Six-fold Screening unfolds optimized Rylene Diimides towards Organic Solar Cell: A DFT Perspective

Sri Vanaja [a], Tanay Kundu [a*] and Amrita Pal [b*]

Cartesian coordinates for optimization (DFT-B3LYP-6-311G++(2p,2d) pop=full) of the Diimide structures

m-PMDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000007	1.446838	0.000023
2	6	0	1.176347	0.702553	-0.000012
3	6	0	1.176229	-0.701669	-0.000038
4	6	0	0.000006	-1.446192	-0.000029
5	6	0	-1.176232	-0.701678	0.000028
6	6	0	-1.176346	0.702541	0.000023
7	6	0	-2.592665	-1.166570	0.000180
8	7	0	-3.380004	0.000666	0.000041
9	6	0	-2.593582	1.166226	-0.000029
10	6	0	2.593575	1.166238	-0.000069
11	7	0	3.379998	0.000632	0.000012
12	6	0	2.592678	-1.166560	-0.000105
13	6	0	4.839541	0.002444	0.000257
14	6	0	-4.839543	0.002431	-0.000082
15	8	0	3.031115	2.322205	-0.000100

16	8	0	3.026498	-2.323780	-0.000196
17	8	0	-3.031067	2.322227	0.000017
18	8	0	-3.026538	-2.323757	0.000073
19	1	0	-0.000026	2.527436	-0.000009
20	1	0	0.000024	-2.526776	-0.000031
21	1	0	5.218125	0.515324	-0.882430
22	1	0	5.170414	-1.032512	-0.005676
23	1	0	5.218521	0.504897	0.888856
24	1	0	-5.218400	0.509982	0.885624
25	1	0	-5.218194	0.510328	-0.885651
26	1	0	-5.170492	-1.032533	-0.000280

---

p-PMDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000105	-1.443797	-0.000013
2	6	0	1.167432	-0.693667	-0.000013
3	6	0	1.167495	0.693499	-0.000013
4	6	0	0.000088	1.443798	-0.000013
5	6	0	-1.167417	0.693712	-0.000013
6	6	0	-1.167482	-0.693538	-0.000013
7	6	0	-2.579365	1.162640	-0.000013
8	7	0	-3.401604	0.000062	-0.000013
9	6	0	-2.579483	-1.162364	-0.000013

10	6	0	2.579376	-1.162646	-0.000013
11	7	0	3.401616	-0.000066	-0.000013
12	6	0	2.579490	1.162380	-0.000013
13	6	0	4.901616	-0.000051	-0.000013
14	6	0	-4.901604	0.000047	-0.000013
15	6	0	5.613134	-1.092883	-0.513099
16	6	0	7.002417	-1.082097	-0.508042
17	6	0	7.708787	0.000069	0.000031
18	6	0	7.002312	1.082223	0.508104
19	6	0	5.613098	1.092895	0.513121
20	6	0	-5.613142	1.092878	-0.513100
21	6	0	-7.002427	1.082088	-0.508040
22	6	0	-7.708804	-0.000074	0.000030
23	6	0	-7.002326	-1.082219	0.508099
24	6	0	-5.613114	-1.092893	0.513117
25	8	0	2.937433	-2.313478	-0.000013
26	8	0	2.937455	2.313291	-0.000013
27	8	0	-2.937458	-2.313284	-0.000013
28	8	0	-2.937439	2.313474	-0.000013
29	1	0	-0.000143	-2.523708	-0.000013
30	1	0	0.000379	2.523709	-0.000013
31	1	0	5.091480	-1.942299	-0.911897
32	1	0	7.529808	-1.936562	-0.909214
33	1	0	8.789783	0.000081	0.000031
34	1	0	7.529571	1.936756	0.909304
35	1	0	5.091401	1.942288	0.911912
36	1	0	-5.091501	1.942299	-0.911899

37	1	0	-7.529810	1.936558	-0.909216
38	1	0	-8.789800	-0.000088	0.000032
39	1	0	-7.529580	-1.936754	0.909300
40	1	0	-5.091437	-1.942293	0.911912

m-NDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.408584	1.236479	-0.000088
2	6	0	-0.711244	0.001660	-0.000292
3	6	0	0.711244	0.001660	-0.000294
4	6	0	1.408584	1.236478	-0.000087
5	6	0	0.703948	2.431100	0.000325
6	6	0	-0.703949	2.431100	0.000324
7	6	0	-1.407483	-1.233732	-0.000188
8	6	0	-0.704008	-2.428848	-0.000119
9	6	0	0.704007	-2.428848	-0.000121
10	6	0	1.407483	-1.233732	-0.000194
11	6	0	-2.888929	1.250377	-0.000577
12	7	0	-3.537694	0.002415	-0.001645
13	6	0	-2.886016	-1.241588	0.000303
14	6	0	2.886016	-1.241589	0.000284
15	7	0	3.537694	0.002415	-0.001648

16	6	0	2.888929	1.250376	-0.000567
17	8	0	3.540059	2.313437	0.001362
18	8	0	3.551132	-2.296163	0.001516
19	8	0	-3.540058	2.313438	0.001359
20	8	0	-3.551132	-2.296162	0.001511
21	6	0	-5.015033	-0.024852	-0.001121
22	6	0	5.015033	-0.024851	-0.001120
23	1	0	1.257680	3.358406	0.000495
24	1	0	-1.257681	3.358406	0.000492
25	1	0	-1.258475	-3.355808	0.000130
26	1	0	1.258475	-3.355808	0.000124
27	1	0	-5.364735	0.999621	-0.033631
28	1	0	-5.373904	-0.521086	0.898093
29	1	0	-5.370720	-0.579803	-0.865960
30	1	0	5.364735	0.999621	-0.033618
31	1	0	5.373901	-0.521094	0.898091
32	1	0	5.370722	-0.579794	-0.865964

---

p-NDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.408314	1.235123	0.000069
2	6	0	-0.711860	0.000000	0.000015
3	6	0	0.711861	0.000000	-0.000016

4	6	0	1.408314	1.235121	-0.000029
5	6	0	0.703797	2.429794	0.000009
6	6	0	-0.703796	2.429794	0.000069
7	6	0	-1.408314	-1.235121	-0.000011
8	6	0	-0.703797	-2.429793	-0.000042
9	6	0	0.703796	-2.429793	-0.000041
10	6	0	1.408314	-1.235121	-0.000032
11	6	0	-2.888514	1.252520	0.000134
12	7	0	-3.542716	0.000001	0.000071
13	6	0	-2.888515	-1.252517	-0.000012
14	6	0	2.888514	-1.252518	-0.000030
15	7	0	3.542717	-0.000000	-0.000073
16	6	0	2.888514	1.252519	-0.000094
17	8	0	3.539892	2.311313	-0.000156
18	8	0	3.539892	-2.311313	0.000019
19	8	0	-3.539891	2.311314	0.000229
20	8	0	-3.539893	-2.311311	-0.000099
21	6	0	-4.999882	0.000001	0.000097
22	6	0	4.999882	-0.000001	-0.000097
23	6	0	-5.687095	-0.000010	-1.212334
24	6	0	-7.082953	-0.000019	-1.209949
25	6	0	-7.781569	-0.000003	0.000146
26	6	0	-7.082910	0.000015	1.210217
27	6	0	-5.687052	0.000010	1.212552
28	6	0	5.687054	-0.000076	-1.212551
29	6	0	7.082912	-0.000070	-1.210214
30	6	0	7.781569	-0.000001	-0.000143

31	6	0	7.082952	0.000068	1.209952
32	6	0	5.687094	0.000075	1.212335
33	1	0	1.258050	3.356840	-0.000015
34	1	0	-1.258049	3.356840	0.000123
35	1	0	-1.258049	-3.356838	-0.000072
36	1	0	1.258048	-3.356839	-0.000041
37	1	0	-5.136416	-0.000024	-2.142327
38	1	0	-7.620762	-0.000033	-2.148034
39	1	0	-8.863112	-0.000004	0.000166
40	1	0	-7.620685	0.000028	2.148321
41	1	0	-5.136339	0.000023	2.142525
42	1	0	5.136341	-0.000130	-2.142525
43	1	0	7.620688	-0.000125	-2.148317
44	1	0	8.863112	-0.000002	-0.000161
45	1	0	7.620759	0.000123	2.148037
46	1	0	5.136412	0.000128	2.142327

---

m-NDI2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000080	-2.405345	-0.708681
2	6	0	0.000010	-1.241018	-1.427910
3	6	0	0.000000	-0.000000	-0.723523
4	6	0	0.000000	0.000000	0.724392

5	6	0	-0.000004	-1.241167	1.428580
6	6	0	-0.000079	-2.405469	0.709412
7	1	0	0.000001	1.253425	-2.509703
8	1	0	-0.000001	-1.253425	-2.509703
9	6	0	-0.000010	1.241018	-1.427910
10	6	0	0.000004	1.241167	1.428580
11	1	0	-0.000003	-1.253811	2.510377
12	6	0	0.000079	2.405469	0.709412
13	6	0	0.000080	2.405345	-0.708681
14	1	0	0.000003	1.253811	2.510377
15	6	0	-0.000024	-3.817924	-1.170980
16	6	0	-0.000004	-3.818803	1.170250
17	6	0	0.000024	3.817924	-1.170980
18	6	0	0.000004	3.818803	1.170250
19	7	0	0.000074	-4.602463	0.000463
20	7	0	-0.000074	4.602463	0.000463
21	6	0	0.000004	-6.061199	0.002638
22	6	0	-0.000004	6.061199	0.002638
23	8	0	-0.000056	-4.260849	-2.326118
24	8	0	-0.000032	-4.265828	2.323960
25	8	0	0.000032	4.265828	2.323960
26	8	0	0.000056	4.260849	-2.326118
27	1	0	0.000446	-6.392885	-1.032119
28	1	0	0.885049	-6.439772	0.511936
29	1	0	-0.885512	-6.439744	0.511076
30	1	0	-0.000446	6.392885	-1.032119
31	1	0	-0.885049	6.439772	0.511936

32	1	0	0.885512	6.439744	0.511076

---

p-NDI2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.404784	-0.707190	0.001973
2	6	0	-1.240813	-1.428123	0.001222
3	6	0	-0.000000	-0.724421	-0.000005
4	6	0	-0.000002	0.724489	0.000003
5	6	0	-1.240818	1.428186	-0.001209
6	6	0	-2.404784	0.707247	-0.001943
7	1	0	1.254975	-2.509809	-0.002542
8	1	0	-1.254968	-2.509813	0.002514
9	6	0	1.240813	-1.428119	-0.001241
10	6	0	1.240811	1.428189	0.001221
11	1	0	-1.254982	2.509876	-0.002499
12	6	0	2.404780	0.707253	0.001946
13	6	0	2.404783	-0.707182	-0.001981
14	1	0	1.254974	2.509879	0.002521
15	6	0	-3.811611	-1.174934	0.002022

16	6	0	-3.811616	1.174989	-0.001968
17	6	0	3.811606	-1.174926	-0.002027
18	6	0	3.811605	1.175002	0.001964
19	7	0	-4.615182	0.000030	0.000008
20	7	0	4.615187	0.000042	-0.000005
21	8	0	-4.228573	-2.337326	0.008215
22	8	0	-4.228564	2.337390	-0.008154
23	8	0	4.228539	2.337407	0.008158
24	8	0	4.228564	-2.337319	-0.008234
25	6	0	6.049764	0.000017	-0.000007
26	6	0	6.746551	0.901304	0.814116
27	6	0	6.746479	-0.901358	-0.814090
28	6	0	8.141777	0.900940	0.804601
29	1	0	6.206032	1.602925	1.428906
30	6	0	8.141703	-0.901118	-0.804562
31	1	0	6.205898	-1.602949	-1.428864
32	6	0	8.843646	-0.000112	0.000014
33	1	0	8.676901	1.603316	1.428842
34	1	0	8.676774	-1.603551	-1.428784
35	1	0	9.925095	-0.000162	0.000019
36	6	0	-6.049763	0.000008	0.000009
37	6	0	-6.746533	0.901180	-0.814248
38	6	0	-6.746474	-0.901236	0.814233
39	6	0	-8.141759	0.900830	-0.804731
40	1	0	-6.205999	1.602700	-1.429141
41	6	0	-8.141700	-0.900989	0.804705
42	1	0	-6.205890	-1.602731	1.429116

43	6	0	-8.843631	-0.000099	-0.000009
44	1	0	-8.676885	1.603116	-1.429072
45	1	0	-8.676781	-1.603322	1.429032
46	1	0	-9.925081	-0.000140	-0.000012

---

m-ADI1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	1.405711	-0.000003
2	6	0	1.225844	0.726445	0.000004
3	6	0	1.225820	-0.725606	0.000003
4	6	0	-0.000000	-1.404903	-0.000005
5	6	0	-1.225820	-0.725606	-0.000010
6	6	0	-1.225844	0.726444	-0.000009
7	6	0	-2.476000	-1.432219	-0.000012
8	6	0	-3.633569	-0.714128	-0.000018
9	6	0	-3.633743	0.714802	-0.000018
10	6	0	-2.476208	1.432835	-0.000011
11	6	0	2.476207	1.432834	0.000011
12	6	0	3.633743	0.714803	0.000019
13	6	0	3.633570	-0.714128	0.000019
14	6	0	2.475999	-1.432218	0.000009
15	6	0	5.045400	1.172017	0.000018

16	7	0	5.827578	0.000292	-0.000011
17	6	0	5.044473	-1.173014	0.000025
18	6	0	-5.044473	-1.173015	-0.000029
19	7	0	-5.827578	0.000292	-0.000013
20	6	0	-5.045400	1.172017	-0.000033
21	8	0	5.498007	2.324592	-0.000006
22	8	0	5.492576	-2.327217	-0.000006
23	8	0	-5.498007	2.324592	-0.000001
24	8	0	-5.492575	-2.327216	-0.000002
25	6	0	7.285884	0.002707	-0.000011
26	6	0	-7.285884	0.002707	0.000065
27	1	0	0.000000	2.488727	-0.000003
28	1	0	-0.000000	-2.487927	-0.000005
29	1	0	-2.488766	-2.514246	-0.000015
30	1	0	-2.489191	2.514869	-0.000013
31	1	0	2.489191	2.514868	0.000007
32	1	0	2.488766	-2.514247	0.000006
33	1	0	7.664300	0.512492	-0.884921
34	1	0	7.617759	-1.031972	-0.000320
35	1	0	7.664329	0.511950	0.885205
36	1	0	-7.664346	0.512493	-0.884825
37	1	0	-7.617759	-1.031972	-0.000227
38	1	0	-7.664283	0.511949	0.885301

---

p-ADI1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000002	-1.405693	-0.000240
2	6	0	-1.225805	-0.726271	-0.000207
3	6	0	-1.225803	0.726285	0.000208
4	6	0	0.000002	1.405703	0.000226
5	6	0	1.225804	0.726282	0.000019
6	6	0	1.225803	-0.726274	-0.000047
7	6	0	2.475673	1.432207	-0.001363
8	6	0	3.632988	0.712428	-0.001990
9	6	0	3.632986	-0.712426	0.001935
10	6	0	2.475669	-1.432202	0.001321
11	6	0	-2.475673	-1.432196	-0.001808
12	6	0	-3.632988	-0.712417	-0.002182
13	6	0	-3.632986	0.712436	0.002214
14	6	0	-2.475670	1.432212	0.001825
15	6	0	-5.037942	-1.176827	-0.002808
16	7	0	-5.840879	0.000012	0.000035
17	6	0	-5.037940	1.176849	0.002854
18	6	0	5.037942	1.176839	-0.002476
19	7	0	5.840879	-0.000002	-0.000035
20	6	0	5.037940	-1.176839	0.002406
21	8	0	-5.459294	-2.338649	-0.010066
22	8	0	-5.459283	2.338674	0.010106
23	8	0	5.459286	-2.338666	0.009278
24	8	0	5.459291	2.338664	-0.009345

25	6	0	-7.274998	0.000006	0.000044
26	6	0	7.274999	-0.000004	-0.000035
27	6	0	-7.972484	-0.911699	-0.802350
28	6	0	-9.367693	-0.910916	-0.793069
29	6	0	-10.069855	-0.000027	0.000066
30	6	0	-9.367703	0.910872	0.793195
31	6	0	-7.972493	0.911688	0.802457
32	6	0	7.972491	0.911958	-0.802132
33	6	0	9.367701	0.911152	-0.792860
34	6	0	10.069855	-0.000010	-0.000035
35	6	0	9.367696	-0.911170	0.792790
36	6	0	7.972486	-0.911970	0.802061
37	1	0	-0.000003	-2.488659	-0.000420
38	1	0	0.000003	2.488670	0.000405
39	1	0	2.490213	2.514131	-0.002795
40	1	0	2.490208	-2.514126	0.002752
41	1	0	-2.490213	-2.514120	-0.003599
42	1	0	-2.490208	2.514136	0.003615
43	1	0	-7.432104	-1.621824	-1.407116
44	1	0	-9.902685	-1.621190	-1.408519
45	1	0	-11.151347	-0.000041	0.000074
46	1	0	-9.902702	1.621132	1.408657
47	1	0	-7.432123	1.621821	1.407220
48	1	0	7.432117	1.622292	-1.406658
49	1	0	9.902698	1.621625	-1.408077
50	1	0	11.151347	-0.000012	-0.000034
51	1	0	9.902690	-1.621646	1.408006

52	1	0	7.432110	-1.622302	1.406586

---

m-ADI2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015088	-1.431320	-0.010574
2	6	0	1.220101	-0.737998	0.041149
3	6	0	1.238537	0.667128	-0.012778
4	6	0	0.015094	1.431341	-0.010664
5	6	0	-1.220111	0.738018	0.041025
6	6	0	-1.238537	-0.667105	-0.012816
7	6	0	-2.482174	-1.365490	-0.074812
8	6	0	-2.523157	-2.734368	-0.146215
9	6	0	-1.331456	-3.479366	-0.154372
10	6	0	-0.117812	-2.853627	-0.085525
11	6	0	2.482182	1.365491	-0.074796
12	6	0	2.523180	2.734373	-0.146171
13	6	0	1.331486	3.479377	-0.154267
14	6	0	0.117832	2.853645	-0.085499
15	6	0	2.519747	-1.469840	0.163013

16	7	0	3.700388	-0.740617	0.029229
17	6	0	3.772691	0.646131	-0.086283
18	6	0	-2.519755	1.469855	0.162877
19	7	0	-3.700396	0.740599	0.029216
20	6	0	-3.772688	-0.646137	-0.086286
21	8	0	2.608781	-2.667550	0.378225
22	8	0	4.843939	1.218091	-0.176174
23	8	0	-4.843937	-1.218109	-0.176103
24	8	0	-2.608807	2.667571	0.378051
25	6	0	4.950604	-1.507102	0.093357
26	6	0	-4.950632	1.507040	0.093486
27	1	0	-3.487661	-3.216910	-0.204130
28	1	0	-1.374374	-4.557366	-0.220373
29	1	0	0.786767	-3.432043	-0.086516
30	1	0	3.487685	3.216912	-0.204073
31	1	0	1.374414	4.557384	-0.220167
32	1	0	-0.786741	3.432071	-0.086455
33	1	0	4.929880	-2.299208	-0.650069
34	1	0	5.058414	-1.962328	1.075323
35	1	0	5.766354	-0.821523	-0.096760
36	1	0	-5.766354	0.821515	-0.096940
37	1	0	-5.058575	1.961914	1.075606
38	1	0	-4.929825	2.299407	-0.649651

---

p-ADI2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.375174	-1.381083	-0.049359
2	6	0	1.374305	-0.377498	0.009552
3	6	0	1.010507	0.979537	-0.054006
4	6	0	-0.375175	1.381132	-0.049330
5	6	0	-1.374314	0.377538	0.009636
6	6	0	-1.010506	-0.979497	-0.053960
7	6	0	-2.015710	-1.990867	-0.129145
8	6	0	-1.681194	-3.318137	-0.210024
9	6	0	-0.331221	-3.709557	-0.213652
10	6	0	0.665084	-2.776817	-0.132671
11	6	0	2.015728	1.990886	-0.129221
12	6	0	1.681234	3.318162	-0.210063
13	6	0	0.331267	3.709601	-0.213644
14	6	0	-0.665053	2.776878	-0.132634
15	6	0	2.821736	-0.733852	0.153624
16	7	0	3.762464	0.294420	-0.006835
17	6	0	3.453843	1.650931	-0.151048
18	6	0	-2.821756	0.733842	0.153820
19	7	0	-3.762467	-0.294435	-0.006689
20	6	0	-3.453830	-1.650942	-0.150896
21	8	0	3.221003	-1.853819	0.408643
22	8	0	4.331707	2.481605	-0.269036
23	8	0	-4.331679	-2.481614	-0.269006
24	8	0	-3.221081	1.853802	0.408773

25	6	0	5.163260	-0.071130	0.051883
26	6	0	-5.163268	0.071102	0.051994
27	6	0	5.825426	-0.421375	-1.115845
28	6	0	7.170945	-0.766982	-1.063202
29	6	0	7.845510	-0.759706	0.153176
30	6	0	7.173098	-0.405389	1.318540
31	6	0	5.827957	-0.059687	1.269802
32	6	0	-5.825406	0.421359	-1.115748
33	6	0	-7.170927	0.766959	-1.063137
34	6	0	-7.845524	0.759665	0.153224
35	6	0	-7.173141	0.405341	1.318602
36	6	0	-5.827996	0.059645	1.269896
37	1	0	-2.477316	-4.044716	-0.280411
38	1	0	-0.077697	-4.757689	-0.287316
39	1	0	1.692994	-3.087323	-0.131485
40	1	0	2.477366	4.044728	-0.280478
41	1	0	0.077759	4.757738	-0.287293
42	1	0	-1.692950	3.087412	-0.131412
43	1	0	5.292130	-0.420529	-2.055947
44	1	0	7.690308	-1.039170	-1.971427
45	1	0	8.892135	-1.028032	0.192958
46	1	0	7.694258	-0.397596	2.265646
47	1	0	5.296490	0.217147	2.169130
48	1	0	-5.292085	0.420527	-2.055835
49	1	0	-7.690268	1.039154	-1.971371
50	1	0	-8.892151	1.027986	0.192982
51	1	0	-7.694325	0.397535	2.265695

52	1	0	-5.296551	-0.217195	2.169235

---

m-PyDI1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.234670	-1.454063	-0.000018
2	6	0	-2.437966	-0.686010	-0.000061
3	6	0	-2.438074	0.685741	0.000064
4	6	0	-1.234825	1.454290	-0.000030
5	6	0	0.000001	0.718455	0.000001
6	6	0	-0.000002	-0.718161	-0.000085
7	6	0	1.234808	1.454290	-0.000071
8	6	0	2.438074	0.685732	0.000002
9	6	0	2.437965	-0.686018	-0.000152
10	6	0	1.234688	-1.454063	-0.000061
11	6	0	1.213107	-2.861114	-0.000099
12	6	0	-0.000020	-3.547531	-0.000072
13	6	0	-1.213125	-2.861111	-0.000053
14	6	0	-1.213137	2.861249	-0.000027
15	6	0	0.000019	3.547575	-0.000080

16	6	0	1.213154	2.861246	-0.000075
17	6	0	3.854725	1.158236	-0.000026
18	7	0	4.649268	-0.001124	0.000114
19	6	0	3.855050	-1.158310	0.000001
20	6	0	-3.855064	-1.158301	0.000121
21	7	0	-4.649266	-0.001115	0.000117
22	6	0	-3.854709	1.158246	0.000075
23	8	0	-4.300132	-2.315138	0.000046
24	8	0	-4.297252	2.315888	0.000016
25	8	0	4.297261	2.315884	0.000004
26	8	0	4.300120	-2.315144	0.000048
27	6	0	-6.107401	-0.002527	0.000022
28	6	0	6.107403	-0.002535	0.000181
29	1	0	2.151486	-3.394888	-0.000065
30	1	0	-0.000005	-4.628761	-0.000075
31	1	0	-2.151524	-3.394846	-0.000023
32	1	0	-2.151350	3.395238	0.000013
33	1	0	0.000003	4.628812	-0.000109
34	1	0	2.151386	3.395197	-0.000102
35	1	0	-6.488621	-0.507988	0.886147
36	1	0	-6.488439	-0.509554	-0.885281
37	1	0	-6.436885	1.033104	-0.000908
38	1	0	6.488544	-0.507721	0.886500
39	1	0	6.488523	-0.509837	-0.884928
40	1	0	6.436884	1.033096	-0.001026

---

p-PyDI1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.234473	-1.450176	-0.109572
2	6	0	2.438282	-0.683459	-0.047002
3	6	0	2.438195	0.683300	0.047354
4	6	0	1.234476	1.449823	0.109723
5	6	0	0.000077	0.716482	0.053554
6	6	0	-0.000077	-0.716481	-0.053569
7	6	0	-1.234473	1.450178	0.109558
8	6	0	-2.438282	0.683460	0.046987
9	6	0	-2.438195	-0.683299	-0.047369
10	6	0	-1.234476	-1.449821	-0.109738
11	6	0	-1.213237	-2.852987	-0.216304
12	6	0	-0.000253	-3.537202	-0.268976
13	6	0	1.212925	-2.852979	-0.216080
14	6	0	1.213237	2.852989	0.216289
15	6	0	0.000253	3.537203	0.268961
16	6	0	-1.212925	2.852981	0.216065
17	6	0	-3.849567	1.159462	0.084470
18	7	0	-4.661225	0.000196	-0.000231
19	6	0	-3.849447	-1.159199	-0.085024
20	6	0	3.849567	-1.159462	-0.084482
21	7	0	4.661225	-0.000196	0.000225
22	6	0	3.849448	1.159200	0.085009

23	8	0	4.269375	-2.320068	-0.165406
24	8	0	4.269351	2.319667	0.165735
25	8	0	-4.269374	2.320069	0.165404
26	8	0	-4.269350	-2.319667	-0.165746
27	6	0	-6.094935	0.000107	-0.000037
28	6	0	6.094935	-0.000108	0.000046
29	6	0	6.791705	-0.933003	0.776840
30	6	0	8.187042	-0.933633	0.766183
31	6	0	8.888678	0.000222	-0.000278
32	6	0	8.186655	0.933921	-0.766570
33	6	0	6.791315	0.932960	-0.776897
34	6	0	-6.791715	0.933008	-0.776815
35	6	0	-8.187052	0.933636	-0.766143
36	6	0	-8.888678	-0.000226	0.000319
37	6	0	-8.186646	-0.933930	0.766595
38	6	0	-6.791306	-0.932968	0.776907
39	1	0	-2.151332	-3.385109	-0.257827
40	1	0	-0.000189	-4.615104	-0.352290
41	1	0	2.150542	-3.385854	-0.257413
42	1	0	2.151332	3.385111	0.257808
43	1	0	0.000189	4.615105	0.352275
44	1	0	-2.150542	3.385856	0.257398
45	1	0	6.250058	-1.656856	1.364833
46	1	0	8.722565	-1.661146	1.360680
47	1	0	9.970156	0.000340	-0.000415
48	1	0	8.721874	1.661552	-1.361197
49	1	0	6.249372	1.656679	-1.364791

50	1	0	-6.250076	1.656866	-1.364807
51	1	0	-8.722582	1.661153	-1.360628
52	1	0	-9.970156	-0.000345	0.000467
53	1	0	-8.721858	-1.661565	1.361223
54	1	0	-6.249357	-1.656692	1.364788

---

m-PyDI2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.684869	-0.192128	0.000006
2	6	0	0.684870	0.192127	-0.000000
3	6	0	1.702733	-0.815177	0.000009
4	6	0	1.327029	-2.196445	0.000029
5	6	0	0.018403	-2.554643	0.000024
6	6	0	-1.030112	-1.579848	0.000015
7	6	0	-1.702731	0.815178	0.000010
8	6	0	-1.327022	2.196457	-0.000004
9	6	0	-0.018401	2.554651	-0.000006
10	6	0	1.030120	1.579846	0.000006
11	6	0	2.381141	1.965979	-0.000024
12	6	0	3.343824	0.981276	-0.000029
13	6	0	3.027145	-0.373818	-0.000011
14	6	0	-2.381140	-1.965978	-0.000000
15	6	0	-3.343819	-0.981270	-0.000003

16	6	0	-3.027147	0.373824	0.000003
17	6	0	4.830454	1.119775	-0.000025
18	7	0	5.328549	-0.186667	-0.000011
19	6	0	4.304245	-1.141588	-0.000024
20	6	0	-4.830453	-1.119775	-0.000003
21	7	0	-5.328550	0.186661	-0.000031
22	6	0	-4.304252	1.141588	0.000025
23	8	0	-5.496154	-2.128343	-0.000010
24	8	0	-4.486781	2.339110	0.000056
25	8	0	4.486768	-2.339111	-0.000011
26	8	0	5.496162	2.128339	0.000015
27	6	0	6.739844	-0.525340	0.000020
28	6	0	-6.739857	0.525331	-0.000030
29	1	0	2.110324	-2.939203	0.000038
30	1	0	-0.257626	-3.600620	0.000020
31	1	0	-2.110326	2.939206	-0.000000
32	1	0	0.257644	3.600623	-0.000005
33	1	0	2.657508	3.011173	-0.000036
34	1	0	-2.657512	-3.011171	-0.000016
35	1	0	6.989892	-1.106048	-0.886080
36	1	0	7.302348	0.403572	0.003525
37	1	0	6.988105	-1.111921	0.882703
38	1	0	-7.302345	-0.403588	-0.003893
39	1	0	-6.988035	1.112204	-0.882539
40	1	0	-6.989966	1.105740	0.886247

---

p-PyDI2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.671811	-0.241580	-0.001285
2	6	0	-0.671811	0.241579	-0.001286
3	6	0	-1.763555	-0.695482	-0.001594
4	6	0	-1.484691	-2.104784	-0.001766
5	6	0	-0.199053	-2.557001	-0.001529
6	6	0	0.919570	-1.655967	-0.001168
7	6	0	1.763555	0.695482	-0.001591
8	6	0	1.484691	2.104784	-0.001763
9	6	0	0.199053	2.557001	-0.001527
10	6	0	-0.919570	1.655967	-0.001168
11	6	0	-2.246740	2.135746	0.000465
12	6	0	-3.279699	1.219278	0.001485
13	6	0	-3.058142	-0.161326	-0.003429
14	6	0	2.246740	-2.135746	0.000467
15	6	0	3.279699	-1.219278	0.001489
16	6	0	3.058142	0.161326	-0.003425
17	6	0	-4.743148	1.467809	0.001586
18	7	0	-5.356575	0.187628	-0.000650
19	6	0	-4.373607	-0.842753	-0.002758
20	6	0	4.743148	-1.467809	0.001592
21	7	0	5.356575	-0.187628	-0.000643
22	6	0	4.373607	0.842753	-0.002752

23	8	0	5.329524	-2.554968	0.008013
24	8	0	4.615790	2.057379	-0.008544
25	8	0	-4.615790	-2.057379	-0.008552
26	8	0	-5.329524	2.554968	0.008008
27	6	0	-6.772524	-0.038210	0.000758
28	6	0	6.772524	0.038210	0.000767
29	6	0	7.600860	-0.742291	0.816542
30	6	0	8.979227	-0.525553	0.807458
31	6	0	9.533229	0.473014	0.002629
32	6	0	8.700036	1.252976	-0.803187
33	6	0	7.321772	1.035630	-0.814176
34	6	0	-7.600861	0.742290	0.816533
35	6	0	-8.979228	0.525552	0.807447
36	6	0	-9.533229	-0.473014	0.002616
37	6	0	-8.700035	-1.252975	-0.803200
38	6	0	-7.321771	-1.035629	-0.814188
39	1	0	-2.319840	-2.788632	-0.001154
40	1	0	0.002516	-3.620160	-0.001288
41	1	0	2.319840	2.788632	-0.001149
42	1	0	-0.002516	3.620160	-0.001286
43	1	0	-2.451315	3.197733	0.002026
44	1	0	2.451315	-3.197733	0.002027
45	1	0	7.175164	-1.518399	1.432153
46	1	0	9.616536	-1.135816	1.432710
47	1	0	10.601543	0.641260	0.003239
48	1	0	9.119835	2.029382	-1.428103
49	1	0	6.678933	1.642916	-1.430860

50	1	0	-7.175165	1.518397	1.432146
51	1	0	-9.616537	1.135814	1.432698
52	1	0	-10.601543	-0.641260	0.003224
53	1	0	-9.119834	-2.029379	-1.428119
54	1	0	-6.678931	-1.642914	-1.430871

---

m-PDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.880787	2.425085	0.000431
2	6	0	-3.577284	1.227380	0.000214
3	6	0	-2.864482	0.001123	-0.000007
4	6	0	-1.433392	0.001007	-0.000008
5	6	0	-0.735592	1.252335	0.000088
6	6	0	-1.481800	2.434212	0.000363
7	6	0	-3.576238	-1.225428	-0.000231
8	6	0	-2.880793	-2.423455	-0.000454
9	6	0	-1.481720	-2.432551	-0.000389
10	6	0	-0.735626	-1.250547	-0.000105
11	6	0	0.735623	-1.250547	0.000094
12	6	0	1.433389	0.001007	-0.000004
13	6	0	0.735591	1.252336	-0.000103
14	6	0	2.864479	0.001126	0.000001
15	6	0	3.577283	1.227388	-0.000216

16	6	0	2.880785	2.425092	-0.000435
17	6	0	1.481797	2.434215	-0.000375
18	6	0	1.481722	-2.432550	0.000381
19	6	0	2.880794	-2.423448	0.000450
20	6	0	3.576236	-1.225420	0.000226
21	6	0	-5.053087	1.245915	0.000240
22	7	0	-5.706039	0.001935	-0.000018
23	6	0	-5.050357	-1.237949	-0.000241
24	6	0	5.050365	-1.237953	0.000248
25	7	0	5.706039	0.001923	-0.000036
26	6	0	5.053081	1.245909	-0.000225
27	8	0	-5.703754	2.312307	0.000497
28	8	0	-5.714866	-2.295926	-0.000431
29	8	0	5.703772	2.312290	-0.000428
30	8	0	5.714859	-2.295934	0.000500
31	6	0	7.181937	-0.024910	-0.000039
32	6	0	-7.181938	-0.024919	-0.000002
33	1	0	-3.440895	3.348746	0.000643
34	1	0	-0.983845	3.391222	0.000543
35	1	0	-3.441436	-3.346884	-0.000668
36	1	0	-0.983594	-3.389473	-0.000579
37	1	0	3.440891	3.348753	-0.000638
38	1	0	0.983838	3.391222	-0.000560
39	1	0	0.983601	-3.389473	0.000572
40	1	0	3.441439	-3.346877	0.000668
41	1	0	7.530422	1.000613	-0.000738
42	1	0	7.540017	-0.550393	0.882572

43	1	0	7.539952	-0.551608	-0.881949
44	1	0	-7.539975	-0.551013	-0.882267
45	1	0	-7.530450	1.000597	0.000033
46	1	0	-7.539973	-0.551066	0.882231

---

p-PDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.880378	2.424111	-0.000462
2	6	0	-3.577135	1.226597	-0.000243
3	6	0	-2.865473	0.000001	-0.000024
4	6	0	-1.433791	0.000001	-0.000024
5	6	0	-0.735652	1.251181	-0.000125
6	6	0	-1.481464	2.433186	-0.000401
7	6	0	-3.577135	-1.226596	0.000196
8	6	0	-2.880376	-2.424109	0.000419
9	6	0	-1.481462	-2.433183	0.000357
10	6	0	-0.735651	-1.251178	0.000078
11	6	0	0.735653	-1.251179	-0.000114
12	6	0	1.433790	0.000001	-0.000024
13	6	0	0.735653	1.251181	0.000067
14	6	0	2.865470	0.000001	-0.000024
15	6	0	3.577135	1.226594	0.000180

16	6	0	2.880381	2.424112	0.000392
17	6	0	1.481467	2.433185	0.000335
18	6	0	1.481466	-2.433183	-0.000379
19	6	0	2.880380	-2.424110	-0.000434
20	6	0	3.577135	-1.226593	-0.000226
21	6	0	-5.052896	1.248585	-0.000263
22	7	0	-5.711216	0.000000	-0.000011
23	6	0	-5.052895	-1.248584	0.000216
24	6	0	5.052895	-1.248582	-0.000249
25	7	0	5.711222	-0.000000	-0.000011
26	6	0	5.052896	1.248583	0.000204
27	8	0	-5.703815	2.310439	-0.000484
28	8	0	-5.703814	-2.310439	0.000498
29	8	0	5.703812	2.310439	0.000426
30	8	0	5.703812	-2.310438	-0.000413
31	6	0	7.167114	-0.000000	0.000015
32	6	0	-7.167123	-0.000001	0.000015
33	6	0	-7.855128	0.000696	1.212080
34	6	0	-9.251007	0.000700	1.210007
35	6	0	-9.949912	-0.000003	0.000066
36	6	0	-9.251051	-0.000705	-1.209900
37	6	0	-7.855171	-0.000699	-1.212024
38	6	0	7.855126	-0.000582	1.212076
39	6	0	9.251005	-0.000590	1.210003
40	6	0	9.949914	-0.000003	0.000065
41	6	0	9.251049	0.000585	-1.209897
42	6	0	7.855169	0.000580	-1.212020

43	1	0	-3.440707	3.347684	-0.000668
44	1	0	-0.983399	3.390141	-0.000593
45	1	0	-3.440706	-3.347683	0.000627
46	1	0	-0.983397	-3.390138	0.000551
47	1	0	3.440711	3.347685	0.000585
48	1	0	0.983403	3.390141	0.000528
49	1	0	0.983401	-3.390138	-0.000570
50	1	0	3.440709	-3.347683	-0.000625
51	1	0	-7.304016	0.001235	2.141798
52	1	0	-9.788772	0.001251	2.148225
53	1	0	-11.031539	-0.000004	0.000086
54	1	0	-9.788849	-0.001257	-2.148099
55	1	0	-7.304094	-0.001236	-2.141762
56	1	0	7.304030	-0.001023	2.141804
57	1	0	9.788757	-0.001054	2.148229
58	1	0	11.031541	-0.000005	0.000085
59	1	0	9.788834	0.001047	-2.148104
60	1	0	7.304106	0.001022	-2.141768

---

m-CorDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.947704	-0.785579
2	6	0	1.146933	1.119946	-0.875371

3	6	0	0.708939	-0.222370	-1.033874
4	6	0	-0.708941	-0.222369	-1.033879
5	6	0	-1.146934	1.119947	-0.875371
6	6	0	-2.374135	1.478376	-0.332097
7	6	0	-2.448847	2.841134	0.163357
8	6	0	-1.316681	3.642250	0.254310
9	6	0	0.000000	3.170018	-0.136328
10	6	0	-1.457241	-1.334063	-0.668056
11	6	0	-2.801631	-0.983848	-0.297398
12	6	0	-3.233070	0.342409	-0.137667
13	6	0	1.457238	-1.334064	-0.668047
14	6	0	0.694228	-2.557564	-0.486099
15	6	0	-0.694236	-2.557565	-0.486120
16	6	0	2.374134	1.478376	-0.332099
17	6	0	3.233066	0.342409	-0.137663
18	6	0	2.801625	-0.983848	-0.297386
19	6	0	1.316684	3.642253	0.254298
20	6	0	2.448849	2.841136	0.163351
21	6	0	-3.914511	-1.880351	0.119961
22	7	0	-4.978365	-1.044385	0.504735
23	6	0	-4.627929	0.309366	0.385164
24	6	0	4.627932	0.309364	0.385149
25	7	0	4.978364	-1.044387	0.504728
26	6	0	3.914513	-1.880353	0.119953
27	8	0	5.364304	1.262400	0.678289
28	8	0	3.937251	-3.118946	0.147456
29	8	0	-5.364268	1.262407	0.678369

30	8	0	-3.937222	-3.118943	0.147564
31	6	0	6.274942	-1.521932	0.971420
32	6	0	-6.274988	-1.521936	0.971290
33	1	0	-3.391843	3.208641	0.541505
34	1	0	-1.414746	4.620533	0.707550
35	1	0	1.222850	-3.474092	-0.267708
36	1	0	-1.222861	-3.474091	-0.267727
37	1	0	1.414750	4.620537	0.707535
38	1	0	3.391846	3.208646	0.541492
39	1	0	6.500565	-1.104839	1.951384
40	1	0	7.063566	-1.234908	0.276771
41	1	0	6.223106	-2.605612	1.035221
42	1	0	-7.063117	-1.238445	0.274600
43	1	0	-6.221926	-2.605320	1.038983
44	1	0	-6.502345	-1.101539	1.949419

---

p-CorDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000011	2.615388	-0.599338
2	6	0	-1.146776	1.824706	-0.859660
3	6	0	-0.708807	0.544713	-1.294992
4	6	0	0.708780	0.544719	-1.295016
5	6	0	1.146755	1.824706	-0.859675

6	6	0	2.374074	2.062540	-0.254823
7	6	0	2.449101	3.292157	0.513305
8	6	0	1.316747	4.056622	0.769674
9	6	0	-0.000002	3.676025	0.289910
10	6	0	1.457057	-0.618636	-1.170201
11	6	0	2.801540	-0.351987	-0.733414
12	6	0	3.233531	0.910305	-0.305568
13	6	0	-1.457094	-0.618636	-1.170190
14	6	0	-0.694365	-1.853034	-1.248228
15	6	0	0.694328	-1.853030	-1.248245
16	6	0	-2.374082	2.062539	-0.254787
17	6	0	-3.233561	0.910323	-0.305532
18	6	0	-2.801569	-0.351982	-0.733369
19	6	0	-1.316741	4.056619	0.769703
20	6	0	-2.449101	3.292162	0.513328
21	6	0	3.909910	-1.317257	-0.521056
22	7	0	4.992531	-0.582877	0.030190
23	6	0	4.626258	0.777322	0.194773
24	6	0	-4.626320	0.777352	0.194760
25	7	0	-4.992514	-0.582857	0.030229
26	6	0	-3.909923	-1.317275	-0.520948
27	8	0	-5.343437	1.666848	0.669089
28	8	0	-3.907132	-2.531345	-0.757441
29	8	0	5.343316	1.666879	0.669091
30	8	0	3.907049	-2.531321	-0.757585
31	6	0	6.269705	-1.135827	0.375432
32	6	0	-6.269674	-1.135810	0.375491

33	6	0	-7.439755	-0.434333	0.060930
34	6	0	-8.679944	-0.972486	0.406283
35	6	0	-8.759726	-2.211384	1.047220
36	6	0	-7.588368	-2.909722	1.350496
37	6	0	-6.341614	-2.373885	1.025114
38	6	0	7.439751	-0.433633	0.062248
39	6	0	8.679940	-0.971829	0.407536
40	6	0	8.759831	-2.211402	1.047145
41	6	0	7.588536	-2.910409	1.349097
42	6	0	6.341762	-2.374640	1.023681
43	1	0	3.392046	3.572994	0.959391
44	1	0	1.415169	4.918936	1.416759
45	1	0	-1.223039	-2.794800	-1.228423
46	1	0	1.223005	-2.794795	-1.228438
47	1	0	-1.415156	4.918932	1.416788
48	1	0	-3.392042	3.572999	0.959428
49	1	0	-7.378702	0.524320	-0.429235
50	1	0	-9.581344	-0.424063	0.169178
51	1	0	-9.723420	-2.627775	1.307023
52	1	0	-7.640688	-3.870388	1.844357
53	1	0	-5.438247	-2.916354	1.253757
54	1	0	7.378692	0.525569	-0.426811
55	1	0	9.581269	-0.422852	0.171438
56	1	0	9.723532	-2.627783	1.306936
57	1	0	7.640896	-3.871604	1.841928
58	1	0	5.438504	-2.917709	1.251262

---

m-BAzDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.515639	-1.134788	-0.235209
2	6	0	1.105610	-2.522211	-0.501298
3	7	0	0.009170	-3.087320	0.186204
4	6	0	-1.174261	-2.491271	0.644233
5	6	0	-1.546138	-1.118471	0.267280
6	6	0	-0.717901	0.004515	0.049402
7	6	0	0.717920	-0.004445	0.049390
8	6	0	-1.515653	1.134791	-0.235322
9	6	0	-1.105603	2.522217	-0.501217
10	7	0	-0.009444	3.087277	0.186747
11	6	0	1.174424	2.491439	0.643977
12	6	0	1.546190	1.118577	0.267085
13	6	0	2.897504	0.701734	0.124265
14	6	0	2.876191	-0.725104	-0.234083
15	6	0	-2.897456	-0.701712	0.124406
16	6	0	-2.876184	0.725069	-0.234217
17	6	0	4.022894	1.516325	0.260500
18	6	0	5.367907	1.202112	0.101606
19	6	0	5.952408	-0.016671	-0.224657
20	6	0	5.331982	-1.234532	-0.483262
21	6	0	3.977272	-1.544523	-0.490017

22	6	0	-4.022794	-1.516329	0.260848
23	6	0	-5.367809	-1.202220	0.101807
24	6	0	-5.952333	0.016465	-0.224821
25	6	0	-5.331968	1.234303	-0.483671
26	6	0	-3.977272	1.544389	-0.490395
27	8	0	1.950494	3.192969	1.282586
28	8	0	-1.788856	3.254293	-1.202589
29	8	0	1.789060	-3.254121	-1.202656
30	8	0	-1.949970	-3.192681	1.283404
31	6	0	0.043967	-4.552562	0.355924
32	6	0	-0.044755	4.552492	0.356567
33	1	0	3.808903	2.535918	0.542605
34	1	0	6.054431	2.024329	0.259820
35	1	0	7.034256	-0.018042	-0.285394
36	1	0	5.994386	-2.058349	-0.717613
37	1	0	3.730813	-2.564177	-0.744666
38	1	0	-3.808755	-2.535822	0.543306
39	1	0	-6.054317	-2.024413	0.260209
40	1	0	-7.034175	0.017759	-0.285665
41	1	0	-5.994413	2.058019	-0.718267
42	1	0	-3.730841	2.564002	-0.745256
43	1	0	1.021407	-4.906057	0.057972
44	1	0	-0.715665	-5.027173	-0.263098
45	1	0	-0.163056	-4.791218	1.393976
46	1	0	0.166994	4.791163	1.393611
47	1	0	0.711359	5.027952	-0.266152
48	1	0	-1.023911	4.905187	0.063280

---

p-BAzDI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.124685	-1.533512	-0.256952
2	6	0	-2.503519	-1.142797	-0.589244
3	7	0	-3.091578	0.000057	0.000012
4	6	0	-2.503467	1.142929	0.589165
5	6	0	-1.124622	1.533559	0.256840
6	6	0	-0.000001	0.718788	0.000005
7	6	0	-0.000037	-0.718795	-0.000044
8	6	0	1.124661	1.533505	-0.256813
9	6	0	2.503489	1.142848	-0.589146
10	7	0	3.091562	-0.000063	-0.000006
11	6	0	2.503447	-1.142999	0.589027
12	6	0	1.124601	-1.533566	0.256686
13	6	0	0.712167	-2.891242	0.183155
14	6	0	-0.712305	-2.891232	-0.183350
15	6	0	-0.712182	2.891252	0.183250
16	6	0	0.712289	2.891208	-0.183257
17	6	0	1.529146	-4.004946	0.385622
18	6	0	1.216794	-5.356792	0.301303
19	6	0	-0.000046	-5.959517	-0.000012
20	6	0	-1.216892	-5.356811	-0.301348

21	6	0	-1.529269	-4.004971	-0.385733
22	6	0	-1.529120	4.005008	0.385637
23	6	0	-1.216713	5.356839	0.301243
24	6	0	0.000148	5.959510	-0.000098
25	6	0	1.216974	5.356751	-0.301405
26	6	0	1.529295	4.004896	-0.385717
27	8	0	3.213018	-1.859486	1.276448
28	8	0	3.213133	1.859275	-1.276553
29	8	0	-3.213162	-1.859027	-1.276857
30	8	0	-3.213053	1.859257	1.276738
31	6	0	-4.545224	0.000056	0.000064
32	6	0	4.545208	-0.000053	0.000054
33	6	0	-5.232718	-0.610087	1.039788
34	6	0	-6.622762	-0.609553	1.038492
35	6	0	-7.319760	0.000031	0.000162
36	6	0	-6.622845	0.609627	-1.038219
37	6	0	-5.232802	0.610184	-1.039613
38	6	0	5.232693	0.609993	1.039842
39	6	0	6.622736	0.609468	1.038554
40	6	0	7.319745	-0.000013	0.000168
41	6	0	6.622838	-0.609513	-1.038274
42	6	0	5.232795	-0.610077	-1.039677
43	1	0	2.547426	-3.774056	0.660440
44	1	0	2.038014	-6.032800	0.503655
45	1	0	-0.000043	-7.043076	0.000020
46	1	0	-2.038108	-6.032839	-0.503648
47	1	0	-2.547560	-3.774123	-0.660526

48	1	0	-2.547413	3.774183	0.660445
49	1	0	-2.037912	6.032889	0.503542
50	1	0	0.000180	7.043069	-0.000132
51	1	0	2.038212	6.032738	-0.503752
52	1	0	2.547573	3.773985	-0.660521
53	1	0	-4.681953	-1.072792	1.846369
54	1	0	-7.159619	-1.081006	1.850065
55	1	0	-8.401065	0.000022	0.000200
56	1	0	-7.159767	1.081069	-1.849754
57	1	0	-4.682103	1.072898	-1.846234
58	1	0	4.681921	1.072615	1.846465
59	1	0	7.159587	1.080844	1.850176
60	1	0	8.401050	0.000003	0.000212
61	1	0	7.159767	-1.080874	-1.849853
62	1	0	4.682103	-1.072715	-1.846346
