400	3.236929	-0.606813
16	6	-3.462168	4.059644	0.355018
17	6	-2.496489	3.510255	1.225618
18	1	-1.423910	1.758054	1.821212
19	1	-4.190441	1.269236	-1.448927
20	1	-4.811635	3.638748	-1.294438
21	1	-2.048808	4.156451	1.972235
22	6	1.635063	-1.220956	0.372687
23	6	0.588395	-2.043634	0.855499
24	6	-0.733324	-1.661364	0.754931
25	6	-1.075323	-0.420751	0.167965
26	6	-0.040581	0.410050	-0.319603
27	6	1.278190	0.014516	-0.222517
28	1	0.825053	-2.982977	1.342127
29	1	-1.512254	-2.296985	1.159268
30	1	-0.286939	1.347332	-0.804328
31	1	2.036341	0.666339	-0.644660
32	6	3.010847	-1.641048	0.490063
33	6	5.258985	-1.475370	0.371536
34	6	3.558664	-2.876791	0.900379
35	1	2.996611	-3.749335	1.198127
36	8	-3.720910	5.365886	0.527346
37	8	-6.383555	-3.824325	-0.782398
38	6	-4.690938	6.008851	-0.305704
39	6	-7.646342	-3.798356	-0.109812
40	1	-4.391870	5.971632	-1.358588
41	1	-5.679535	5.554222	-0.181472
42	1	-8.194152	-2.877352	-0.335973
43	1	-7.517718	-3.900063	0.973067
44	6	6.556728	-0.925807	0.150902
45	6	6.895375	0.323653	-0.298356
46	6	5.893898	1.287678	-0.623066
47	6	8.302321	0.767208	-0.482705
48	7	4.980734	1.975499	-0.850948
49	8	8.608518	1.869968	-0.878411
50	8	9.193878	-0.195481	-0.159913
51	1	7.381731	-1.595693	0.370211
52	1	10.076652	0.182196	-0.311047
53	6	4.944087	-2.773478	0.825050
54	1	5.669674	-3.539381	1.059788
55	7	4.062490	-0.822412	0.175950
56	1	3.994754	0.145735	-0.110993

57	1	-8.199391	-4.654802	-0.492742
58	1	-4.721541	7.045111	0.027699
Optimized Cartesian coordinates for compound D3 in the cationic state.				
Center Number	**Atomic Number**	**Coordinates (Angstroms)**		
		X	**Y**	**Z**
1	6	-3.402916	-2.157320	-0.962509
2	6	-4.305924	-3.189287	-1.106066
3	6	-5.526109	-3.177938	-0.394006
4	6	-5.819499	-2.100823	0.465037
5	6	-4.911324	-1.061786	0.603324
6	6	-3.693776	-1.072816	-0.103780
7	1	-2.479750	-2.162166	-1.531023
8	1	-4.109039	-4.018541	-1.776159
9	1	-6.739157	-2.079835	1.035886
10	1	-5.127435	-0.247302	1.285609
11	7	-2.775100	-0.009076	0.042060
12	6	-2.652673	2.238310	1.018626
13	6	-3.246676	1.320164	0.122409
14	6	-4.316412	1.744668	-0.689314
15	6	-4.784081	3.048177	-0.619102
16	6	-4.189155	3.958900	0.276169
17	6	-3.119090	3.533271	1.094980
18	1	-1.846272	1.914377	1.666823
19	1	-4.757866	1.053875	-1.398852
20	1	-5.592224	3.356554	-1.270098
21	1	-2.688468	4.244975	1.790300
22	6	1.385115	-0.795795	0.237796
23	6	0.447214	-1.662851	0.846996
24	6	-0.911009	-1.415437	0.779053
25	6	-1.391699	-0.272903	0.105028
26	6	-0.470024	0.604320	-0.502698
27	6	0.885759	0.340971	-0.438797
28	1	0.792419	-2.522442	1.409815
29	1	-1.607808	-2.078863	1.278377
30	1	-0.828321	1.468011	-1.050871
31	1	1.571300	1.012629	-0.945107
32	6	2.809435	-1.072431	0.312948
33	6	5.269971	-1.084776	0.278053
34	6	3.439811	-2.255705	0.684298
35	1	2.922786	-3.166497	0.962908
36	8	-4.558786	5.237887	0.427004
37	8	-6.327796	-4.231286	-0.604299
38	6	-5.638372	5.762284	-0.355580
39	6	-7.593058	-4.304322	0.063594
40	1	-5.404862	5.717755	-1.424360
41	1	-6.568902	5.222569	-0.151464
42	1	-8.231110	-3.457984	-0.211131
43	1	-7.461318	-4.338029	1.150072
44	6	6.694288	-0.882004	0.195065
45	6	7.389728	0.226665	-0.176866
46	6	6.753561	1.443635	-0.568944
47	6	8.885574	0.254051	-0.204266
48	7	6.186435	2.411329	-0.880264
49	8	9.526896	1.225942	-0.530313
50	8	9.428165	-0.921823	0.173931
51	1	7.264524	-1.761360	0.476263
52	1	10.392875	-0.812385	0.126160
53	16	4.026187	0.110454	-0.085481
54	7	4.787589	-2.256965	0.662577
55	1	-5.743147	6.801397	-0.047674
56	1	-8.049476	-5.232128	-0.277667

Optimized Cartesian coordinates for compound D4 in the cationic state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3.175632	-2.089115	0.979935
2	6	4.140705	-3.045690	1.174416
3	6	5.382365	-2.949746	0.519357
4	6	5.635261	-1.866142	-0.333569
5	6	4.664486	-0.900881	-0.522418
6	6	3.425615	-0.997370	0.126092
7	1	2.230343	-2.157141	1.505371
8	1	3.977140	-3.882990	1.842251
9	1	6.575930	-1.781974	-0.861157
10	1	4.850565	-0.077712	-1.202299
11	7	2.442416	-0.011952	-0.074339
12	6	2.174024	2.195142	-1.084377
13	6	2.814194	1.340410	-0.165490
14	6	3.826602	1.851525	0.659072
15	6	4.194793	3.180793	0.580256
16	6	3.555367	4.026899	-0.337234
17	6	2.542812	3.514291	-1.169487
18	1	1.409393	1.801620	-1.743593
19	1	4.301901	1.204671	1.387096
20	1	4.962791	3.558304	1.241911
21	1	2.077176	4.184414	-1.882169
22	6	-1.613421	-1.108543	-0.397343
23	6	-0.601159	-1.913199	-0.950470
24	6	0.726360	-1.563790	-0.842816
25	6	1.090101	-0.378963	-0.181347
26	6	0.090577	0.435439	0.372764
27	6	-1.234756	0.070392	0.268922
28	1	-0.866927	-2.812414	-1.493486
29	1	1.490003	-2.182805	-1.298190
30	1	0.364150	1.333957	0.912660
31	1	-1.979808	0.703413	0.738671
32	6	-3.002282	-1.500728	-0.517956
33	6	-5.202686	-1.384702	-0.403795
34	6	-3.597922	-2.683063	-0.947303
35	1	-3.109042	-3.584439	-1.288497
36	8	3.832348	5.321669	-0.496925
37	8	6.246471	-3.933870	0.773876
38	6	4.846781	5.926408	0.298537
39	6	7.531754	-3.914487	0.161782
40	1	4.592520	5.877598	1.361431
41	1	5.817022	5.452271	0.123509
42	1	8.091797	-3.021161	0.453634
43	1	7.447950	-3.964027	-0.927893
44	6	-6.545016	-0.912234	-0.183673
45	6	-6.938113	0.286072	0.302206
46	6	-5.978289	1.279205	0.675925
47	6	-8.364074	0.663294	0.487273
48	7	-5.094104	1.980967	0.935189
49	8	-8.712391	1.731698	0.921170
50	8	-9.203382	-0.313676	0.118823
51	1	-7.311331	-1.631890	-0.448504
52	1	-10.104661	0.012499	0.271284
53	7	-4.939204	-2.601182	-0.872474
54	7	-4.050390	-0.692985	-0.174692
55	1	-4.004959	0.264336	0.151516
56	1	4.888364	6.966674	-0.017207
57	1	8.046016	-4.801026	0.526755

Optimized Cartesian coordinates for compound D1 in the anionic state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.196087	-2.256699	-0.909267
2	6	-3.904420	-3.440320	-1.057795
3	6	-5.144448	-3.614463	-0.429361
4	6	-5.655902	-2.582725	0.362466
5	6	-4.930105	-1.400375	0.525129
6	6	-3.695900	-1.206954	-0.112887
7	1	-2.239448	-2.134257	-1.404756
8	1	-3.515080	-4.246425	-1.671564
9	1	-6.606396	-2.687155	0.873243
10	1	-5.331528	-0.614891	1.156241
11	7	-2.955794	-0.012429	0.049145
12	6	-3.093324	2.239008	1.010226
13	6	-3.600679	1.243519	0.151994
14	6	-4.738861	1.551230	-0.607424
15	6	-5.367073	2.794730	-0.504985
16	6	-4.848871	3.771890	0.349310
17	6	-3.702367	3.482194	1.100960
18	1	-2.207195	2.027398	1.598379
19	1	-5.141618	0.808429	-1.287620
20	1	-6.245070	2.988596	-1.110579
21	1	-3.306779	4.247334	1.761337
22	6	1.331978	-0.187816	0.193434
23	6	0.516530	-0.972798	1.055046
24	6	-0.866557	-0.909198	1.014088
25	6	-1.525402	-0.070894	0.096955
26	6	-0.741923	0.708345	-0.768875
27	6	0.643077	0.659450	-0.716161
28	1	0.985973	-1.632136	1.777769
29	1	-1.456570	-1.516287	1.695177
30	1	-1.233264	1.361028	-1.485115
31	1	1.214816	1.277388	-1.402040
32	16	3.798518	0.742469	-0.791186
33	6	2.767008	-0.252862	0.245974
34	6	5.307680	0.056062	-0.102720
35	6	4.952868	-0.895233	0.883732
36	6	3.583976	-1.051862	1.060703
37	1	5.719327	-1.430322	1.425908
38	1	3.171007	-1.751245	1.780798
39	6	6.519950	0.529373	-0.609170
40	6	7.892817	0.251609	-0.338799
41	6	6.406179	1.281259	-1.388057
42	8	8.828362	0.988869	-1.119891
43	8	8.428272	-0.678088	0.623323
44	1	9.557015	1.617400	-1.785096
45	8	7.823938	-1.417784	1.403056
46	8	9.809615	-0.705646	0.633654
47	6	10.008291	-1.363775	1.317435
48	6	-5.380371	5.028258	0.521168
49	1	-5.769279	-4.819331	-0.652041
50	1	-6.516568	5.371414	-0.246085
51	1	-7.010473	-5.043014	-0.014558
52	1	-6.311074	5.328632	-1.324589
53	1	-7.372952	4.718683	-0.025962
54	1	-7.770585	-4.314050	-0.328819
55	1	-6.921948	-5.007085	1.080133
56	6	-7.331803	-6.042993	-0.313010
57	7	-6.771671	6.397236	0.027447
Optimized Cartesian coordinates for compound D2 in the anionic state.				

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.943889	-2.154478	-0.946734
2	6	-3.800070	-3.205617	-1.241595
3	6	-5.127199	-3.193671	-0.793209
4	6	-5.577412	-2.111137	-0.033050
5	6	-4.706828	-1.063732	0.277571
6	6	-3.379791	-1.055816	-0.178624
7	1	-1.920098	-2.175052	-1.303080
8	1	-3.458828	-4.049182	-1.833363
9	1	-6.594747	-2.073208	0.339682
10	1	-5.066644	-0.238506	0.882484
11	7	-2.490120	-0.003950	0.138627
12	6	-2.385267	2.210285	1.185868
13	6	-2.935474	1.336354	0.227347
14	6	-3.907663	1.849246	-0.644033
15	6	-4.338038	3.175146	-0.554571
16	6	-3.780786	4.028536	0.401339
17	6	-2.796042	3.532995	1.266145
18	1	-1.621235	1.839539	1.860079
19	1	-4.335872	1.203657	-1.403244
20	1	-5.092126	3.528112	-1.248750
21	1	-2.366563	4.203682	2.003568
22	6	1.651134	-0.893920	0.831374
23	6	0.612158	-1.532284	1.562372
24	6	-0.722979	-1.238791	1.344989
25	6	-1.106433	-0.299620	0.369162
26	6	-0.096952	0.337952	-0.369785
27	6	1.242956	0.059319	-0.142352
28	1	0.870799	-2.262479	2.323155
29	1	-1.490861	-1.740112	1.928041
30	1	-0.373641	1.065080	-1.128160
31	1	1.984167	0.580246	-0.741150
32	6	3.032125	-1.204263	1.073121
33	6	5.310461	-1.086583	0.829695
34	6	3.622175	-2.122454	1.967908
35	1	3.079189	-2.768821	2.644470
36	8	-4.124701	5.349441	0.572237
37	8	-5.894514	-4.279404	-1.149630
38	6	-5.075321	5.900281	-0.316333
39	6	-7.232921	-4.312789	-0.698978
40	1	-4.736488	5.852660	-1.360415
41	1	-6.049331	5.396360	-0.240519
42	1	-7.817474	-3.465237	-1.083848
43	1	-7.297409	-4.312517	0.398151
44	6	6.572234	-0.692598	0.363465
45	6	6.902794	0.272772	-0.634374
46	6	5.897225	0.995766	-1.319441
47	6	8.258714	0.573871	-1.009585
48	7	4.999652	1.547447	-1.835406
49	8	8.643910	1.384118	-1.853855
50	8	9.205429	-0.161780	-0.309050
51	1	7.414080	-1.193109	0.827412
52	1	10.038640	0.162998	-0.683289
53	6	5.004088	-2.056344	1.825635
54	1	5.744887	-2.632362	2.364411
55	7	4.082959	-0.597097	0.400991
56	1	3.997886	0.119347	-0.304981
57	1	-7.661328	-5.242187	-1.080131
58	1	-5.193442	6.946754	-0.027598

Optimized Cartesian coordinates for compound D3 in the anionic state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-3.227594	-2.181747	-0.953285
2	6	-4.027775	-3.293861	-1.171413
3	6	-5.305230	-3.376937	-0.601844
4	6	-5.762079	-2.327875	0.200667
5	6	-4.944529	-1.219473	0.434018
6	6	-3.670371	-1.117735	-0.142800
7	1	-2.242836	-2.128281	-1.404137
8	1	-3.682717	-4.112351	-1.795135
9	1	-6.740802	-2.363574	0.665358
10	1	-5.304511	-0.419653	1.072277
11	7	-2.837758	0.002738	0.092162
12	6	-2.845486	2.250665	1.074293
13	6	-3.375486	1.310109	0.169262
14	6	-4.430612	1.719341	-0.658471
15	6	-4.958173	3.010322	-0.579235
16	6	-4.417827	3.932646	0.320945
17	6	-3.352678	3.540173	1.142425
18	1	-2.021846	1.960352	1.717161
19	1	-4.847699	1.019527	-1.374594
20	1	-5.774749	3.282964	-1.238002
21	1	-2.938732	4.263383	1.837795
22	6	1.386428	-0.593616	0.536473
23	6	0.439843	-1.332665	1.293707
24	6	-0.924516	-1.131267	1.156566
25	6	-1.427238	-0.190694	0.240918
26	6	-0.510151	0.548572	-0.520662
27	6	0.857054	0.360287	-0.369729
28	1	0.786795	-2.066773	2.013745
29	1	-1.620238	-1.707915	1.759502
30	1	-0.878768	1.279790	-1.234313
31	1	1.537847	0.948969	-0.976838
32	6	2.805497	-0.805196	0.682294
33	6	5.313916	-0.827750	0.609880
34	6	3.476379	-1.736559	1.478963
35	1	2.961643	-2.449447	2.117858
36	8	-4.851866	5.227582	0.475213
37	8	-6.019525	-4.515692	-0.890096
38	6	-5.890000	5.678544	-0.371659
39	6	-7.302199	-4.652030	-0.312233
40	1	-5.606844	5.623039	-1.431713
41	1	-6.817187	5.106821	-0.225385
42	1	-7.985193	-3.853904	-0.635207
43	1	-7.259351	-4.654024	0.785728
44	6	6.688573	-0.674170	0.420370
45	6	7.431114	0.211899	-0.390903
46	6	6.836987	1.191247	-1.229814
47	6	8.879709	0.177459	-0.420361
48	7	6.345314	1.997224	-1.920022
49	8	9.623678	0.895563	-1.083021
50	8	9.431119	-0.785535	0.403976
51	1	7.272139	-1.371018	1.011788
52	1	10.383203	-0.668926	0.262980
53	16	4.023794	0.133914	-0.188886
54	7	4.811271	-1.761959	1.452794
55	1	-6.070104	6.721888	-0.104992
56	1	-7.691117	-5.612990	-0.655025

Optimized Cartesian coordinates for compound D4 in the anionic state.				
Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.968823	-2.141728	0.943304
2	6	3.832900	-3.183568	1.221700
3	6	5.143723	-3.166005	0.745082
4	6	5.570194	-2.090478	-0.026092
5	6	4.689284	-1.053270	-0.321231
6	6	3.381056	-1.051897	0.162473
7	1	1.954407	-2.163953	1.324098
8	1	3.512071	-4.026699	1.823607
9	1	6.578303	-2.048747	-0.419786
10	1	5.029074	-0.227921	-0.936344
11	7	2.484588	-0.004400	-0.134309
12	6	2.365398	2.206807	-1.164056
13	6	2.922915	1.334942	-0.218160
14	6	3.899011	1.838756	0.640518
15	6	4.328192	3.160423	0.553138
16	6	3.762308	4.013394	-0.388087
17	6	2.772551	3.525012	-1.241383
18	1	1.596442	1.837871	-1.832823
19	1	4.334792	1.187775	1.389823
20	1	5.090475	3.509638	1.238553
21	1	2.336750	4.200649	-1.969059
22	6	-1.637425	-0.898769	-0.751550
23	6	-0.622075	-1.558632	-1.471934
24	6	0.713382	-1.262345	-1.278319
25	6	1.103310	-0.302295	-0.339907
26	6	0.112367	0.356441	0.387135
27	6	-1.228026	0.073908	0.180758
28	1	-0.895052	-2.307284	-2.208134
29	1	1.474765	-1.779609	-1.853924
30	1	0.399888	1.103801	1.119938
31	1	-1.966647	0.609069	0.768821
32	6	-3.027075	-1.213825	-0.967086
33	6	-5.258350	-1.131495	-0.771116
34	6	-3.653040	-2.158089	-1.770961
35	1	-3.169209	-2.874673	-2.423714
36	8	4.103960	5.327451	-0.553691
37	8	5.922188	-4.238502	1.086730
38	6	5.059485	5.868757	0.324339
39	6	7.243081	-4.264633	0.606515
40	1	4.731139	5.811866	1.369741
41	1	6.030419	5.364795	0.233441
42	1	7.828453	-3.411746	0.973525
43	1	7.279311	-4.268180	-0.490362
44	6	-6.548605	-0.753666	-0.366589
45	6	-6.913162	0.261038	0.561943
46	6	-5.935187	1.044765	1.215018
47	6	-8.273756	0.556250	0.898114
48	7	-5.052396	1.634252	1.699738
49	8	-8.681554	1.407132	1.683014
50	8	-9.190537	-0.228860	0.239470
51	1	-7.350052	-1.314374	-0.827139
52	1	-10.034436	0.100491	0.579454
53	7	-4.991571	-2.118112	-1.661195
54	7	-4.077725	-0.572354	-0.336533
55	1	-4.026330	0.196118	0.316519
56	1	5.176270	6.916482	0.044849
57	1	7.688765	-5.187623	0.979437