Supporting Information for

Tandem Scholl Reaction for the Synthesis of Twisted Nanographenes

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Cartesian coordinates

(*P*)-**1a** (B3LYP/6-31G(d,p), gas phase) $E = -1936.826074$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.427326	-3.150500	-0.249017
2	6	0	-2.444428	-1.736621	-0.417939
3	6	0	-1.218828	-1.033114	-0.463593
4	6	0	-0.013440	-1.702935	-0.005262
5	6	0	-0.019275	-3.130550	-0.008562
6	6	0	-1.246830	-3.830174	-0.143315
7	6	0	1.197892	-1.044956	0.455769
8	6	0	2.418341	-1.757919	0.405322
9	6	0	2.389080	-3.171365	0.229271
10	6	0	1.203154	-3.840630	0.121862
11	6	0	3.689061	-1.043745	0.541718
12	6	0	-3.710163	-1.010705	-0.550136
13	6	0	4.920800	-1.665616	0.228015
14	6	0	6.137122	-0.996495	0.266474
15	6	0	6.110055	0.367721	0.630548
16	6	0	4.924994	1.002754	0.944277
17	6	0	3.689810	0.320423	0.922212
18	6	0	-3.699542	0.358227	-0.923616
19	6	0	-4.925545	1.049810	-0.938861
20	6	0	-6.121767	0.425324	-0.627009
21	6	0	-6.159731	-0.936433	-0.272842
22	6	0	-4.944742	-1.617229	-0.239743
23	6	0	2.435121	0.945920	1.322897
24	6	0	2.403030	2.195995	1.978428
25	6	0	1.225298	2.739069	2.450034
26	6	0	0.002121	2.043776	2.330934
27	6	0	0.026831	0.827073	1.663403
28	6	0	1.205631	0.268929	1.111760
29	6	0	-2.438243	0.973287	-1.323295

30	6	0	-1.215403	0.284328	-1.114971
31	6	0	-0.032019	0.832562	-1.665947
32	6	0	0.003808	2.051054	-2.330257
33	6	0	-1.212700	2.757728	-2.447074
34	6	0	-2.395272	2.224034	-1.976104
35	6	0	-1.280048	2.646205	2.931802
36	6	0	-1.063762	2.941274	4.435204
37	6	0	-2.491535	1.704891	2.801729
38	6	0	-1.606841	3.965626	2.191426
39	6	0	1.291531	2.643011	-2.929721
40	6	0	1.630730	3.957390	-2.185992
41	6	0	2.494160	1.690026	-2.802228
42	6	0	1.077896	2.943974	-4.432331
43	6	0	7.476533	-1.667890	-0.084542
44	6	0	8.118545	-0.938192	-1.288625
45	6	0	7.312444	-3.153357	-0.456242
46	6	0	8.426881	-1.578794	1.133466
47	6	0	-7.464749	-1.669827	0.091842
48	6	0	-7.381396	-2.180830	1.549829
49	6	0	-7.665872	-2.871662	-0.861362
50	6	0	-8.699274	-0.755709	-0.025464
51	1	0	-3.354266	-3.708563	-0.295692
52	1	0	-1.233028	-4.916442	-0.127298
53	1	0	3.311205	-3.737540	0.272113
54	1	0	1.180549	-4.926662	0.100275
55	1	0	4.908750	-2.698157	-0.090528
56	1	0	7.031883	0.940540	0.659768
57	1	0	4.953991	2.056016	1.199587
58	1	0	-4.945567	2.104850	-1.187908
59	1	0	-7.032831	1.011288	-0.653909
60	1	0	-4.948413	-2.653504	0.074932
61	1	0	3.327796	2.732851	2.156737
62	1	0	1.258455	3.700704	2.952798
63	1	0	-0.886280	0.257919	1.576812
64	1	0	0.875861	0.254838	-1.581270
65	1	0	-1.237436	3.720811	-2.947549

66	1	0	-3.315504	2.769179	-2.152895
67	1	0	-0.246497	3.648450	4.604105
68	1	0	-1.971093	3.375297	4.870027
69	1	0	-0.830272	2.023339	4.984515
70	1	0	-3.369606	2.171959	3.259677
71	1	0	-2.738967	1.495113	1.757424
72	1	0	-2.320973	0.751441	3.312509
73	1	0	-0.794513	4.693476	2.282397
74	1	0	-1.774674	3.781931	1.125483
75	1	0	-2.512183	4.422343	2.607614
76	1	0	0.825165	4.692958	-2.274963
77	1	0	1.796977	3.769412	-1.120542
78	1	0	2.540227	4.406746	-2.601136
79	1	0	3.376632	2.150131	-3.258757
80	1	0	2.739445	1.474880	-1.758497
81	1	0	2.314700	0.739678	-3.315742
82	1	0	0.267290	3.659230	-4.599283
83	1	0	0.835706	2.029694	-4.983968
84	1	0	1.989222	3.370555	-4.866167
85	1	0	8.304520	0.118142	-1.073686
86	1	0	9.078826	-1.399187	-1.545962
87	1	0	7.469586	-0.990438	-2.168819
88	1	0	6.679123	-3.285649	-1.339571
89	1	0	8.291497	-3.585595	-0.686396
90	1	0	6.881045	-3.733809	0.365905
91	1	0	8.002486	-2.096809	1.999595
92	1	0	8.618926	-0.542418	1.426145
93	1	0	9.391689	-2.042322	0.898676
94	1	0	-7.243844	-1.349427	2.248718
95	1	0	-8.303416	-2.706277	1.823393
96	1	0	-6.548325	-2.875565	1.691252
97	1	0	-7.735165	-2.538906	-1.902077
98	1	0	-6.841008	-3.587096	-0.795059
99	1	0	-8.589974	-3.405512	-0.612479
100	1	0	-8.641246	0.098655	0.656731
101	1	0	-8.827980	-0.373178	-1.043268

102	1	0	-9.601314	-1.320346	0.231202

TS between (*P*)-**1a** and (*M*)-**1a** (B3LYP/6-31G(d,p), gas phase) $E = -1936.749024$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.038305	-1.760424	2.644956
2	6	0	2.110966	-1.177819	1.350003
3	6	0	1.270972	-0.079747	1.040160
4	6	0	-0.032050	-0.045130	1.709379
5	6	0	-0.141646	-0.803719	2.923817
6	6	0	0.985187	-1.479123	3.466597
7	6	0	-1.292351	0.285236	1.041683
8	6	0	-2.416160	-0.516227	1.357234
9	6	0	-2.507576	-1.097251	2.651447
10	6	0	-1.413454	-1.131703	3.467345
11	6	0	-3.395482	-0.821970	0.309323
12	6	0	2.937922	-1.767739	0.292724
13	6	0	-4.318272	-1.881831	0.453824
14	6	0	-5.129267	-2.318649	-0.588947
15	6	0	-4.989477	-1.668861	-1.834336
16	6	0	-4.106818	-0.617073	-2.001095
17	6	0	-3.309559	-0.157835	-0.937145
18	6	0	3.034171	-1.111710	-0.956522
19	6	0	3.629236	-1.794451	-2.032370
20	6	0	4.152114	-3.065314	-1.873297
21	6	0	4.115222	-3.722819	-0.624673
22	6	0	3.497424	-3.057484	0.429849
23	6	0	-2.519767	1.066060	-0.983841
24	6	0	-2.838634	2.101548	-1.882440
25	6	0	-2.452818	3.403602	-1.632896
26	6	0	-1.747774	3.736971	-0.458014
27	6	0	-1.238347	2.681851	0.299022
28	6	0	-1.579417	1.332094	0.045251

29	6	0	2.665711	0.298000	-0.990033
30	6	0	1.862243	0.841478	0.046562
31	6	0	1.976635	2.230694	0.312306
32	6	0	2.811281	3.068434	-0.431581
33	6	0	3.376695	2.533194	-1.608207
34	6	0	3.307990	1.181921	-1.877290
35	6	0	-1.672718	5.214194	-0.023819
36	6	0	-3.062932	5.880440	-0.180656
37	6	0	-0.662200	5.966603	-0.915217
38	6	0	-1.285498	5.357756	1.460861
39	6	0	3.336649	4.432005	0.066732
40	6	0	3.302274	5.502993	-1.047634
41	6	0	2.573891	4.965355	1.289223
42	6	0	4.813744	4.222479	0.494712
43	6	0	-6.130160	-3.478818	-0.441150
44	6	0	-7.554189	-2.969719	-0.769174
45	6	0	-6.148217	-4.064313	0.983191
46	6	0	-5.753782	-4.613559	-1.423432
47	6	0	4.720160	-5.131515	-0.485481
48	6	0	3.995817	-6.102229	-1.448375
49	6	0	4.591512	-5.689853	0.944073
50	6	0	6.223849	-5.079357	-0.847168
51	1	0	2.818411	-2.438241	2.972664
52	1	0	0.908611	-1.930133	4.451729
53	1	0	-3.447782	-1.521254	2.985328
54	1	0	-1.465496	-1.588337	4.451526
55	1	0	-4.360636	-2.400922	1.401430
56	1	0	-5.580659	-1.993924	-2.684988
57	1	0	-4.026897	-0.144277	-2.974825
58	1	0	3.675791	-1.321868	-3.008448
59	1	0	4.596524	-3.558142	-2.732601
60	1	0	3.398987	-3.562468	1.380937
61	1	0	-3.505127	1.902884	-2.715027
62	1	0	-2.792702	4.184824	-2.304785
63	1	0	-0.673078	2.887188	1.198229
64	1	0	1.505745	2.604202	1.212708

65	1	0	3.975847	3.161474	-2.258785
66	1	0	3.876755	0.783762	-2.710880
67	1	0	-3.824228	5.344948	0.395391
68	1	0	-3.022542	6.912067	0.186341
69	1	0	-3.394366	5.919010	-1.221505
70	1	0	-0.583322	7.018743	-0.617926
71	1	0	0.328341	5.513550	-0.846329
72	1	0	-0.965887	5.935928	-1.966761
73	1	0	-2.022055	4.868286	2.106429
74	1	0	-0.308206	4.930505	1.690259
75	1	0	-1.250382	6.417326	1.734817
76	1	0	3.944539	5.239016	-1.892359
77	1	0	2.291888	5.656270	-1.434597
78	1	0	3.662490	6.460592	-0.656097
79	1	0	3.021576	5.907313	1.622559
80	1	0	1.527258	5.163904	1.057168
81	1	0	2.615085	4.269089	2.132694
82	1	0	5.428142	3.872384	-0.339805
83	1	0	4.886320	3.481005	1.296734
84	1	0	5.241171	5.163806	0.859618
85	1	0	-7.621632	-2.574697	-1.787006
86	1	0	-8.280876	-3.785152	-0.679833
87	1	0	-7.852305	-2.171690	-0.081423
88	1	0	-6.427012	-3.312532	1.728900
89	1	0	-6.883619	-4.873321	1.039527
90	1	0	-5.176631	-4.483283	1.264743
91	1	0	-4.751040	-4.997987	-1.210625
92	1	0	-5.766540	-4.273737	-2.463113
93	1	0	-6.462826	-5.444662	-1.336372
94	1	0	4.087783	-5.786107	-2.491524
95	1	0	4.421417	-7.108862	-1.367085
96	1	0	2.928739	-6.163783	-1.211490
97	1	0	5.101317	-5.055248	1.676436
98	1	0	3.545142	-5.793739	1.249202
99	1	0	5.048348	-6.683484	0.993911
100	1	0	6.385138	-4.726569	-1.869952

101	1	0	6.765103	-4.407181	-0.173407
102	1	0	6.670931	-6.076495	-0.764632

(*P*,*P*)-**2** (B3LYP/6-31G(d,p), gas phase) $E = -3871.268665$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.860650	2.450193	-0.089987
2	6	0	-1.455309	2.402397	-0.226357
3	6	0	-0.733757	1.236278	-0.050107
4	6	0	-1.452539	0.000004	0.000036
5	6	0	-2.882175	0.000012	0.000057
6	6	0	-3.561016	1.261668	0.216864
7	6	0	-0.733770	-1.236278	0.050159
8	6	0	-1.455330	-2.402390	0.226424
9	6	0	-2.860674	-2.450172	0.090081
10	6	0	-3.561035	-1.261636	-0.216739
11	6	0	-3.595307	3.709144	-0.246232
12	6	0	-4.873262	1.388736	0.857408
13	6	0	-5.417776	0.346211	1.646226
14	6	0	-6.633540	0.450654	2.307734
15	6	0	-7.341363	1.664580	2.168658
16	6	0	-6.812521	2.721828	1.455816
17	6	0	-5.564897	2.627621	0.803111
18	6	0	-4.957833	3.773082	0.133293
19	6	0	-5.659161	4.972079	-0.115636
20	6	0	-5.043945	6.065849	-0.691866
21	6	0	-3.682790	6.029983	-1.065577
22	6	0	-2.994379	4.845477	-0.835148
23	6	0	-4.873297	-1.388680	-0.857249
24	6	0	-5.564950	-2.627554	-0.802945
25	6	0	-6.812600	-2.721730	-1.455605
26	6	0	-7.341452	-1.664461	-2.168409
27	6	0	-6.633610	-0.450547	-2.307498

28	6	0	-5.417820	-0.346133	-1.646033
29	6	0	-4.957879	-3.773034	-0.133163
30	6	0	-3.595341	-3.709119	0.246322
31	6	0	-2.994408	-4.845474	0.835191
32	6	0	-3.682827	-6.029975	1.065618
33	6	0	-5.043996	-6.065814	0.691955
34	6	0	-5.659216	-4.972025	0.115767
35	6	0	2.860634	-2.450189	-0.090529
36	6	0	1.455289	-2.402366	-0.226842
37	6	0	0.733744	-1.236277	-0.050358
38	6	0	1.452527	-0.000013	-0.000012
39	6	0	2.882164	-0.000023	-0.000044
40	6	0	3.561013	-1.261718	0.216500
41	6	0	0.733759	1.236260	0.050366
42	6	0	1.455326	2.402337	0.226837
43	6	0	2.860667	2.450141	0.090479
44	6	0	3.561019	1.261668	-0.216606
45	6	0	3.595284	-3.709115	-0.247021
46	6	0	4.873291	-1.388895	0.856955
47	6	0	5.417850	-0.346498	1.645911
48	6	0	6.633659	-0.451044	2.307321
49	6	0	7.341478	-1.664945	2.168000
50	6	0	6.812592	-2.722078	1.455019
51	6	0	5.564928	-2.627767	0.802408
52	6	0	4.957829	-3.773117	0.132428
53	6	0	5.659146	-4.972070	-0.116740
54	6	0	5.043902	-6.065742	-0.693126
55	6	0	3.682729	-6.029815	-1.066761
56	6	0	2.994328	-4.845349	-0.836098
57	6	0	4.873264	1.388846	-0.857130
58	6	0	5.564915	2.627712	-0.802591
59	6	0	6.812533	2.722035	-1.455286
60	6	0	7.341355	1.664925	-2.168349
61	6	0	6.633518	0.451034	-2.307662
62	6	0	5.417759	0.346472	-1.646158
63	6	0	4.957868	3.773048	-0.132540

64	6	0	3.595344	3.709049	0.246979
65	6	0	2.994432	4.845265	0.836138
66	6	0	3.682860	6.029715	1.066806
67	6	0	5.044012	6.065641	0.693091
68	6	0	5.659212	4.971983	0.116631
69	6	0	-3.035353	7.265037	-1.716252
70	6	0	-3.035384	-7.265052	1.716243
71	6	0	3.035262	-7.264760	-1.717611
72	6	0	3.035446	7.264640	1.717747
73	6	0	-7.222244	-0.682139	3.166848
74	6	0	-7.222331	0.682272	-3.166568
75	6	0	7.222201	-0.681592	-3.167008
76	6	0	7.222422	0.681615	3.166571
77	1	0	-0.921171	3.327068	-0.394087
78	1	0	-0.921194	-3.327066	0.394141
79	1	0	-4.838286	-0.558804	1.750681
80	1	0	-8.302611	1.793361	2.656479
81	1	0	-7.360137	3.657261	1.435666
82	1	0	-6.711726	5.042320	0.134577
83	1	0	-5.631136	6.962466	-0.865129
84	1	0	-1.963948	4.774666	-1.154076
85	1	0	-7.360230	-3.657154	-1.435450
86	1	0	-8.302722	-1.793216	-2.656193
87	1	0	-4.838322	0.558877	-1.750489
88	1	0	-1.963964	-4.774688	1.154080
89	1	0	-5.631194	-6.962425	0.865223
90	1	0	-6.711790	-5.042246	-0.134412
91	1	0	0.921142	-3.327005	-0.394718
92	1	0	0.921202	3.326987	0.394735
93	1	0	4.838363	0.558498	1.750555
94	1	0	8.302761	-1.793799	2.655732
95	1	0	7.360209	-3.657505	1.434677
96	1	0	6.711723	-5.042353	0.133407
97	1	0	5.631087	-6.962328	-0.866576
98	1	0	1.963880	-4.774488	-1.154960
99	1	0	7.360162	3.657456	-1.434946

100	1	0	8.302602	1.793790	-2.656147
101	1	0	4.838256	-0.558514	-1.750792
102	1	0	1.964004	4.774395	1.155063
103	1	0	5.631215	6.962215	0.866537
104	1	0	6.711776	5.042265	-0.133575
105	6	0	-6.268265	1.884184	-3.292550
106	1	0	-6.056298	2.344666	-2.323572
107	1	0	-5.316406	1.599836	-3.753148
108	1	0	-6.725751	2.650423	-3.926925
109	6	0	-8.538342	1.171021	-2.514673
110	1	0	-8.984909	1.973931	-3.112425
111	1	0	-9.274990	0.365451	-2.435370
112	1	0	-8.353268	1.556238	-1.506929
113	6	0	-7.519369	0.157092	-4.591371
114	1	0	-8.234920	-0.670265	-4.586062
115	1	0	-7.943915	0.956854	-5.208471
116	1	0	-6.603781	-0.195972	-5.077038
117	6	0	-6.268249	-1.884119	3.292702
118	1	0	-6.056555	-2.344704	2.323713
119	1	0	-5.316254	-1.599810	3.753044
120	1	0	-6.725645	-2.650263	3.927255
121	6	0	-8.538359	-1.170793	2.515080
122	1	0	-8.984945	-1.973637	3.112908
123	1	0	-9.274939	-0.365156	2.435818
124	1	0	-8.353406	-1.556070	1.507339
125	6	0	-7.519100	-0.156967	4.591688
126	1	0	-8.234613	0.670423	4.586471
127	1	0	-7.943610	-0.956720	5.208825
128	1	0	-6.603444	0.196051	5.077262
129	6	0	-1.549552	7.043178	-2.054885
130	1	0	-0.957256	6.818661	-1.161409
131	1	0	-1.410483	6.227750	-2.772053
132	1	0	-1.134735	7.950674	-2.504989
133	6	0	-3.133455	8.464677	-0.743660
134	1	0	-2.687142	9.358093	-1.194649
135	1	0	-4.171128	8.702725	-0.492302

136	1	0	-2.603574	8.254725	0.191153
137	6	0	-3.782143	7.607286	-3.027642
138	1	0	-4.840481	7.819929	-2.850634
139	1	0	-3.339310	8.492044	-3.498712
140	1	0	-3.722762	6.777553	-3.739353
141	6	0	-1.549567	-7.043223	2.054826
142	1	0	-0.957303	-6.818693	1.161332
143	1	0	-1.410459	-6.227815	2.772009
144	1	0	-1.134746	-7.950736	2.504892
145	6	0	-3.133541	-8.464672	0.743632
146	1	0	-2.687224	-9.358103	1.194587
147	1	0	-4.171227	-8.702700	0.492308
148	1	0	-2.603692	-8.254709	-0.191196
149	6	0	-3.782132	-7.607315	3.027655
150	1	0	-4.840479	-7.819938	2.850681
151	1	0	-3.339296	-8.492090	3.498690
152	1	0	-3.722711	-6.777598	3.739380
153	6	0	1.549637	7.042740	2.056322
154	1	0	0.957344	6.818423	1.162794
155	1	0	1.410546	6.227165	2.773318
156	1	0	1.134836	7.950149	2.506616
157	6	0	3.782237	7.606588	3.029214
158	1	0	4.840578	7.819254	2.852256
159	1	0	3.339413	8.491246	3.500479
160	1	0	3.722843	6.776697	3.740741
161	6	0	3.133579	8.464490	0.745415
162	1	0	2.687294	9.357820	1.196601
163	1	0	4.171258	8.702565	0.494107
164	1	0	2.603688	8.254756	-0.189441
165	6	0	3.781980	-7.606783	-3.029099
166	1	0	4.840328	-7.819454	-2.852186
167	1	0	3.339119	-8.491457	-3.500299
168	1	0	3.722561	-6.776925	-3.740663
169	6	0	3.133426	-8.464565	-0.745225
170	1	0	2.687105	-9.357910	-1.196345
171	1	0	4.171115	-8.702642	-0.493958

172	1	0	2.603586	-8.254775	0.189647
173	6	0	1.549438	-7.042856	-2.056121
174	1	0	0.957197	-6.818468	-1.162576
175	1	0	1.410322	-6.227328	-2.773166
176	1	0	1.134597	-7.950288	-2.506331
177	6	0	7.519370	0.156228	4.591312
178	1	0	8.234904	-0.671141	4.585929
179	1	0	7.943884	0.955898	5.208553
180	1	0	6.603746	-0.196892	5.076874
181	6	0	8.538497	1.170361	2.514787
182	1	0	8.985133	1.973105	3.112711
183	1	0	9.275065	0.364731	2.435340
184	1	0	8.353471	1.555801	1.507121
185	6	0	6.268453	1.883590	3.292676
186	1	0	6.056733	2.344355	2.323779
187	1	0	5.316470	1.599217	3.753004
188	1	0	6.725886	2.649610	3.927352
189	6	0	7.518932	-0.156186	-4.591784
190	1	0	8.234467	0.671183	-4.586503
191	1	0	7.943346	-0.955848	-5.209103
192	1	0	6.603236	0.196945	-5.077204
193	6	0	8.538389	-1.170299	-2.515413
194	1	0	8.984998	-1.972979	-3.113443
195	1	0	9.274915	-0.364627	-2.436017
196	1	0	8.353510	-1.555811	-1.507749
197	6	0	6.268260	-1.883600	-3.292989
198	1	0	6.056852	-2.344507	-2.324092
199	1	0	5.316124	-1.599214	-3.752994
200	1	0	6.725545	-2.649511	-3.927903

(*P*,*M*)-**2** (B3LYP/6-31G(d,p), gas phase) $E = -3871.266586$

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

1	6	0	2.838416	-2.448392	0.066713
2	6	0	1.429169	-2.413430	-0.031757
3	6	0	0.710752	-1.236432	0.071555
4	6	0	1.429204	0.000011	0.000011
5	6	0	2.859356	0.000017	0.000006
6	6	0	3.540068	-1.243646	0.294918
7	6	0	0.710742	1.236450	-0.071526
8	6	0	1.429148	2.413454	0.031775
9	6	0	2.838395	2.448428	-0.066717
10	6	0	3.540053	1.243686	-0.294916
11	6	0	3.579310	-3.708184	-0.041372
12	6	0	4.853169	-1.332861	0.940514
13	6	0	5.397404	-0.246393	1.667579
14	6	0	6.608906	-0.315666	2.341780
15	6	0	7.312528	-1.538387	2.281011
16	6	0	6.785004	-2.634090	1.627511
17	6	0	5.542581	-2.573945	0.961694
18	6	0	4.940643	-3.751286	0.344818
19	6	0	5.647826	-4.955539	0.144948
20	6	0	5.042096	-6.068825	-0.403627
21	6	0	3.686825	-6.048143	-0.798894
22	6	0	2.988446	-4.862372	-0.604565
23	6	0	4.853154	1.332902	-0.940520
24	6	0	5.542564	2.573987	-0.961714
25	6	0	6.784993	2.634119	-1.627519
26	6	0	7.312517	1.538404	-2.281002
27	6	0	6.608899	0.315685	-2.341760
28	6	0	5.397388	0.246424	-1.667571
29	6	0	4.940615	3.751332	-0.344859
30	6	0	3.579284	3.708227	0.041339
31	6	0	2.988415	4.862423	0.604509
32	6	0	3.686786	6.048203	0.798814
33	6	0	5.042055	6.068886	0.403542
34	6	0	5.647788	4.955594	-0.145017
35	6	0	-2.869229	2.327514	-0.786245
36	6	0	-1.475986	2.355155	-0.538931

37	6	0	-0.753568	1.219761	-0.225194
38	6	0	-1.466861	-0.000002	0.000017
39	6	0	-2.891878	-0.000014	0.000004
40	6	0	-3.565525	1.104562	-0.654812
41	6	0	-0.753558	-1.219756	0.225236
42	6	0	-1.475963	-2.355156	0.538989
43	6	0	-2.869207	-2.327533	0.786293
44	6	0	-3.565523	-1.104594	0.654812
45	6	0	-3.594158	3.543544	-1.171359
46	6	0	-4.864649	0.972457	-1.321659
47	6	0	-5.401934	-0.293911	-1.659929
48	6	0	-6.609342	-0.454544	-2.324785
49	6	0	-7.316065	0.718021	-2.670331
50	6	0	-6.792004	1.968367	-2.412341
51	6	0	-5.552385	2.134942	-1.757753
52	6	0	-4.947262	3.450278	-1.580307
53	6	0	-5.643461	4.647683	-1.851247
54	6	0	-5.031747	5.880995	-1.754309
55	6	0	-3.678296	5.998778	-1.371039
56	6	0	-2.996952	4.822975	-1.082700
57	6	0	-4.864677	-0.972509	1.321604
58	6	0	-5.552420	-2.135005	1.757654
59	6	0	-6.792074	-1.968454	2.412182
60	6	0	-7.316168	-0.718116	2.670151
61	6	0	-6.609440	0.454462	2.324652
62	6	0	-5.401997	0.293850	1.659858
63	6	0	-4.947262	-3.450330	1.580252
64	6	0	-3.594119	-3.543569	1.171423
65	6	0	-2.996866	-4.822987	1.082893
66	6	0	-3.678209	-5.998798	1.371206
67	6	0	-5.031711	-5.881043	1.754301
68	6	0	-5.643467	-4.647744	1.851137
69	6	0	3.058567	-7.300617	-1.434764
70	6	0	3.058520	7.300688	1.434656
71	6	0	-3.031847	7.391687	-1.275834
72	6	0	-3.031700	-7.391689	1.276144

73	6	0	7.197101	0.864559	3.134958
74	6	0	7.197079	-0.864531	-3.134946
75	6	0	-7.190140	1.831968	2.689212
76	6	0	-7.190008	-1.832055	-2.689355
77	1	0	0.896249	-3.351906	-0.103606
78	1	0	0.896219	3.351924	0.103628
79	1	0	4.820712	0.665298	1.713989
80	1	0	8.269615	-1.641241	2.782949
81	1	0	7.329116	-3.571115	1.665509
82	1	0	6.698435	-5.013093	0.406620
83	1	0	5.634131	-6.968152	-0.542875
84	1	0	1.961826	-4.800497	-0.938829
85	1	0	7.329128	3.571131	-1.665506
86	1	0	8.269607	1.641253	-2.782939
87	1	0	4.820697	-0.665267	-1.713959
88	1	0	1.961797	4.800544	0.938778
89	1	0	5.634083	6.968221	0.542769
90	1	0	6.698394	5.013155	-0.406703
91	1	0	-0.941284	3.278947	-0.708442
92	1	0	-0.941246	-3.278938	0.708496
93	1	0	-4.824193	-1.169124	-1.404763
94	1	0	-8.271347	0.647912	-3.181322
95	1	0	-7.337705	2.837898	-2.760146
96	1	0	-6.689398	4.610588	-2.133340
97	1	0	-5.614086	6.770703	-1.973283
98	1	0	-1.972325	4.890553	-0.746313
99	1	0	-7.337766	-2.837998	2.759968
100	1	0	-8.271478	-0.648024	3.181090
101	1	0	-4.824260	1.169074	1.404722
102	1	0	-1.972192	-4.890558	0.746649
103	1	0	-5.614055	-6.770762	1.973219
104	1	0	-6.689438	-4.610660	2.133102
105	6	0	-3.093666	-8.078299	2.661644
106	1	0	-4.122807	-8.192507	3.014363
107	1	0	-2.646083	-9.077298	2.612003
108	1	0	-2.546626	-7.497237	3.411054

109	6	0	-1.556826	-7.327880	0.838945
110	1	0	-1.447745	-6.883795	-0.155968
111	1	0	-0.947593	-6.751531	1.543006
112	1	0	-1.141266	-8.339574	0.794208
113	6	0	-3.802636	-8.249650	0.244679
114	1	0	-3.358895	-9.249013	0.172658
115	1	0	-4.853961	-8.372737	0.520489
116	1	0	-3.769709	-7.790535	-0.748695
117	6	0	3.112238	-8.467970	-0.420384
118	1	0	2.682422	-9.375262	-0.859697
119	1	0	4.138287	-8.698352	-0.118812
120	1	0	2.545093	-8.226339	0.484422
121	6	0	1.589446	-7.081354	-1.839667
122	1	0	0.963350	-6.829569	-0.977807
123	1	0	1.486194	-6.285074	-2.584072
124	1	0	1.187685	-7.999057	-2.280988
125	6	0	3.852606	-7.689545	-2.704754
126	1	0	4.901064	-7.906996	-2.481518
127	1	0	3.418846	-8.584271	-3.165278
128	1	0	3.828948	-6.881732	-3.443273
129	6	0	8.518147	1.309250	2.462123
130	1	0	8.964869	2.144655	3.013425
131	1	0	9.252015	0.497736	2.434478
132	1	0	8.339489	1.634665	1.432366
133	6	0	6.246671	2.074897	3.183901
134	1	0	6.041621	2.477726	2.188148
135	1	0	5.291300	1.821433	3.655144
136	1	0	6.703406	2.876018	3.774208
137	6	0	7.484780	0.424597	4.590224
138	1	0	8.197881	-0.403451	4.638505
139	1	0	7.908326	1.258649	5.160862
140	1	0	6.565480	0.103570	5.090858
141	6	0	7.484594	-0.424605	-4.590239
142	1	0	8.197642	0.403482	-4.638617
143	1	0	7.908107	-1.258660	-5.160895
144	1	0	6.565236	-0.103626	-5.090811

145	6	0	6.246743	-2.074947	-3.183701
146	1	0	6.041904	-2.477777	-2.187903
147	1	0	5.291262	-1.821572	-3.654772
148	1	0	6.703435	-2.876034	-3.774083
149	6	0	8.518247	-1.309113	-2.462221
150	1	0	8.964955	-2.144504	-3.013563
151	1	0	9.252064	-0.497551	-2.434708
152	1	0	8.339712	-1.634517	-1.432447
153	6	0	-8.511824	2.038139	1.910536
154	1	0	-9.248789	1.265562	2.151164
155	1	0	-8.953679	3.009915	2.159137
156	1	0	-8.335329	2.008219	0.830637
157	6	0	-6.234930	2.986975	2.336629
158	1	0	-5.278721	2.897252	2.862614
159	1	0	-6.032248	3.039985	1.263300
160	1	0	-6.686413	3.939517	2.632712
161	6	0	-7.474258	1.894215	4.208867
162	1	0	-7.892477	2.871174	4.475888
163	1	0	-8.190499	1.131136	4.526999
164	1	0	-6.554469	1.750216	4.785118
165	6	0	1.589405	7.081420	1.839572
166	1	0	0.963297	6.829655	0.977715
167	1	0	1.486161	6.285121	2.583959
168	1	0	1.187650	7.999112	2.280920
169	6	0	3.852562	7.689665	2.704627
170	1	0	4.901013	7.907135	2.481379
171	1	0	3.418785	8.584392	3.165132
172	1	0	3.828929	6.881872	3.443168
173	6	0	3.112171	8.468012	0.420237
174	1	0	2.682357	9.375317	0.859529
175	1	0	4.138216	8.698389	0.118647
176	1	0	2.545016	8.226349	-0.484553
177	6	0	-3.802960	8.249594	-0.244459
178	1	0	-3.359256	9.248966	-0.172338
179	1	0	-4.854248	8.372662	-0.520419
180	1	0	-3.770170	7.790450	0.748907

181	6	0	-3.093632	8.078337	-2.661324
182	1	0	-4.122726	8.192520	-3.014190
183	1	0	-2.646094	9.077351	-2.611588
184	1	0	-2.546461	7.497316	-3.410671
185	6	0	-1.557037	7.327909	-0.838420
186	1	0	-1.448087	6.883778	0.156487
187	1	0	-0.947680	6.751616	-1.542420
188	1	0	-1.141517	8.339614	-0.793572
189	6	0	-6.234792	-2.987051	-2.336760
190	1	0	-5.278543	-2.897268	-2.862665
191	1	0	-6.032188	-3.040117	-1.263419
192	1	0	-6.686222	-3.939589	-2.632930
193	6	0	-8.511704	-2.038231	-1.910662
194	1	0	-9.248658	-1.265650	-2.151304
195	1	0	-8.953558	-3.010005	-2.159285
196	1	0	-8.335195	-2.008328	-0.830770
197	6	0	-7.474156	-1.894304	-4.208993
198	1	0	-7.892348	-2.871276	-4.475999
199	1	0	-8.190420	-1.131245	-4.527120
200	1	0	-6.554388	-1.750286	-4.785282

TS between (*P*,*P*)-**2** and (*P*,*M*)-**2** (B3LYP/6-31G(d,p), gas phase) $E = -3871.194719$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.967856	-2.119404	0.836598
2	6	0	-1.555966	-2.154939	0.825627
3	6	0	-0.817254	-1.170086	0.202193
4	6	0	-1.521909	0.026116	-0.143866
5	6	0	-2.945747	0.029866	-0.312341
6	6	0	-3.641565	-1.225940	-0.033768
7	6	0	-0.777742	1.245636	-0.058783
8	6	0	-1.482026	2.363582	0.340449
9	6	0	-2.893882	2.374729	0.363663

10	6	0	-3.600046	1.335642	-0.290844
11	6	0	-3.749672	-2.897814	1.804034
12	6	0	-4.959104	-1.717233	-0.477946
13	6	0	-5.298201	-1.766464	-1.855211
14	6	0	-6.374651	-2.517121	-2.333646
15	6	0	-7.256237	-3.061505	-1.376186
16	6	0	-6.940841	-3.052191	-0.032911
17	6	0	-5.733004	-2.494621	0.424833
18	6	0	-5.159347	-2.913022	1.698150
19	6	0	-5.907144	-3.473480	2.749234
20	6	0	-5.286078	-4.035864	3.850030
21	6	0	-3.879258	-4.074620	3.959074
22	6	0	-3.142711	-3.493164	2.931333
23	6	0	-4.909555	1.747415	-0.817587
24	6	0	-5.658633	2.725637	-0.111467
25	6	0	-6.872640	3.167353	-0.668914
26	6	0	-7.214960	2.853761	-1.969718
27	6	0	-6.346773	2.100057	-2.786154
28	6	0	-5.265225	1.479258	-2.161097
29	6	0	-5.055533	3.414562	1.023201
30	6	0	-3.645552	3.376096	1.129399
31	6	0	-3.010649	4.195238	2.088371
32	6	0	-3.718057	5.026136	2.951795
33	6	0	-5.126113	5.013284	2.853714
34	6	0	-5.774425	4.231346	1.914767
35	6	0	2.800650	2.363776	-0.659001
36	6	0	1.414803	2.383003	-0.374342
37	6	0	0.685478	1.226539	-0.186517
38	6	0	1.383502	-0.019462	-0.115489
39	6	0	2.803447	-0.058489	-0.240974
40	6	0	3.467540	1.121170	-0.763563
41	6	0	0.644583	-1.225917	0.090521
42	6	0	1.327726	-2.425177	0.107976
43	6	0	2.740114	-2.481533	0.169964
44	6	0	3.479180	-1.275276	0.169645
45	6	0	3.543978	3.610982	-0.859767

46	6	0	4.718137	1.080983	-1.529163
47	6	0	5.189608	-0.117696	-2.118287
48	6	0	6.342489	-0.183996	-2.888420
49	6	0	7.063376	1.015563	-3.075561
50	6	0	6.600559	2.212213	-2.566718
51	6	0	5.414119	2.287382	-1.806098
52	6	0	4.867903	3.563994	-1.358712
53	6	0	5.586986	4.775268	-1.444882
54	6	0	5.022773	5.981454	-1.079332
55	6	0	3.698996	6.054917	-0.593634
56	6	0	2.995658	4.861486	-0.491823
57	6	0	4.839472	-1.306717	0.715829
58	6	0	5.508298	-2.549623	0.869311
59	6	0	6.806125	-2.543014	1.424135
60	6	0	7.408312	-1.376673	1.850982
61	6	0	6.730872	-0.139451	1.785604
62	6	0	5.464009	-0.139179	1.218751
63	6	0	4.831640	-3.790956	0.509540
64	6	0	3.443132	-3.766649	0.232793
65	6	0	2.780273	-4.984710	-0.045240
66	6	0	3.431200	-6.211591	-0.068910
67	6	0	4.818742	-6.208726	0.192668
68	6	0	5.493922	-5.036588	0.469312
69	6	0	-3.226420	-4.716705	5.196427
70	6	0	-3.033426	5.916096	4.004692
71	6	0	3.106895	7.415775	-0.187090
72	6	0	2.714419	-7.536823	-0.381910
73	6	0	-6.528245	-2.974040	-3.800041
74	6	0	-6.573383	2.088285	-4.311000
75	6	0	7.405936	1.130342	2.333121
76	6	0	6.849524	-1.487237	-3.530661
77	1	0	-1.043649	-2.957877	1.341590
78	1	0	-0.944606	3.245853	0.665430
79	1	0	-4.604181	-1.316925	-2.553904
80	1	0	-8.143743	-3.596935	-1.696577
81	1	0	-7.571747	-3.601837	0.657482

82	1	0	-6.991530	-3.459386	2.704054
83	1	0	-5.902573	-4.450541	4.641682
84	1	0	-2.065523	-3.451876	3.018030
85	1	0	-7.492464	3.867165	-0.118544
86	1	0	-8.118733	3.284638	-2.387588
87	1	0	-4.581015	0.875105	-2.741706
88	1	0	-1.934888	4.137477	2.182743
89	1	0	-5.721965	5.623632	3.525421
90	1	0	-6.858889	4.246383	1.873852
91	1	0	0.886700	3.326088	-0.423601
92	1	0	0.756752	-3.343615	0.142441
93	1	0	4.601973	-1.011911	-1.975428
94	1	0	7.978713	1.015747	-3.659268
95	1	0	7.149430	3.118396	-2.796544
96	1	0	6.613770	4.768612	-1.792801
97	1	0	5.621656	6.883275	-1.162359
98	1	0	1.997005	4.882576	-0.079265
99	1	0	7.337740	-3.478216	1.558402
100	1	0	8.406105	-1.429521	2.275488
101	1	0	4.908317	0.785411	1.175481
102	1	0	1.726857	-4.954038	-0.284582
103	1	0	5.377712	-7.139234	0.170011
104	1	0	6.562728	-5.084123	0.644681
105	6	0	-6.890551	3.521023	-4.808453
106	1	0	-7.826916	3.909524	-4.399769
107	1	0	-6.090717	4.218211	-4.539533
108	1	0	-6.987787	3.520515	-5.899765
109	6	0	-7.768512	1.172513	-4.650488
110	1	0	-7.943621	1.140551	-5.732089
111	1	0	-7.589267	0.154372	-4.300232
112	1	0	-8.686203	1.529038	-4.171243
113	6	0	-5.315916	1.629611	-5.074891
114	1	0	-5.003626	0.617258	-4.814296
115	1	0	-5.510423	1.642956	-6.152334
116	1	0	-4.472024	2.298778	-4.877758
117	6	0	-6.164027	-4.481723	-3.850832

118	1	0	-5.134297	-4.646013	-3.517706
119	1	0	-6.821088	-5.076249	-3.209475
120	1	0	-6.256349	-4.860730	-4.875366
121	6	0	-5.585091	-2.238598	-4.764491
122	1	0	-5.709260	-2.634634	-5.777643
123	1	0	-5.799022	-1.170060	-4.801725
124	1	0	-4.534031	-2.371435	-4.489635
125	6	0	-7.981244	-2.808152	-4.301567
126	1	0	-8.317948	-1.770475	-4.237339
127	1	0	-8.052969	-3.122132	-5.348601
128	1	0	-8.685777	-3.421210	-3.732723
129	6	0	-1.687963	-4.672119	5.141473
130	1	0	-1.295934	-5.203202	4.267856
131	1	0	-1.309188	-3.645236	5.116874
132	1	0	-1.273520	-5.153491	6.033028
133	6	0	-3.661164	-6.198803	5.291708
134	1	0	-3.214230	-6.671140	6.173770
135	1	0	-4.747124	-6.301074	5.374561
136	1	0	-3.340032	-6.758388	4.407107
137	6	0	-3.684971	-3.966317	6.469572
138	1	0	-4.771394	-3.998932	6.593248
139	1	0	-3.234893	-4.417477	7.361110
140	1	0	-3.384805	-2.914176	6.432377
141	6	0	-1.497861	5.804606	3.962914
142	1	0	-1.155934	4.787280	4.179168
143	1	0	-1.094241	6.102972	2.989548
144	1	0	-1.060114	6.465566	4.717841
145	6	0	-3.507961	5.501860	5.417993
146	1	0	-3.035297	6.132655	6.179351
147	1	0	-4.591533	5.601876	5.529743
148	1	0	-3.245596	4.460069	5.628510
149	6	0	-3.414936	7.393992	3.749711
150	1	0	-4.495965	7.551647	3.805385
151	1	0	-2.945095	8.043414	4.496997
152	1	0	-3.081205	7.718828	2.758818
153	6	0	1.207943	-7.346720	-0.638829

154	1	0	0.697296	-6.917142	0.229274
155	1	0	1.018918	-6.700774	-1.502395
156	1	0	0.744525	-8.316456	-0.846559
157	6	0	3.341654	-8.175514	-1.644076
158	1	0	4.408535	-8.377734	-1.511710
159	1	0	2.848939	-9.126687	-1.875068
160	1	0	3.231942	-7.516400	-2.511328
161	6	0	2.880234	-8.502198	0.816115
162	1	0	2.384936	-9.457092	0.607194
163	1	0	3.932512	-8.713279	1.027758
164	1	0	2.435754	-8.079975	1.723223
165	6	0	3.112525	8.360722	-1.412586
166	1	0	2.502853	7.951701	-2.224717
167	1	0	2.703963	9.340406	-1.140336
168	1	0	4.122869	8.518479	-1.801105
169	6	0	1.657700	7.300547	0.321667
170	1	0	1.280929	8.293380	0.587380
171	1	0	0.989513	6.887910	-0.441264
172	1	0	1.588309	6.672560	1.216201
173	6	0	3.965651	8.035670	0.940971
174	1	0	3.974006	7.390632	1.825572
175	1	0	5.003023	8.186080	0.628198
176	1	0	3.562266	9.011227	1.234957
177	6	0	7.024511	-1.285059	-5.054673
178	1	0	7.742759	-0.493417	-5.286909
179	1	0	7.388896	-2.208100	-5.519336
180	1	0	6.072254	-1.021155	-5.526270
181	6	0	8.214871	-1.855899	-2.901607
182	1	0	8.605298	-2.776850	-3.349802
183	1	0	8.958620	-1.068166	-3.057310
184	1	0	8.115816	-2.014950	-1.823142
185	6	0	5.882623	-2.666020	-3.315970
186	1	0	5.753311	-2.904256	-2.256621
187	1	0	4.895710	-2.464217	-3.745311
188	1	0	6.279695	-3.560267	-3.807429
189	6	0	7.811836	0.910338	3.809905

190	1	0	8.511699	0.077739	3.926193
191	1	0	8.298147	1.808536	4.206713
192	1	0	6.934301	0.698171	4.429411
193	6	0	8.670823	1.426589	1.491634
194	1	0	9.177745	2.322793	1.867500
195	1	0	9.385936	0.598903	1.529245
196	1	0	8.408787	1.595799	0.442408
197	6	0	6.484228	2.362154	2.271737
198	1	0	6.199123	2.611705	1.245865
199	1	0	5.569900	2.213940	2.855766
200	1	0	7.004678	3.230694	2.688469

3c' (B3LYP/6-31G(d,p), gas phase) $E = -2308.145241$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.753320	1.896384	-0.011096
2	6	0	0.394935	2.322010	0.118725
3	6	0	-0.652390	1.379265	0.298587
4	6	0	-0.373483	-0.017725	-0.000734
5	6	0	0.980453	-0.362695	-0.002314
6	6	0	2.067048	0.558576	0.024114
7	6	0	-1.292120	-1.109217	-0.299701
8	6	0	-0.832968	-2.445928	-0.140332
9	6	0	0.562701	-2.726048	-0.019236
10	6	0	1.463886	-1.694005	-0.034640
11	6	0	-1.806239	-3.541212	-0.111283
12	6	0	0.071006	3.751601	0.080023
13	6	0	-1.449175	-4.832440	0.341304
14	6	0	-2.366494	-5.866737	0.453692
15	6	0	-3.706955	-5.602976	0.109520
16	6	0	-4.087366	-4.352060	-0.334967
17	6	0	-3.156755	-3.298519	-0.469575
18	6	0	-1.220340	4.195457	0.464114

19	6	0	-1.528234	5.566732	0.326988
20	6	0	-0.601784	6.474321	-0.147395
21	6	0	0.689335	6.053536	-0.522098
22	6	0	0.995155	4.705588	-0.405425
23	6	0	-3.524099	-1.992445	-1.002324
24	6	0	-4.758749	-1.774561	-1.652794
25	6	0	-5.071847	-0.559673	-2.229171
26	6	0	-4.145611	0.501811	-2.212835
27	6	0	-2.935394	0.300868	-1.568576
28	6	0	-2.602520	-0.913440	-0.922777
29	6	0	-2.164235	3.234020	1.020562
30	6	0	-1.884261	1.843384	0.937587
31	6	0	-2.755240	0.942845	1.595207
32	6	0	-3.899583	1.355406	2.258831
33	6	0	-4.191355	2.733628	2.282593
34	6	0	-3.337257	3.643701	1.692017
35	6	0	-4.462347	1.808315	-2.899011
36	6	0	-4.801495	0.367176	2.957426
37	6	0	-1.956605	-7.232204	0.949559
38	6	0	1.694725	7.045708	-1.054313
39	6	0	3.305104	-0.250050	0.014664
40	6	0	2.927537	-1.606047	-0.019675
41	6	0	3.881153	-2.638192	-0.038622
42	6	0	5.216246	-2.306656	-0.031052
43	6	0	5.671345	-0.953668	0.009001
44	6	0	4.685169	0.101605	0.039591
45	6	0	7.048240	-0.608362	0.025365
46	6	0	7.452720	0.705742	0.077835
47	6	0	6.493336	1.741154	0.123117
48	6	0	5.150141	1.443304	0.105091
49	17	0	6.387127	-3.625461	-0.071094
50	1	0	2.522727	2.652595	-0.065580
51	1	0	0.902420	-3.754420	0.009246
52	1	0	-0.429745	-5.026170	0.655322
53	1	0	-4.451635	-6.389086	0.206041
54	1	0	-5.131792	-4.178596	-0.567947

55	1	0	-2.520526	5.921625	0.581148
56	1	0	-0.875795	7.521781	-0.245166
57	1	0	1.971986	4.379895	-0.744951
58	1	0	-5.469108	-2.588619	-1.740058
59	1	0	-6.027839	-0.432958	-2.731262
60	1	0	-2.204413	1.098540	-1.588484
61	1	0	-2.504509	-0.109861	1.608107
62	1	0	-5.079456	3.087352	2.800501
63	1	0	-3.561085	4.700352	1.783453
64	1	0	-4.651747	1.662404	-3.968958
65	1	0	-5.361601	2.269743	-2.474433
66	1	0	-3.641635	2.522708	-2.796693
67	1	0	-4.880958	0.586299	4.028678
68	1	0	-5.817572	0.400972	2.547194
69	1	0	-4.432779	-0.655939	2.849420
70	1	0	-2.132121	-8.000360	0.187181
71	1	0	-0.896238	-7.261604	1.214080
72	1	0	-2.531710	-7.524393	1.835709
73	1	0	1.933844	7.809275	-0.304690
74	1	0	2.629218	6.555880	-1.340840
75	1	0	1.308561	7.572311	-1.934604
76	1	0	3.578741	-3.679032	-0.067837
77	1	0	7.784178	-1.402952	-0.001444
78	1	0	8.511300	0.946513	0.090171
79	1	0	6.816857	2.776475	0.175840
80	1	0	4.429349	2.248428	0.156045

(*P*,*S*,*M*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.903612$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.031942	-2.119520	1.498844
2	6	0	-7.341476	-1.611562	1.232158
3	6	0	-7.552737	-0.620870	0.236428

4	6	0	-6.394913	0.111831	-0.255491
5	6	0	-5.164577	-0.514118	-0.040893
6	6	0	-4.948260	-1.644197	0.799891
7	6	0	-6.325613	1.398528	-0.937510
8	6	0	-5.157838	1.706357	-1.688330
9	6	0	-3.961285	0.943456	-1.519043
10	6	0	-3.945948	-0.105783	-0.638101
11	6	0	-5.187350	2.823973	-2.635921
12	6	0	-8.490467	-2.124791	1.984847
13	6	0	-4.178755	2.987829	-3.613613
14	6	0	-4.220603	3.989187	-4.572420
15	6	0	-5.323822	4.865415	-4.566856
16	6	0	-6.325414	4.731119	-3.625679
17	6	0	-6.281985	3.725804	-2.634843
18	6	0	-9.809036	-1.824246	1.556834
19	6	0	-10.890239	-2.255538	2.356223
20	6	0	-10.691569	-2.972877	3.519446
21	6	0	-9.389720	-3.291101	3.953449
22	6	0	-8.321181	-2.857621	3.182465
23	6	0	-7.292859	3.610845	-1.591125
24	6	0	-8.231915	4.637562	-1.348006
25	6	0	-9.135922	4.564044	-0.307073
26	6	0	-9.127573	3.464085	0.573212
27	6	0	-8.216304	2.447239	0.337290
28	6	0	-7.311093	2.465138	-0.750293
29	6	0	-10.001490	-1.120234	0.295035
30	6	0	-8.887484	-0.525201	-0.356201
31	6	0	-9.083653	0.040906	-1.638085
32	6	0	-10.324555	0.095751	-2.252395
33	6	0	-11.428278	-0.449140	-1.566850
34	6	0	-11.263345	-1.052022	-0.335671
35	6	0	-10.072660	3.414001	1.749035
36	6	0	-10.495070	0.700045	-3.624977
37	6	0	-3.133136	4.132012	-5.609510
38	6	0	-9.175220	-4.062512	5.233113
39	6	0	-3.505385	-1.960727	0.717191

40	6	0	-2.912999	-1.029172	-0.155606
41	6	0	-1.539333	-1.068724	-0.451279
42	6	0	-0.726126	-2.031703	0.119047
43	6	0	-1.291534	-2.993156	1.025802
44	6	0	-2.702831	-2.968260	1.325526
45	6	0	-0.481053	-3.977899	1.654077
46	6	0	-1.017661	-4.906818	2.516198
47	6	0	-2.402968	-4.897266	2.791930
48	6	0	-3.218878	-3.952473	2.212361
49	6	0	6.074649	-2.138535	-1.441209
50	6	0	7.335944	-1.471398	-1.350918
51	6	0	7.464409	-0.242635	-0.649974
52	6	0	6.392883	0.142233	0.257416
53	6	0	5.167131	-0.485789	0.023719
54	6	0	4.962275	-1.601855	-0.838354
55	6	0	6.406235	1.081863	1.371961
56	6	0	5.166714	1.603358	1.834563
57	6	0	3.932316	0.990364	1.456545
58	6	0	3.943272	-0.097254	0.623368
59	6	0	5.164382	2.775067	2.714872
60	6	0	8.516562	-2.050919	-1.999369
61	6	0	3.981783	3.511317	2.958385
62	6	0	3.963890	4.668473	3.722896
63	6	0	5.182564	5.123293	4.264049
64	6	0	6.354648	4.427006	4.043910
65	6	0	6.378976	3.238194	3.282092
66	6	0	9.699011	-1.279559	-2.137475
67	6	0	10.845786	-1.898206	-2.681754
68	6	0	10.831788	-3.215403	-3.096339
69	6	0	9.662939	-3.992851	-2.978758
70	6	0	8.536335	-3.397697	-2.430436
71	6	0	7.591944	2.451542	3.096813
72	6	0	8.752945	2.681149	3.867807
73	6	0	9.873269	1.882946	3.749854
74	6	0	9.880381	0.783301	2.869181
75	6	0	8.749533	0.555621	2.101465

76	6	0	7.603758	1.384196	2.158426
77	6	0	9.677407	0.126150	-1.752369
78	6	0	8.574525	0.637585	-1.016713
79	6	0	8.522531	2.029248	-0.766269
80	6	0	9.530006	2.899185	-1.151496
81	6	0	10.642807	2.365443	-1.831134
82	6	0	10.702763	1.019530	-2.133490
83	6	0	11.081068	-0.127700	2.787457
84	6	0	9.437123	4.380006	-0.874405
85	6	0	2.686330	5.437568	3.957094
86	6	0	9.654829	-5.436533	-3.419613
87	6	0	3.519413	-1.922221	-0.776917
88	6	0	2.915720	-1.008042	0.106373
89	6	0	1.538776	-1.055354	0.385548
90	6	0	0.737300	-2.020255	-0.198065
91	6	0	1.313301	-2.959382	-1.121601
92	6	0	2.723762	-2.911978	-1.422192
93	6	0	0.512429	-3.936240	-1.774043
94	6	0	1.055066	-4.827195	-2.671801
95	6	0	2.434850	-4.777793	-2.970106
96	6	0	3.242574	-3.843489	-2.362682
97	1	0	-5.932406	-2.930418	2.205492
98	1	0	-3.055815	1.244884	-2.031848
99	1	0	-3.353683	2.285721	-3.653348
100	1	0	-5.393033	5.647878	-5.318435
101	1	0	-7.171014	5.408294	-3.666457
102	1	0	-11.904559	-2.005785	2.066327
103	1	0	-11.547676	-3.283647	4.113065
104	1	0	-7.321023	-3.059842	3.548918
105	1	0	-8.224403	5.527661	-1.966592
106	1	0	-9.836670	5.379301	-0.144437
107	1	0	-8.178389	1.619801	1.033662
108	1	0	-8.225703	0.421230	-2.177041
109	1	0	-12.413263	-0.425583	-2.026610
110	1	0	-12.123040	-1.515618	0.134482
111	1	0	-9.936435	2.499994	2.332521

112	1	0	-11.117320	3.446087	1.418051
113	1	0	-9.922657	4.268368	2.419550
114	1	0	-10.897946	-0.030430	-4.336351
115	1	0	-11.194800	1.543697	-3.601187
116	1	0	-9.544811	1.066985	-4.020907
117	1	0	-2.631697	5.103609	-5.527694
118	1	0	-2.372070	3.354438	-5.502857
119	1	0	-3.539239	4.066823	-6.625538
120	1	0	-9.626396	-5.060171	5.175624
121	1	0	-8.111543	-4.189989	5.451432
122	1	0	-9.634339	-3.553243	6.088270
123	1	0	-1.106667	-0.342973	-1.133850
124	1	0	0.582292	-3.987277	1.442552
125	1	0	-0.376836	-5.648531	2.983445
126	1	0	-2.825826	-5.637359	3.465125
127	1	0	-4.278617	-3.964538	2.430828
128	1	0	6.008619	-3.028931	-2.049267
129	1	0	3.003865	1.342689	1.889624
130	1	0	3.050768	3.193252	2.503061
131	1	0	5.202215	6.037956	4.851343
132	1	0	7.277460	4.819269	4.455990
133	1	0	11.770034	-1.337451	-2.762896
134	1	0	11.735314	-3.660641	-3.505344
135	1	0	7.656100	-4.015905	-2.294380
136	1	0	8.759456	3.479135	4.601387
137	1	0	10.744603	2.083831	4.368370
138	1	0	7.647016	2.439129	-0.279744
139	1	0	11.445976	3.024856	-2.150863
140	1	0	11.543995	0.654423	-2.711488
141	1	0	10.925883	-0.929000	2.060645
142	1	0	11.977947	0.426527	2.486911
143	1	0	11.299767	-0.589302	3.757582
144	1	0	10.272793	4.718492	-0.250674
145	1	0	9.472631	4.963527	-1.801868
146	1	0	8.509960	4.631642	-0.353390
147	1	0	2.773607	6.472846	3.607734

148	1	0	1.840759	4.979127	3.437447
149	1	0	2.438847	5.480377	5.024358
150	1	0	8.689898	-5.911131	-3.222125
151	1	0	9.856926	-5.524783	-4.493658
152	1	0	10.426412	-6.016969	-2.900787
153	1	0	1.097424	-0.344527	1.078164
154	1	0	-0.549253	-3.967057	-1.556285
155	1	0	0.421282	-5.563013	-3.157623
156	1	0	2.858680	-5.474716	-3.687331
157	1	0	4.292908	-3.805668	-2.620439
158	1	0	8.734610	-0.311065	1.453684

TS (*ortho–peri*) between (*P*,*S*,*M*)-**4'** and (*M*,*R*,*P*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.867133$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.031942	-2.119520	1.498844
2	6	0	-7.341476	-1.611562	1.232158
3	6	0	-7.552737	-0.620870	0.236428
4	6	0	-6.394913	0.111831	-0.255491
5	6	0	-5.164577	-0.514118	-0.040893
6	6	0	-4.948260	-1.644197	0.799891
7	6	0	-6.325613	1.398528	-0.937510
8	6	0	-5.157838	1.706357	-1.688330
9	6	0	-3.961285	0.943456	-1.519043
10	6	0	-3.945948	-0.105783	-0.638101
11	6	0	-5.187350	2.823973	-2.635921
12	6	0	-8.490467	-2.124791	1.984847
13	6	0	-4.178755	2.987829	-3.613613
14	6	0	-4.220603	3.989187	-4.572420
15	6	0	-5.323822	4.865415	-4.566856
16	6	0	-6.325414	4.731119	-3.625679
17	6	0	-6.281985	3.725804	-2.634843
18	6	0	-9.809036	-1.824246	1.556834

19	6	0	-10.890239	-2.255538	2.356223
20	6	0	-10.691569	-2.972877	3.519446
21	6	0	-9.389720	-3.291101	3.953449
22	6	0	-8.321181	-2.857621	3.182465
23	6	0	-7.292859	3.610845	-1.591125
24	6	0	-8.231915	4.637562	-1.348006
25	6	0	-9.135922	4.564044	-0.307073
26	6	0	-9.127573	3.464085	0.573212
27	6	0	-8.216304	2.447239	0.337290
28	6	0	-7.311093	2.465138	-0.750293
29	6	0	-10.001490	-1.120234	0.295035
30	6	0	-8.887484	-0.525201	-0.356201
31	6	0	-9.083653	0.040906	-1.638085
32	6	0	-10.324555	0.095751	-2.252395
33	6	0	-11.428278	-0.449140	-1.566850
34	6	0	-11.263345	-1.052022	-0.335671
35	6	0	-10.072660	3.414001	1.749035
36	6	0	-10.495070	0.700045	-3.624977
37	6	0	-3.133136	4.132012	-5.609510
38	6	0	-9.175220	-4.062512	5.233113
39	6	0	-3.505385	-1.960727	0.717191
40	6	0	-2.912999	-1.029172	-0.155606
41	6	0	-1.539333	-1.068724	-0.451279
42	6	0	-0.726126	-2.031703	0.119047
43	6	0	-1.291534	-2.993156	1.025802
44	6	0	-2.702831	-2.968260	1.325526
45	6	0	-0.481053	-3.977899	1.654077
46	6	0	-1.017661	-4.906818	2.516198
47	6	0	-2.402968	-4.897266	2.791930
48	6	0	-3.218878	-3.952473	2.212361
49	6	0	6.074649	-2.138535	-1.441209
50	6	0	7.335944	-1.471398	-1.350918
51	6	0	7.464409	-0.242635	-0.649974
52	6	0	6.392883	0.142233	0.257416
53	6	0	5.167131	-0.485789	0.023719
54	6	0	4.962275	-1.601855	-0.838354

55	6	0	6.406235	1.081863	1.371961
56	6	0	5.166714	1.603358	1.834563
57	6	0	3.932316	0.990364	1.456545
58	6	0	3.943272	-0.097254	0.623368
59	6	0	5.164382	2.775067	2.714872
60	6	0	8.516562	-2.050919	-1.999369
61	6	0	3.981783	3.511317	2.958385
62	6	0	3.963890	4.668473	3.722896
63	6	0	5.182564	5.123293	4.264049
64	6	0	6.354648	4.427006	4.043910
65	6	0	6.378976	3.238194	3.282092
66	6	0	9.699011	-1.279559	-2.137475
67	6	0	10.845786	-1.898206	-2.681754
68	6	0	10.831788	-3.215403	-3.096339
69	6	0	9.662939	-3.992851	-2.978758
70	6	0	8.536335	-3.397697	-2.430436
71	6	0	7.591944	2.451542	3.096813
72	6	0	8.752945	2.681149	3.867807
73	6	0	9.873269	1.882946	3.749854
74	6	0	9.880381	0.783301	2.869181
75	6	0	8.749533	0.555621	2.101465
76	6	0	7.603758	1.384196	2.158426
77	6	0	9.677407	0.126150	-1.752369
78	6	0	8.574525	0.637585	-1.016713
79	6	0	8.522531	2.029248	-0.766269
80	6	0	9.530006	2.899185	-1.151496
81	6	0	10.642807	2.365443	-1.831134
82	6	0	10.702763	1.019530	-2.133490
83	6	0	11.081068	-0.127700	2.787457
84	6	0	9.437123	4.380006	-0.874405
85	6	0	2.686330	5.437568	3.957094
86	6	0	9.654829	-5.436533	-3.419613
87	6	0	3.519413	-1.922221	-0.776917
88	6	0	2.915720	-1.008042	0.106373
89	6	0	1.538776	-1.055354	0.385548
90	6	0	0.737300	-2.020255	-0.198065

91	6	0	1.313301	-2.959382	-1.121601
92	6	0	2.723762	-2.911978	-1.422192
93	6	0	0.512429	-3.936240	-1.774043
94	6	0	1.055066	-4.827195	-2.671801
95	6	0	2.434850	-4.777793	-2.970106
96	6	0	3.242574	-3.843489	-2.362682
97	1	0	-5.932406	-2.930418	2.205492
98	1	0	-3.055815	1.244884	-2.031848
99	1	0	-3.353683	2.285721	-3.653348
100	1	0	-5.393033	5.647878	-5.318435
101	1	0	-7.171014	5.408294	-3.666457
102	1	0	-11.904559	-2.005785	2.066327
103	1	0	-11.547676	-3.283647	4.113065
104	1	0	-7.321023	-3.059842	3.548918
105	1	0	-8.224403	5.527661	-1.966592
106	1	0	-9.836670	5.379301	-0.144437
107	1	0	-8.178389	1.619801	1.033662
108	1	0	-8.225703	0.421230	-2.177041
109	1	0	-12.413263	-0.425583	-2.026610
110	1	0	-12.123040	-1.515618	0.134482
111	1	0	-9.936435	2.499994	2.332521
112	1	0	-11.117320	3.446087	1.418051
113	1	0	-9.922657	4.268368	2.419550
114	1	0	-10.897946	-0.030430	-4.336351
115	1	0	-11.194800	1.543697	-3.601187
116	1	0	-9.544811	1.066985	-4.020907
117	1	0	-2.631697	5.103609	-5.527694
118	1	0	-2.372070	3.354438	-5.502857
119	1	0	-3.539239	4.066823	-6.625538
120	1	0	-9.626396	-5.060171	5.175624
121	1	0	-8.111543	-4.189989	5.451432
122	1	0	-9.634339	-3.553243	6.088270
123	1	0	-1.106667	-0.342973	-1.133850
124	1	0	0.582292	-3.987277	1.442552
125	1	0	-0.376836	-5.648531	2.983445
126	1	0	-2.825826	-5.637359	3.465125

127	1	0	-4.278617	-3.964538	2.430828
128	1	0	6.008619	-3.028931	-2.049267
129	1	0	3.003865	1.342689	1.889624
130	1	0	3.050768	3.193252	2.503061
131	1	0	5.202215	6.037956	4.851343
132	1	0	7.277460	4.819269	4.455990
133	1	0	11.770034	-1.337451	-2.762896
134	1	0	11.735314	-3.660641	-3.505344
135	1	0	7.656100	-4.015905	-2.294380
136	1	0	8.759456	3.479135	4.601387
137	1	0	10.744603	2.083831	4.368370
138	1	0	7.647016	2.439129	-0.279744
139	1	0	11.445976	3.024856	-2.150863
140	1	0	11.543995	0.654423	-2.711488
141	1	0	10.925883	-0.929000	2.060645
142	1	0	11.977947	0.426527	2.486911
143	1	0	11.299767	-0.589302	3.757582
144	1	0	10.272793	4.718492	-0.250674
145	1	0	9.472631	4.963527	-1.801868
146	1	0	8.509960	4.631642	-0.353390
147	1	0	2.773607	6.472846	3.607734
148	1	0	1.840759	4.979127	3.437447
149	1	0	2.438847	5.480377	5.024358
150	1	0	8.689898	-5.911131	-3.222125
151	1	0	9.856926	-5.524783	-4.493658
152	1	0	10.426412	-6.016969	-2.900787
153	1	0	1.097424	-0.344527	1.078164
154	1	0	-0.549253	-3.967057	-1.556285
155	1	0	0.421282	-5.563013	-3.157623
156	1	0	2.858680	-5.474716	-3.687331
157	1	0	4.292908	-3.805668	-2.620439
158	1	0	8.734610	-0.311065	1.453684

TS (*peri–peri*) between (*P*,*S*,*M*)-**4'** and (*M*,*R*,*P*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.851898$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.027077	2.479810	0.625506
2	6	0	7.066538	1.512067	0.464525
3	6	0	6.830926	0.296369	-0.232280
4	6	0	5.449563	-0.104646	-0.461716
5	6	0	4.515937	0.931696	-0.390561
6	6	0	4.776117	2.243019	0.106575
7	6	0	4.895788	-1.421971	-0.749735
8	6	0	3.600336	-1.500441	-1.331290
9	6	0	2.729008	-0.367319	-1.325963
10	6	0	3.159075	0.815274	-0.784577
11	6	0	3.155992	-2.763242	-1.927629
12	6	0	8.402259	1.775610	1.009165
13	6	0	2.025894	-2.819486	-2.775995
14	6	0	1.627305	-3.983615	-3.416246
15	6	0	2.395585	-5.146997	-3.213028
16	6	0	3.505569	-5.124150	-2.391637
17	6	0	3.907591	-3.948110	-1.721170
18	6	0	9.495474	0.954085	0.631794
19	6	0	10.747637	1.177733	1.245115
20	6	0	10.930431	2.180961	2.176333
21	6	0	9.859502	3.014990	2.553197
22	6	0	8.622134	2.792366	1.967121
23	6	0	5.033177	-3.919578	-0.795549
24	6	0	5.629831	-5.105443	-0.312981
25	6	0	6.640070	-5.080077	0.627768
26	6	0	7.089063	-3.857197	1.164224
27	6	0	6.516912	-2.687764	0.689530
28	6	0	5.517194	-2.673773	-0.311926
29	6	0	9.299176	-0.058814	-0.397929
30	6	0	7.982925	-0.384664	-0.822893
31	6	0	7.829729	-1.281127	-1.906942
32	6	0	8.903949	-1.899067	-2.526771
33	6	0	10.199220	-1.605804	-2.055977

34	6	0	10.386805	-0.700025	-1.030799
35	6	0	8.146850	-3.832657	2.240693
36	6	0	8.704052	-2.842889	-3.687542
37	6	0	0.420695	-4.009885	-4.322758
38	6	0	10.059193	4.101830	3.581531
39	6	0	3.508482	2.989653	-0.007410
40	6	0	2.537176	2.118372	-0.516589
41	6	0	1.196530	2.507451	-0.610797
42	6	0	0.733112	3.766152	-0.198226
43	6	0	1.780370	4.775248	-0.017417
44	6	0	3.157519	4.355273	0.180244
45	6	0	1.586184	6.176292	-0.132544
46	6	0	2.583578	7.101520	0.096658
47	6	0	3.878897	6.678134	0.442714
48	6	0	4.154711	5.330981	0.449680
49	6	0	-6.088875	2.462576	-0.584659
50	6	0	-7.051456	1.407314	-0.627441
51	6	0	-6.698958	0.079022	-0.265720
52	6	0	-5.455682	-0.125628	0.462824
53	6	0	-4.532812	0.918580	0.366673
54	6	0	-4.804141	2.215406	-0.160978
55	6	0	-5.023477	-1.260020	1.271526
56	6	0	-3.632210	-1.436361	1.504164
57	6	0	-2.709894	-0.376780	1.239196
58	6	0	-3.173280	0.818771	0.757155
59	6	0	-3.148071	-2.717825	2.025126
60	6	0	-8.423622	1.691207	-1.059904
61	6	0	-1.775317	-3.056102	1.991572
62	6	0	-1.297448	-4.290902	2.404957
63	6	0	-2.230621	-5.240527	2.866032
64	6	0	-3.577931	-4.940932	2.911058
65	6	0	-4.071085	-3.680474	2.508122
66	6	0	-9.311623	0.623193	-1.346690
67	6	0	-10.652033	0.930631	-1.667066
68	6	0	-11.102713	2.234673	-1.727377
69	6	0	-10.231860	3.308636	-1.458202

70	6	0	-8.917594	3.014628	-1.125835
71	6	0	-5.480062	-3.321859	2.610921
72	6	0	-6.396043	-4.104539	3.348213
73	6	0	-7.712791	-3.722351	3.510321
74	6	0	-8.180186	-2.510452	2.964465
75	6	0	-7.291610	-1.739966	2.231883
76	6	0	-5.949358	-2.125767	2.003458
77	6	0	-8.802281	-0.742596	-1.340173
78	6	0	-7.512305	-1.011036	-0.807704
79	6	0	-6.994798	-2.321879	-0.935099
80	6	0	-7.717634	-3.363770	-1.493838
81	6	0	-9.017966	-3.091846	-1.962776
82	6	0	-9.534464	-1.812912	-1.899520
83	6	0	-9.602717	-2.061887	3.195726
84	6	0	-7.128950	-4.747830	-1.620838
85	6	0	0.173493	-4.624689	2.349027
86	6	0	-10.730786	4.732301	-1.511055
87	6	0	-3.539726	2.973259	-0.069262
88	6	0	-2.558734	2.114037	0.443381
89	6	0	-1.217482	2.505693	0.510215
90	6	0	-0.762422	3.762440	0.083685
91	6	0	-1.815380	4.763818	-0.102791
92	6	0	-3.192461	4.336132	-0.285875
93	6	0	-1.624374	6.167244	-0.013017
94	6	0	-2.623124	7.086149	-0.259515
95	6	0	-3.915129	6.652415	-0.605202
96	6	0	-4.187989	5.304888	-0.585596
97	1	0	6.262819	3.416593	1.109988
98	1	0	1.711506	-0.472319	-1.683287
99	1	0	1.462252	-1.915300	-2.976255
100	1	0	2.118650	-6.069178	-3.717795
101	1	0	4.087107	-6.032044	-2.278178
102	1	0	11.587656	0.538636	0.997773
103	1	0	11.907331	2.320453	2.632476
104	1	0	7.790876	3.404442	2.298619
105	1	0	5.265033	-6.066554	-0.656822

106	1	0	7.067888	-6.014236	0.983377
107	1	0	6.829585	-1.748960	1.127488
108	1	0	6.835311	-1.471432	-2.289449
109	1	0	11.061651	-2.071247	-2.526813
110	1	0	11.400115	-0.452593	-0.735821
111	1	0	8.387383	-2.809821	2.541261
112	1	0	9.073385	-4.305895	1.895222
113	1	0	7.821651	-4.379394	3.133703
114	1	0	9.216516	-2.483716	-4.587745
115	1	0	9.109034	-3.836639	-3.463264
116	1	0	7.644596	-2.961581	-3.928064
117	1	0	-0.344766	-4.697637	-3.944385
118	1	0	-0.035928	-3.020657	-4.412121
119	1	0	0.685828	-4.349735	-5.330519
120	1	0	10.791804	4.842326	3.239309
121	1	0	9.125788	4.630004	3.793808
122	1	0	10.435664	3.693272	4.526393
123	1	0	0.481829	1.775267	-0.964906
124	1	0	0.651408	6.539140	-0.517387
125	1	0	2.370059	8.158735	-0.030938
126	1	0	4.665348	7.401922	0.633967
127	1	0	5.174650	4.999733	0.595113
128	1	0	-6.373846	3.427118	-0.979321
129	1	0	-1.663733	-0.500155	1.492185
130	1	0	-1.058863	-2.347306	1.592335
131	1	0	-1.887310	-6.223575	3.178572
132	1	0	-4.269261	-5.704565	3.249042
133	1	0	-11.356467	0.128127	-1.854110
134	1	0	-12.143173	2.433788	-1.971642
135	1	0	-8.266152	3.841669	-0.866962
136	1	0	-6.055307	-5.011236	3.834804
137	1	0	-8.385811	-4.345361	4.094315
138	1	0	-5.981063	-2.516277	-0.610450
139	1	0	-9.607162	-3.888483	-2.410375
140	1	0	-10.513045	-1.626820	-2.326999
141	1	0	-9.804808	-1.105989	2.705977

142	1	0	-10.317250	-2.795406	2.804227
143	1	0	-9.816547	-1.945378	4.264728
144	1	0	-7.739300	-5.487212	-1.089246
145	1	0	-7.079627	-5.066977	-2.668622
146	1	0	-6.118225	-4.791534	-1.207369
147	1	0	0.354944	-5.531037	1.760328
148	1	0	0.753754	-3.814092	1.900787
149	1	0	0.576528	-4.808801	3.352042
150	1	0	-9.948616	5.442383	-1.229441
151	1	0	-11.073690	4.995550	-2.518694
152	1	0	-11.580204	4.883297	-0.834994
153	1	0	-0.498169	1.781134	0.870453
154	1	0	-0.689520	6.538107	0.363669
155	1	0	-2.412326	8.146075	-0.151539
156	1	0	-4.700904	7.369919	-0.821401
157	1	0	-5.203719	4.969312	-0.745918
158	1	0	-7.634070	-0.789215	1.844513

(*P*,*S*,*P*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.903412$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.227948	-0.021577	-0.430194
2	6	0	-6.497337	0.237338	0.092620
3	6	0	5.892758	2.010976	-1.571010
4	1	0	5.697632	2.900025	-2.152706
5	6	0	-6.540486	1.241308	1.148653
6	6	0	4.214739	-1.893792	0.600367
7	1	0	3.368083	-2.547540	0.772255
8	6	0	4.894044	1.110567	-1.286688
9	6	0	4.081509	-0.770771	-0.173120
10	6	0	7.240533	1.740567	-1.178179
11	6	0	6.497330	-0.237341	0.092599
12	6	0	3.451214	0.983349	-1.586891

13	6	0	-4.081508	0.770734	-0.173104
14	6	0	5.227941	0.021545	-0.430228
15	6	0	-2.972812	0.155073	-0.911087
16	6	0	7.577213	0.538811	-0.499814
17	6	0	-5.892795	-2.011002	-1.570966
18	1	0	-5.697687	-2.900061	-2.152674
19	6	0	8.298975	2.707215	-1.487118
20	6	0	-4.214725	1.893770	0.600364
21	1	0	-3.368085	2.547516	0.772232
22	6	0	-7.577229	-0.538799	-0.499793
23	6	0	-1.624428	0.541763	-0.986546
24	1	0	-1.276681	1.415718	-0.443242
25	6	0	-7.240566	-1.740567	-1.178145
26	6	0	-0.721183	-0.200116	-1.728355
27	6	0	2.972804	-0.155129	-0.911107
28	6	0	-1.175499	-1.356537	-2.450953
29	6	0	8.960155	0.069071	-0.592355
30	6	0	-9.660599	-2.338427	-1.337706
31	6	0	-8.299024	-2.707201	-1.487078
32	6	0	-3.451231	-0.983418	-1.586844
33	6	0	-4.894063	-1.110614	-1.286641
34	6	0	-8.978594	-4.992107	-2.088614
35	6	0	9.988760	0.957075	-1.007799
36	6	0	7.998274	4.036925	-1.863196
37	1	0	6.963101	4.349739	-1.941046
38	6	0	-9.287952	1.293848	-0.399282
39	1	0	-8.495717	1.992402	-0.163400
40	6	0	-5.453483	2.150839	1.264915
41	6	0	-7.551381	1.255805	2.207888
42	6	0	8.978504	4.992123	-2.088694
43	6	0	-7.998345	-4.036921	-1.863127
44	1	0	-6.963173	-4.349757	-1.940958
45	6	0	-7.652367	2.370094	3.084287
46	6	0	9.660556	2.338469	-1.337734
47	6	0	5.453503	-2.150849	1.264912
48	6	0	-2.561159	-1.756511	-2.385381

49	6	0	0.721169	0.200040	-1.728367
50	6	0	-8.960162	-0.069033	-0.592355
51	6	0	10.324638	4.611436	-1.923207
52	1	0	11.113576	5.343799	-2.075196
53	6	0	10.577482	-1.782178	-0.536505
54	6	0	1.624421	-0.541825	-0.986550
55	1	0	1.276678	-1.415767	-0.443227
56	6	0	-2.078666	-3.606240	-3.904463
57	1	0	-2.420969	-4.467782	-4.470437
58	6	0	-8.359727	0.123895	2.468369
59	1	0	-8.228362	-0.761709	1.860545
60	6	0	10.888927	-3.244808	-0.331638
61	6	0	-9.988778	-0.957020	-1.007799
62	6	0	8.624128	6.406647	-2.478794
63	6	0	6.540489	-1.241298	1.148643
64	6	0	-5.610260	3.356049	2.083877
65	6	0	-10.577449	1.782252	-0.536564
66	6	0	8.359697	-0.123832	2.468357
67	1	0	8.228307	0.761768	1.860531
68	6	0	7.652396	-2.370046	3.084284
69	6	0	-0.288514	-2.117109	-3.261772
70	1	0	0.749866	-1.811531	-3.321959
71	6	0	-4.695073	4.430557	1.996195
72	1	0	-3.846359	4.356414	1.325769
73	6	0	-10.324717	-4.611396	-1.923125
74	1	0	-11.113672	-5.343759	-2.075087
75	6	0	-6.738920	3.495534	2.931260
76	6	0	-6.908963	4.711123	3.629530
77	1	0	-7.783729	4.853466	4.253859
78	6	0	9.287970	-1.293798	-0.399255
79	1	0	8.495744	-1.992365	-0.163375
80	6	0	2.561140	1.756413	-2.385452
81	6	0	-11.594970	0.876002	-0.894976
82	1	0	-12.615297	1.231677	-1.015636
83	6	0	-2.969852	-2.892908	-3.135847
84	1	0	-4.009399	-3.192915	-3.117022

85	6	0	7.551381	-1.255763	2.207882
86	6	0	-10.651125	-3.321439	-1.553520
87	1	0	-11.695920	-3.070480	-1.409683
88	6	0	5.610313	-3.356057	2.083875
89	6	0	10.651065	3.321495	-1.553575
90	1	0	11.695865	3.070553	-1.409747
91	6	0	-9.417812	1.221999	4.316790
92	1	0	-10.135366	1.218580	5.133633
93	6	0	-0.722804	-3.215324	-3.968483
94	1	0	-0.025202	-3.776347	-4.583150
95	6	0	11.301089	0.451325	-1.136911
96	1	0	12.097322	1.106703	-1.470876
97	6	0	1.175480	1.356441	-2.451000
98	6	0	-11.301095	-0.451244	-1.136945
99	1	0	-12.097334	-1.106614	-1.470916
100	6	0	11.594988	-0.875913	-0.894911
101	1	0	12.615327	-1.231569	-1.015541
102	6	0	-8.609315	2.324111	4.122148
103	1	0	-8.691031	3.155940	4.812339
104	6	0	-8.624234	-6.406622	-2.478762
105	6	0	6.738977	-3.495509	2.931259
106	6	0	-10.888875	3.244889	-0.331720
107	6	0	9.288980	-0.084488	3.495490
108	6	0	-4.860438	5.614450	2.699679
109	6	0	-9.289009	0.084578	3.495503
110	6	0	10.127159	1.144937	3.748960
111	6	0	-10.127230	-1.144817	3.748981
112	6	0	9.417814	-1.221904	4.316779
113	1	0	10.135367	-1.218464	5.133618
114	6	0	-5.996444	5.742193	3.523085
115	1	0	-6.162251	6.666256	4.071296
116	6	0	6.909054	-4.711090	3.629535
117	1	0	7.783828	-4.853405	4.253866
118	6	0	4.860563	-5.614484	2.699679
119	6	0	-3.870335	6.747329	2.577818
120	6	0	8.609345	-2.324036	4.122141

121	1	0	8.691084	-3.155862	4.812341
122	6	0	4.695165	-4.430598	1.996194
123	1	0	3.846438	-4.356499	1.325742
124	6	0	2.969837	2.892775	-3.135969
125	1	0	4.009384	3.192761	-3.117179
126	6	0	0.288491	2.116991	-3.261837
127	1	0	-0.749890	1.811416	-3.322004
128	6	0	5.996570	-5.742190	3.523092
129	1	0	6.162405	-6.666244	4.071304
130	6	0	2.078648	3.606084	-3.904604
131	1	0	2.420952	4.467599	-4.470620
132	6	0	0.722782	3.215178	-3.968591
133	1	0	0.025177	3.776183	-4.583270
134	6	0	3.870497	-6.747394	2.577817
135	1	0	9.031463	7.131838	-1.764928
136	1	0	9.034882	6.661873	-3.462844
137	1	0	7.541347	6.551771	-2.521963
138	1	0	3.071022	-6.507431	1.871788
139	1	0	4.356827	-7.667648	2.234124
140	1	0	3.405393	-6.973709	3.544560
141	1	0	-3.405380	6.973768	3.544603
142	1	0	-3.070751	6.507258	1.871948
143	1	0	-4.356595	7.667542	2.233919
144	1	0	-7.541453	-6.551836	-2.521652
145	1	0	-9.031832	-7.131857	-1.765094
146	1	0	-9.034731	-6.661698	-3.462959
147	1	0	-9.992402	3.810894	-0.066429
148	1	0	-11.316137	3.693315	-1.236347
149	1	0	-11.621637	3.384320	0.471734
150	1	0	-11.196894	-0.915719	3.676822
151	1	0	-9.906506	-1.934771	3.026712
152	1	0	-9.952938	-1.547523	4.753723
153	1	0	9.992411	-3.810861	-0.066589
154	1	0	11.316427	-3.693187	-1.236175
155	1	0	11.621492	-3.384240	0.471993
156	1	0	9.952908	1.547590	4.753730

157	1	0	11.196830	0.915898	3.676716
158	1	0	9.906347	1.934913	3.026741

(*P*,*R*,*P*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.903431$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.922679	-1.935274	-1.685425
2	6	0	7.222567	-1.809947	-1.103580
3	6	0	7.480411	-0.848804	-0.089987
4	6	0	6.514465	0.224347	0.096137
5	6	0	5.239842	-0.032690	-0.414720
6	6	0	4.898792	-1.113600	-1.278566
7	6	0	6.676278	1.524935	0.734571
8	6	0	5.512533	2.216370	1.170269
9	6	0	4.217476	1.823155	0.711437
10	6	0	4.095734	0.757522	-0.141063
11	6	0	5.652211	3.347518	2.091615
12	6	0	8.308006	-2.691312	-1.545393
13	6	0	4.538783	3.873144	2.787222
14	6	0	4.652479	4.890284	3.723349
15	6	0	5.936862	5.404284	3.989830
16	6	0	7.044091	4.911923	3.327487
17	6	0	6.935241	3.889153	2.359869
18	6	0	9.515658	-2.754176	-0.803914
19	6	0	10.574064	-3.541336	-1.308069
20	6	0	10.449831	-4.258024	-2.481983
21	6	0	9.253736	-4.217374	-3.225030
22	6	0	8.214372	-3.434037	-2.745218
23	6	0	8.080964	3.404968	1.600040
24	6	0	9.314434	4.093150	1.593664
25	6	0	10.372957	3.680061	0.809380
26	6	0	10.242217	2.564875	-0.041581
27	6	0	9.039199	1.877254	-0.034978

28	6	0	7.951790	2.241512	0.794105
29	6	0	9.606992	-2.040519	0.463822
30	6	0	8.602809	-1.098623	0.815399
31	6	0	8.651830	-0.515310	2.103604
32	6	0	9.669676	-0.775620	3.007144
33	6	0	10.687397	-1.669601	2.619747
34	6	0	10.644449	-2.292795	1.388368
35	6	0	3.450703	-0.990911	-1.555429
36	6	0	2.977477	0.139166	-0.862086
37	6	0	1.626795	0.521847	-0.915542
38	6	0	0.719752	-0.205717	-1.666514
39	6	0	1.166180	-1.359410	-2.397993
40	6	0	2.549402	-1.768381	-2.337085
41	6	0	0.270590	-2.115989	-3.203063
42	6	0	0.691355	-3.227377	-3.897135
43	6	0	2.038860	-3.643239	-3.815667
44	6	0	2.939339	-2.930726	-3.057219
45	6	0	-5.922685	1.935326	-1.685388
46	6	0	-7.222573	1.809981	-1.103545
47	6	0	-7.480419	0.848803	-0.089985
48	6	0	-6.514471	-0.224352	0.096106
49	6	0	-5.239846	0.032703	-0.414739
50	6	0	-4.898796	1.113641	-1.278550
51	6	0	-6.676276	-1.524956	0.734516
52	6	0	-5.512529	-2.216388	1.170210
53	6	0	-4.217474	-1.823159	0.711384
54	6	0	-4.095735	-0.757509	-0.141096
55	6	0	-5.652200	-3.347543	2.091551
56	6	0	-8.308009	2.691362	-1.545327
57	6	0	-4.538763	-3.873172	2.787146
58	6	0	-4.652449	-4.890313	3.723272
59	6	0	-5.936834	-5.404297	3.989783
60	6	0	-7.044070	-4.911931	3.327457
61	6	0	-6.935229	-3.889166	2.359829
62	6	0	-9.515664	2.754203	-0.803844
63	6	0	-10.574065	3.541384	-1.307971

64	6	0	-10.449829	4.258116	-2.481861
65	6	0	-9.253737	4.217489	-3.224908
66	6	0	-8.214374	3.434129	-2.745123
67	6	0	-8.080961	-3.404979	1.600015
68	6	0	-9.314448	-4.093123	1.593695
69	6	0	-10.372977	-3.680039	0.809413
70	6	0	-10.242216	-2.564911	-0.041615
71	6	0	-9.039191	-1.877298	-0.035036
72	6	0	-7.951784	-2.241541	0.794048
73	6	0	-9.607003	2.040496	0.463863
74	6	0	-8.602819	1.098585	0.815405
75	6	0	-8.651855	0.515207	2.103576
76	6	0	-9.669723	0.775454	3.007112
77	6	0	-10.687430	1.669466	2.619757
78	6	0	-10.644464	2.292729	1.388412
79	6	0	-3.450704	0.990969	-1.555405
80	6	0	-2.977478	-0.139128	-0.862095
81	6	0	-1.626795	-0.521805	-0.915559
82	6	0	-0.719751	0.205783	-1.666507
83	6	0	-1.166178	1.359501	-2.397948
84	6	0	-2.549400	1.768470	-2.337028
85	6	0	-0.270587	2.116108	-3.202990
86	6	0	-0.691351	3.227524	-3.897019
87	6	0	-2.038854	3.643388	-3.815532
88	6	0	-2.939335	2.930846	-3.057113
89	6	0	11.377390	2.151857	-0.946612
90	6	0	9.684203	-0.142161	4.377102
91	6	0	3.445738	5.423588	4.456773
92	6	0	9.126059	-4.990284	-4.515350
93	6	0	-11.377310	-2.152081	-0.946832
94	6	0	-9.684315	0.141826	4.376992
95	6	0	-3.445683	-5.423699	4.456594
96	6	0	-9.126050	4.990448	-4.515199
97	1	0	5.754021	-2.733937	-2.392868
98	1	0	3.350547	2.414359	0.980914
99	1	0	3.555655	3.447086	2.622275

100	1	0	6.058865	6.188573	4.732741
101	1	0	8.019648	5.314749	3.575041
102	1	0	11.517984	-3.574912	-0.775943
103	1	0	11.287904	-4.848823	-2.843192
104	1	0	7.315962	-3.365124	-3.348223
105	1	0	9.428923	4.992465	2.187904
106	1	0	11.303667	4.241970	0.822360
107	1	0	8.919633	1.044922	-0.716138
108	1	0	7.846576	0.139304	2.410544
109	1	0	11.496026	-1.897315	3.309963
110	1	0	11.410444	-3.021313	1.148440
111	1	0	1.284272	1.392173	-0.363128
112	1	0	-0.764881	-1.800729	-3.263523
113	1	0	-0.012878	-3.786540	-4.505860
114	1	0	2.365855	-4.527868	-4.354417
115	1	0	3.965823	-3.268403	-3.000572
116	1	0	-5.754029	2.734003	-2.392814
117	1	0	-3.350540	-2.414359	0.980855
118	1	0	-3.555637	-3.447114	2.622191
119	1	0	-6.058832	-6.188573	4.732708
120	1	0	-8.019625	-5.314742	3.575037
121	1	0	-11.517985	3.574944	-0.775844
122	1	0	-11.287900	4.848932	-2.843045
123	1	0	-7.315963	3.365236	-3.348131
124	1	0	-9.428965	-4.992391	2.188001
125	1	0	-11.303710	-4.241909	0.822457
126	1	0	-8.919624	-1.044985	-0.716217
127	1	0	-7.846603	-0.139419	2.410495
128	1	0	-11.496064	1.897148	3.309977
129	1	0	-11.410451	3.021268	1.148520
130	1	0	-1.284272	-1.392149	-0.363172
131	1	0	0.764883	1.800850	-3.263463
132	1	0	0.012883	3.786709	-4.505723
133	1	0	-2.365847	4.528041	-4.354244
134	1	0	-3.965816	3.268527	-3.000444
135	1	0	11.114293	1.274254	-1.542435

136	1	0	11.652773	2.958316	-1.636402
137	1	0	12.274965	1.905215	-0.367446
138	1	0	9.657507	-0.900366	5.168600
139	1	0	8.828535	0.522777	4.518853
140	1	0	10.595040	0.448493	4.529927
141	1	0	3.560874	5.321963	5.542092
142	1	0	2.533637	4.895596	4.166088
143	1	0	3.294725	6.489683	4.250011
144	1	0	9.226176	-6.068596	-4.343761
145	1	0	9.907465	-4.706748	-5.229784
146	1	0	8.157756	-4.817441	-4.992675
147	1	0	-11.114673	-1.273753	-1.541792
148	1	0	-12.275395	-1.906751	-0.367918
149	1	0	-11.651623	-2.958186	-1.637474
150	1	0	-8.828161	-0.522424	4.519034
151	1	0	-10.594721	-0.449618	4.529338
152	1	0	-9.658605	0.899953	5.168593
153	1	0	-2.533676	-4.895304	4.166345
154	1	0	-3.561018	-5.322726	5.541950
155	1	0	-3.294349	-6.489636	4.249242
156	1	0	-8.157621	4.817866	-4.992361
157	1	0	-9.226481	6.068729	-4.343610
158	1	0	-9.907258	4.706716	-5.229774

TS (*ortho–peri*) between (*P*,*S*,*P*)-**4'** and (*P*,*R*,*P*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.866793$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.376859	-0.231121	0.196781
2	6	0	6.745113	0.033971	0.106090
3	6	0	-5.647862	2.615910	-0.124568
4	1	0	-5.273220	3.629517	-0.131458
5	6	0	7.092367	1.424418	-0.159802
6	6	0	-4.749207	-2.072886	-0.259500

7	1	0	-4.000761	-2.856153	-0.266019
8	6	0	-4.794542	1.540658	-0.209251
9	6	0	-4.377008	-0.755030	-0.294561
10	6	0	-7.044007	2.413108	0.102182
11	6	0	-6.749198	-0.027518	-0.111321
12	6	0	-3.339215	1.337914	-0.328039
13	6	0	4.370020	0.764621	0.262006
14	6	0	-5.382328	0.241402	-0.210227
15	6	0	3.085463	0.053495	0.318855
16	6	0	-7.576130	1.106576	0.275387
17	6	0	5.632741	-2.604227	0.052176
18	1	0	5.244973	-3.608357	-0.046079
19	6	0	-7.945686	3.567637	0.168430
20	6	0	4.747310	2.081125	0.297527
21	1	0	4.005906	2.865035	0.396901
22	6	0	7.608721	-1.124784	0.289300
23	6	0	1.782592	0.561283	0.272236
24	1	0	1.660896	1.632445	0.252502
25	6	0	7.048757	-2.415034	0.085089
26	6	0	0.660353	-0.270540	0.202954
27	6	0	-3.092387	-0.044140	-0.329680
28	6	0	0.897746	-1.667515	0.587905
29	6	0	-8.841235	0.978943	1.000870
30	6	0	9.326963	-3.431585	0.212204
31	6	0	7.944829	-3.564250	-0.078367
32	6	0	3.333966	-1.327675	0.321344
33	6	0	4.789061	-1.530491	0.214448
34	6	0	8.318541	-5.875708	-0.827372
35	6	0	-9.679882	2.112483	1.178611
36	6	0	-7.548719	4.841383	-0.300333
37	1	0	-6.551331	4.975124	-0.703680
38	6	0	9.416088	0.103399	1.520339
39	1	0	8.744402	0.945787	1.623362
40	6	0	6.120409	2.428292	0.105048
41	6	0	8.316958	1.834699	-0.850216
42	6	0	-8.404148	5.933168	-0.319856

43	6	0	7.479246	-4.796518	-0.592673
44	1	0	6.433768	-4.904661	-0.858761
45	6	0	8.686186	3.206383	-0.896591
46	6	0	-9.273963	3.403761	0.637733
47	6	0	-6.135676	-2.416918	-0.316999
48	6	0	2.240096	-2.210062	0.544415
49	6	0	-0.666882	0.273682	-0.205180
50	6	0	8.963378	-1.049430	0.835900
51	6	0	-9.723442	5.748593	0.138026
52	1	0	-10.421991	6.581321	0.116404
53	6	0	-10.362383	-0.365151	2.389523
54	6	0	-1.791330	-0.554916	-0.271438
55	1	0	-1.672941	-1.626455	-0.252126
56	6	0	1.425603	-4.394379	1.277785
57	1	0	1.617208	-5.434302	1.524695
58	6	0	9.088802	0.908593	-1.591139
59	1	0	8.765420	-0.123145	-1.634343
60	6	0	-10.707081	-1.665416	3.074179
61	6	0	9.811996	-2.188684	0.799368
62	6	0	-7.952105	7.278236	-0.834622
63	6	0	-7.130001	-1.404513	-0.404485
64	6	0	6.536797	3.831957	0.166866
65	6	0	10.672271	0.187161	2.099124
66	6	0	-9.292912	-0.811723	-1.530504
67	1	0	-8.975624	0.222765	-1.549816
68	6	0	-8.809980	-3.145990	-1.035942
69	6	0	-0.095338	-2.518422	1.150599
70	1	0	-1.057997	-2.106049	1.413559
71	6	0	5.696555	4.825345	0.721001
72	1	0	4.715404	4.549754	1.090941
73	6	0	9.690194	-5.721416	-0.545839
74	1	0	10.374561	-6.544229	-0.736875
75	6	0	7.835567	4.205952	-0.262755
76	6	0	8.237459	5.549432	-0.096438
77	1	0	9.238655	5.849602	-0.384179
78	6	0	-9.199346	-0.227027	1.648954

79	1	0	-8.524308	-1.070727	1.591151
80	6	0	-2.241881	2.217009	-0.550345
81	6	0	11.521493	-0.933265	2.005129
82	1	0	12.510761	-0.898546	2.454859
83	6	0	2.449445	-3.582012	0.848642
84	1	0	3.457973	-3.973479	0.810868
85	6	0	-8.433727	-1.777985	-0.955353
86	6	0	10.176415	-4.529998	-0.044632
87	1	0	11.241320	-4.438093	0.136467
88	6	0	-6.544837	-3.824090	-0.290282
89	6	0	-10.143153	4.515898	0.597988
90	1	0	-11.172835	4.403685	0.917955
91	6	0	10.609297	2.626919	-2.282171
92	1	0	11.492852	2.942537	-2.831568
93	6	0	0.149733	-3.836531	1.478700
94	1	0	-0.639780	-4.430546	1.929635
95	6	0	-10.867301	1.959137	1.927629
96	1	0	-11.512275	2.815021	2.090306
97	6	0	-0.901292	1.669578	-0.595155
98	6	0	11.093363	-2.090337	1.385003
99	1	0	11.749994	-2.952838	1.385261
100	6	0	-11.211297	0.753181	2.505358
101	1	0	-12.128319	0.676111	3.084355
102	6	0	9.849905	3.565284	-1.612085
103	1	0	10.140248	4.607825	-1.673890
104	6	0	7.792446	-7.174365	-1.388915
105	6	0	-7.888500	-4.177410	-0.576326
106	6	0	11.118924	1.430189	2.829580
107	6	0	-10.510615	-1.137105	-2.105989
108	6	0	6.093416	6.146626	0.864845
109	6	0	10.223453	1.272060	-2.298711
110	6	0	-11.397140	-0.079955	-2.718107
111	6	0	11.016116	0.257092	-3.085980
112	6	0	-10.893982	-2.492768	-2.124176
113	1	0	-11.841671	-2.778852	-2.573798
114	6	0	7.392543	6.496955	0.447210

115	1	0	7.737683	7.521063	0.565524
116	6	0	-8.270449	-5.530639	-0.444498
117	1	0	-9.300838	-5.816942	-0.622031
118	6	0	-6.024103	-6.176748	0.197068
119	6	0	5.177372	7.182153	1.470805
120	6	0	-10.057211	-3.466457	-1.616439
121	1	0	-10.356249	-4.504632	-1.704270
122	6	0	-5.644555	-4.847296	0.087498
123	1	0	-4.622063	-4.592759	0.342168
124	6	0	-2.441132	3.593326	-0.841618
125	1	0	-3.443957	3.995954	-0.786240
126	6	0	0.094666	2.515612	-1.160322
127	1	0	1.054372	2.098008	-1.426228
128	6	0	-7.367052	-6.506400	-0.072349
129	1	0	-7.697758	-7.537537	0.023972
130	6	0	-1.413941	4.401098	-1.271437
131	1	0	-1.598891	5.444864	-1.507068
132	6	0	-0.143216	3.835941	-1.484169
133	1	0	0.648163	4.426531	-1.936098
134	6	0	-5.041190	-7.244405	0.612451
135	1	0	-8.589144	7.626487	-1.655740
136	1	0	-7.999498	8.040643	-0.048013
137	1	0	-6.922860	7.242202	-1.201627
138	1	0	-4.052694	-6.823072	0.814170
139	1	0	-5.375305	-7.764809	1.517520
140	1	0	-4.926765	-8.004531	-0.169312
141	1	0	4.965483	7.989532	0.759887
142	1	0	4.222040	6.745063	1.773331
143	1	0	5.628924	7.646074	2.355336
144	1	0	6.717742	-7.121763	-1.582663
145	1	0	8.290456	-7.433145	-2.330474
146	1	0	7.967002	-8.006124	-0.696220
147	1	0	10.342959	2.199723	2.820098
148	1	0	11.366074	1.212502	3.875268
149	1	0	12.018061	1.857104	2.369977
150	1	0	12.055419	0.212590	-2.740027

151	1	0	10.589903	-0.744641	-2.989655
152	1	0	11.043991	0.511124	-4.152183
153	1	0	-10.796685	-1.534728	4.159029
154	1	0	-11.667196	-2.057055	2.718256
155	1	0	-9.947022	-2.428464	2.888522
156	1	0	-11.573159	-0.273153	-3.782857
157	1	0	-12.378643	-0.056194	-2.230283
158	1	0	-10.954997	0.915174	-2.625097

TS (*peri–peri*) between (*P*,*S*,*P*)-**4'** and (*P*,*R*,*P*)-**4'** (B3LYP/6-31G(d,p), gas phase) $E = -3695.852016$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.523961	0.918460	-0.381419
2	6	0	5.455889	-0.118119	-0.470356
3	6	0	-6.046604	2.456810	-0.632369
4	1	0	-6.288327	3.389281	-1.122160
5	6	0	4.898326	-1.432546	-0.764231
6	6	0	-2.726719	-0.371616	1.309571
7	1	0	-1.705248	-0.473449	1.656141
8	6	0	-4.790301	2.225406	-0.123805
9	6	0	-3.163374	0.806420	0.763548
10	6	0	-7.083449	1.489668	-0.452892
11	6	0	-5.455890	-0.118119	0.470359
12	6	0	-3.522625	2.974478	-0.026955
13	6	0	3.163370	0.806419	-0.763523
14	6	0	-4.523962	0.918459	0.381429
15	6	0	2.545764	2.108496	-0.480697
16	6	0	-6.839740	0.280034	0.251704
17	6	0	6.046615	2.456817	0.632353
18	1	0	6.288348	3.389292	1.122131
19	6	0	-8.424839	1.747500	-0.986312
20	6	0	2.726709	-0.371619	-1.309538
21	1	0	1.705234	-0.473454	-1.656096

22	6	0	6.839741	0.280036	-0.251717
23	6	0	1.205486	2.501601	-0.564094
24	1	0	0.487179	1.773474	-0.919256
25	6	0	7.083457	1.489672	0.452872
26	6	0	0.747616	3.759462	-0.142525
27	6	0	-2.545767	2.108497	0.480723
28	6	0	1.798492	4.764165	0.041809
29	6	0	-7.985283	-0.396508	0.859959
30	6	0	9.513567	0.928568	0.590739
31	6	0	8.424850	1.747500	0.986286
32	6	0	3.522627	2.974480	0.026968
33	6	0	4.790305	2.225410	0.123806
34	6	0	9.898666	2.972406	2.526181
35	6	0	-9.306033	-0.075192	0.445702
36	6	0	-8.655219	2.755705	-1.950810
37	1	0	-7.827797	3.365444	-2.295972
38	6	0	7.820378	-1.283353	-1.950179
39	1	0	6.821937	-1.469803	-2.323973
40	6	0	3.596970	-1.505354	-1.333143
41	6	0	5.523863	-2.688324	-0.344282
42	6	0	-9.898646	2.972415	-2.526209
43	6	0	8.655236	2.755703	1.950785
44	1	0	7.827817	3.365443	2.295951
45	6	0	5.034688	-3.929436	-0.834618
46	6	0	-9.513561	0.928572	-0.590771
47	6	0	-3.596979	-1.505351	1.333168
48	6	0	3.175722	4.339208	0.228024
49	6	0	-0.747618	3.759462	0.142553
50	6	0	7.985278	-0.396509	-0.859980
51	6	0	-10.965069	2.140989	-2.131308
52	1	0	-11.946663	2.275850	-2.578700
53	6	0	-8.887779	-1.896607	2.586247
54	6	0	-1.205489	2.501603	0.564127
55	1	0	-0.487184	1.773478	0.919296
56	6	0	3.904253	6.657882	0.508758
57	1	0	4.693545	7.377884	0.702618

58	6	0	6.533812	-2.711740	0.646701
59	1	0	6.850948	-1.777108	1.090382
60	6	0	-8.675256	-2.830675	3.752654
61	6	0	9.306032	-0.075191	-0.445735
62	6	0	-10.109536	4.050159	-3.561880
63	6	0	-4.898329	-1.432546	0.764241
64	6	0	3.145418	-2.762735	-1.935378
65	6	0	8.887759	-1.896611	-2.586273
66	6	0	-6.533789	-2.711743	-0.646718
67	1	0	-6.850922	-1.777111	-1.090402
68	6	0	-5.034684	-3.929436	0.834623
69	6	0	1.607232	6.166785	-0.057908
70	1	0	0.671388	6.535770	-0.433721
71	6	0	2.005237	-2.811588	-2.770399
72	1	0	1.438321	-1.906155	-2.954873
73	6	0	10.965084	2.140975	2.131275
74	1	0	11.946680	2.275831	2.578666
75	6	0	3.899256	-3.949338	-1.748297
76	6	0	3.489734	-5.119245	-2.424788
77	1	0	4.072555	-6.028060	-2.326335
78	6	0	-7.820392	-1.283349	1.950164
79	1	0	-6.821955	-1.469795	2.323969
80	6	0	-3.175722	4.339206	-0.228010
81	6	0	10.187994	-1.608202	-2.126315
82	1	0	11.045231	-2.070070	-2.609993
83	6	0	4.176732	5.310100	0.500910
84	1	0	5.196585	4.975094	0.637689
85	6	0	-5.523857	-2.688325	0.344282
86	6	0	10.772039	1.146003	1.193270
87	1	0	11.608984	0.508465	0.931865
88	6	0	-3.145432	-2.762731	1.935409
89	6	0	-10.772030	1.146014	-1.193303
90	1	0	-11.608981	0.508482	-0.931899
91	6	0	6.656148	-5.103304	0.560993
92	1	0	7.087402	-6.040818	0.903425
93	6	0	2.607885	7.087564	0.174715

94	1	0	2.395815	8.146463	0.059187
95	6	0	-10.386700	-0.711473	1.095242
96	1	0	-11.403149	-0.467163	0.808547
97	6	0	-1.798493	4.764164	-0.041788
98	6	0	10.386693	-0.711470	-1.095285
99	1	0	11.403144	-0.467156	-0.808602
100	6	0	-10.188009	-1.608202	2.126275
101	1	0	-11.045251	-2.070071	2.609945
102	6	0	5.636205	-5.119784	-0.369420
103	1	0	5.267397	-6.077560	-0.718184
104	6	0	10.109561	4.050140	3.561860
105	6	0	-3.899265	-3.949336	1.748317
106	6	0	8.675225	-2.830675	-3.752681
107	6	0	-7.110730	-3.885570	-1.104381
108	6	0	1.598779	-3.970111	-3.415751
109	6	0	7.110766	-3.885565	1.104352
110	6	0	-8.179635	-3.871215	-2.170039
111	6	0	8.179675	-3.871209	2.170006
112	6	0	-6.656112	-5.103308	-0.561021
113	1	0	-7.087353	-6.040824	-0.903467
114	6	0	2.369985	-5.134877	-3.232916
115	1	0	2.086866	-6.052592	-3.742356
116	6	0	-3.489750	-5.119242	2.424814
117	1	0	-4.072569	-6.028057	2.326354
118	6	0	-1.598809	-3.970104	3.415801
119	6	0	0.378901	-3.989439	-4.304427
120	6	0	-5.636186	-5.119786	0.369409
121	1	0	-5.267375	-6.077561	0.718173
122	6	0	-2.005261	-2.811582	2.770444
123	1	0	-1.438349	-1.906148	2.954925
124	6	0	-4.176732	5.310098	-0.500900
125	1	0	-5.196585	4.975091	-0.637681
126	6	0	-1.607234	6.166783	0.057933
127	1	0	-0.671392	6.535766	0.433754
128	6	0	-2.370012	-5.134871	3.232957
129	1	0	-2.086899	-6.052585	3.742402

130	6	0	-3.904253	6.657880	-0.508745
131	1	0	-4.693545	7.377882	-0.702607
132	6	0	-2.607886	7.087563	-0.174695
133	1	0	-2.395818	8.146461	-0.059164
134	6	0	-0.378938	-3.989431	4.304486
135	1	0	-10.494193	3.633063	-4.499706
136	1	0	-10.840005	4.792559	-3.219196
137	1	0	-9.178916	4.577802	-3.787344
138	1	0	0.067951	-2.995812	4.394348
139	1	0	-0.625175	-4.340119	5.313284
140	1	0	0.388652	-4.665104	3.908984
141	1	0	-0.388656	-4.665169	-3.908960
142	1	0	-0.068032	-2.995833	-4.394227
143	1	0	0.625145	-4.340055	-5.313248
144	1	0	9.178963	4.577850	3.787258
145	1	0	10.494123	3.633021	4.499715
146	1	0	10.840108	4.792485	3.219224
147	1	0	7.613437	-2.944177	-3.985262
148	1	0	9.181427	-2.466184	-4.654284
149	1	0	9.078749	-3.827451	-3.539418
150	1	0	9.103264	-4.339298	1.809879
151	1	0	8.422012	-2.851328	2.479122
152	1	0	7.864582	-4.428067	3.060400
153	1	0	-7.613486	-2.943949	3.985426
154	1	0	-9.181710	-2.466339	4.654176
155	1	0	-9.078513	-3.827535	3.539272
156	1	0	-8.421894	-2.851339	-2.479233
157	1	0	-7.864581	-4.428167	-3.060386
158	1	0	-9.103263	-4.339204	-1.809879

S1' (B3LYP/6-31G(d,p), gas phase) $E = -1467.430268$ Hartree

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

1	6	0	2.159262	-2.212434	1.629712
2	6	0	2.509236	-1.419682	0.498158
3	6	0	1.548683	-0.584389	-0.045403
4	6	0	0.241294	-0.499521	0.498011
5	6	0	-0.094026	-1.299881	1.636053
6	6	0	0.900773	-2.151009	2.182030
7	6	0	-0.750032	0.353031	-0.057785
8	6	0	-2.027848	0.426786	0.468078
9	6	0	-2.344761	-0.375904	1.604122
10	6	0	-1.407614	-1.206476	2.168592
11	6	0	-3.028044	1.376869	-0.099765
12	6	0	3.866867	-1.552825	-0.105883
13	6	0	-4.353585	1.006369	-0.433744
14	6	0	-5.224193	2.008383	-0.893790
15	6	0	-4.816044	3.329630	-1.040833
16	6	0	-3.502971	3.705663	-0.736180
17	6	0	-2.637138	2.716097	-0.265006
18	6	0	4.318681	-2.847639	-0.411583
19	6	0	5.543817	-3.096028	-1.034165
20	6	0	6.339950	-1.993516	-1.365088
21	6	0	5.920678	-0.703250	-1.060246
22	6	0	4.694403	-0.448551	-0.423275
23	6	0	-4.865607	-0.391651	-0.363614
24	6	0	4.359860	0.964666	-0.085476
25	6	0	-4.174074	-1.463087	-0.953077
26	6	0	-4.693731	-2.753684	-0.923089
27	6	0	-5.921617	-3.031295	-0.305781
28	6	0	-6.609896	-1.964935	0.283123
29	6	0	-6.095431	-0.669044	0.252432
30	6	0	4.471744	1.973488	-1.053008
31	6	0	4.217872	3.308407	-0.735320
32	6	0	3.847854	3.686451	0.559101
33	6	0	3.742498	2.677895	1.528556
34	6	0	3.990425	1.345520	1.215777
35	6	0	-6.487999	-4.431276	-0.298608
36	6	0	-3.035288	5.129802	-0.919810

37	6	0	5.999299	-4.505283	-1.329412
38	6	0	3.557996	5.127348	0.906513
39	1	0	2.912059	-2.861999	2.066552
40	1	0	1.790626	0.022140	-0.912868
41	1	0	0.655078	-2.756518	3.050794
42	1	0	-0.490920	0.951284	-0.927383
43	1	0	-3.341368	-0.315736	2.027890
44	1	0	-1.663671	-1.804451	3.039529
45	1	0	-6.237233	1.729062	-1.168185
46	1	0	-5.521821	4.072886	-1.403649
47	1	0	-1.625246	2.992392	0.019105
48	1	0	3.666814	-3.686485	-0.181317
49	1	0	7.298810	-2.145476	-1.854648
50	1	0	6.568013	0.137212	-1.292845
51	1	0	-3.223781	-1.279203	-1.443406
52	1	0	-4.136386	-3.561805	-1.390950
53	1	0	-7.560342	-2.149942	0.777882
54	1	0	-6.645252	0.137599	0.729274
55	1	0	4.749005	1.707577	-2.069282
56	1	0	4.307624	4.067069	-1.509060
57	1	0	3.466927	2.942461	2.546783
58	1	0	3.908227	0.589032	1.989505
59	1	0	-6.932476	-4.685891	-1.268924
60	1	0	-5.712109	-5.176662	-0.095664
61	1	0	-7.269597	-4.542846	0.458307
62	1	0	-3.805721	5.846495	-0.617723
63	1	0	-2.134617	5.333935	-0.334011
64	1	0	-2.796678	5.336788	-1.970573
65	1	0	5.161256	-5.207789	-1.317423
66	1	0	6.483367	-4.572581	-2.309060
67	1	0	6.728076	-4.851005	-0.585648
68	1	0	3.848281	5.800636	0.095167
69	1	0	2.489880	5.284205	1.100553
70	1	0	4.095427	5.437342	1.809374

Radical cation of **S1'** (UB3LYP/6-31G(d,p), gas phase) $E = -1467.190970$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.192284	-2.310276	1.595035
2	6	0	2.576303	-1.449081	0.538481
3	6	0	1.609916	-0.574042	0.011416
4	6	0	0.287398	-0.537260	0.517281
5	6	0	-0.073118	-1.404819	1.595307
6	6	0	0.910513	-2.280502	2.114185
7	6	0	-0.685087	0.339707	-0.018490
8	6	0	-1.999931	0.370582	0.468552
9	6	0	-2.334083	-0.497445	1.540722
10	6	0	-1.398685	-1.350326	2.091349
11	6	0	-2.974938	1.332352	-0.095405
12	6	0	3.923700	-1.533381	-0.060621
13	6	0	-4.326108	0.992412	-0.391613
14	6	0	-5.189079	2.027077	-0.797887
15	6	0	-4.747975	3.333169	-0.946064
16	6	0	-3.406770	3.676231	-0.693207
17	6	0	-2.548538	2.662390	-0.274506
18	6	0	4.461370	-2.808235	-0.313497
19	6	0	5.672693	-2.990317	-0.977302
20	6	0	6.370981	-1.840540	-1.398221
21	6	0	5.875059	-0.572389	-1.144737
22	6	0	4.662634	-0.377540	-0.454625
23	6	0	-4.853683	-0.391566	-0.363901
24	6	0	4.258983	0.999066	-0.108372
25	6	0	-4.165637	-1.458079	-0.972575
26	6	0	-4.700552	-2.740977	-0.978511
27	6	0	-5.938479	-3.017764	-0.376749
28	6	0	-6.624108	-1.954267	0.230613
29	6	0	-6.101439	-0.665777	0.228565
30	6	0	4.394944	2.043986	-1.047997
31	6	0	4.068020	3.349504	-0.713757

32	6	0	3.614609	3.682993	0.578514
33	6	0	3.487749	2.649021	1.516322
34	6	0	3.797633	1.334583	1.185838
35	6	0	-6.529386	-4.403683	-0.412655
36	6	0	-2.932741	5.098079	-0.851589
37	6	0	6.219022	-4.365108	-1.259278
38	6	0	3.312815	5.112531	0.941500
39	1	0	2.927635	-2.983972	2.021795
40	1	0	1.863525	0.058309	-0.832203
41	1	0	0.649178	-2.934053	2.941687
42	1	0	-0.407749	0.984869	-0.846907
43	1	0	-3.341632	-0.477941	1.939064
44	1	0	-1.676991	-1.991667	2.922659
45	1	0	-6.216020	1.779193	-1.045762
46	1	0	-5.443624	4.098477	-1.279350
47	1	0	-1.523526	2.917635	-0.020567
48	1	0	3.884243	-3.682698	-0.028648
49	1	0	7.320446	-1.950567	-1.914680
50	1	0	6.458187	0.295712	-1.433862
51	1	0	-3.218515	-1.270991	-1.468107
52	1	0	-4.156455	-3.543348	-1.469504
53	1	0	-7.579961	-2.141068	0.712309
54	1	0	-6.648227	0.135212	0.717147
55	1	0	4.732128	1.816152	-2.054374
56	1	0	4.164249	4.131827	-1.461650
57	1	0	3.156792	2.880602	2.524678
58	1	0	3.729462	0.563574	1.945053
59	1	0	-7.177104	-4.527896	-1.289510
60	1	0	-5.752563	-5.170955	-0.472128
61	1	0	-7.141844	-4.601650	0.471458
62	1	0	-3.469546	5.771304	-0.173948
63	1	0	-1.864391	5.192553	-0.642535
64	1	0	-3.111840	5.460707	-1.869828
65	1	0	5.556960	-5.148366	-0.883562
66	1	0	6.354753	-4.522176	-2.334997
67	1	0	7.200903	-4.497930	-0.791230

68	1	0	2.793178	5.630617	0.129515
69	1	0	2.700350	5.179613	1.843981
70	1	0	4.240259	5.667064	1.131292

Radical cation of **1a'** (UB3LYP/6-31G(d,p), gas phase) $E = -1464.812820$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.431174	2.966834	-0.029277
2	6	0	2.472133	1.564108	-0.171057
3	6	0	1.232355	0.854554	-0.359104
4	6	0	-0.000001	1.517212	-0.000012
5	6	0	-0.000003	2.944680	-0.000016
6	6	0	1.230363	3.644541	-0.028855
7	6	0	-1.232355	0.854553	0.359086
8	6	0	-2.472134	1.564104	0.171038
9	6	0	-2.431179	2.966828	0.029250
10	6	0	-1.230370	3.644539	0.028820
11	6	0	-3.724338	0.822494	0.155061
12	6	0	3.724337	0.822499	-0.155068
13	6	0	-4.916898	1.409727	-0.325814
14	6	0	-6.108480	0.701182	-0.417821
15	6	0	-6.098820	-0.648986	-0.019659
16	6	0	-4.944473	-1.249173	0.459303
17	6	0	-3.738161	-0.534706	0.569835
18	6	0	3.738164	-0.534702	-0.569835
19	6	0	4.944479	-1.249164	-0.459307
20	6	0	6.098825	-0.648971	0.019649
21	6	0	6.108478	0.701196	0.417817
22	6	0	4.916897	1.409739	0.325800
23	6	0	-2.526811	-1.115820	1.147897
24	6	0	-2.545319	-2.337824	1.843351
25	6	0	-1.407577	-2.845662	2.450654
26	6	0	-0.187751	-2.140266	2.422115

27	6	0	-0.155697	-0.940563	1.729740
28	6	0	-1.286676	-0.420806	1.050901
29	6	0	2.526817	-1.115821	-1.147900
30	6	0	1.286680	-0.420809	-1.050910
31	6	0	0.155704	-0.940570	-1.729753
32	6	0	0.187763	-2.140276	-2.422123
33	6	0	1.407593	-2.845664	-2.450665
34	6	0	2.545331	-2.337824	-1.843356
35	6	0	1.021328	-2.667045	3.153268
36	6	0	-1.021332	-2.667094	-3.153221
37	6	0	-7.369810	1.339303	-0.942304
38	6	0	7.369782	1.339289	0.942396
39	1	0	3.353998	3.531326	0.010925
40	1	0	1.216676	4.729972	-0.003047
41	1	0	-3.354004	3.531318	-0.010951
42	1	0	-1.216685	4.729969	0.003005
43	1	0	-4.906367	2.435702	-0.676277
44	1	0	-7.010592	-1.234925	-0.095436
45	1	0	-4.984172	-2.294757	0.740947
46	1	0	4.984185	-2.294745	-0.740962
47	1	0	7.010604	-1.234902	0.095410
48	1	0	4.906367	2.435720	0.676246
49	1	0	-3.472942	-2.888164	1.944004
50	1	0	-1.469340	-3.785297	2.992853
51	1	0	0.758608	-0.360137	1.744421
52	1	0	-0.758600	-0.360141	-1.744447
53	1	0	1.469364	-3.785292	-2.992876
54	1	0	3.472958	-2.888157	-1.944016
55	1	0	0.824223	-2.761797	4.226638
56	1	0	1.297772	-3.662462	2.788744
57	1	0	1.885225	-2.010269	3.026604
58	1	0	-0.824003	-2.762660	-4.226475
59	1	0	-1.298241	-3.662159	-2.788078
60	1	0	-1.885016	-2.009915	-3.027206
61	1	0	-7.758726	0.793235	-1.808386
62	1	0	-8.156764	1.335226	-0.180121

63	1	0	-7.201726	2.375555	-1.244871
64	1	0	7.757977	0.793870	1.809217
65	1	0	8.157166	1.334166	0.180671
66	1	0	7.201954	2.375888	1.243916

S2' (B3LYP/6-31G(d,p), gas phase) $E = -1849.748952$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.662723	0.433349	-0.421965
2	6	0	-1.698899	1.477868	-0.383510
3	6	0	-0.329343	1.150602	-0.475231
4	6	0	0.062837	-0.231792	-0.274861
5	6	0	-0.921255	-1.243166	-0.500333
6	6	0	-2.308583	-0.885346	-0.570442
7	6	0	1.389118	-0.666333	0.130236
8	6	0	1.803756	-1.976123	-0.196298
9	6	0	0.826065	-2.921844	-0.615092
10	6	0	-0.498627	-2.590247	-0.670329
11	6	0	3.217343	-2.340920	-0.099639
12	6	0	-2.109894	2.876342	-0.252454
13	6	0	3.712674	-3.535412	-0.671048
14	6	0	5.060743	-3.862027	-0.668089
15	6	0	5.960396	-2.953682	-0.076035
16	6	0	5.505959	-1.780759	0.494861
17	6	0	4.133623	-1.448751	0.512955
18	6	0	-1.152777	3.908150	-0.426282
19	6	0	-1.553747	5.240853	-0.188069
20	6	0	-2.848261	5.553685	0.178938
21	6	0	-3.817073	4.542601	0.333640
22	6	0	-3.427484	3.228573	0.119646
23	6	0	3.622632	-0.254815	1.177333
24	6	0	4.426210	0.505058	2.056262
25	6	0	3.921330	1.584437	2.753200

26	6	0	2.565085	1.944213	2.630418
27	6	0	1.771355	1.210580	1.762885
28	6	0	2.267576	0.131676	0.994223
29	6	0	0.186700	3.561488	-0.888983
30	6	0	0.595116	2.200833	-0.919031
31	6	0	1.844651	1.891153	-1.505170
32	6	0	2.710828	2.860521	-1.985857
33	6	0	2.315326	4.208991	-1.891249
34	6	0	1.080726	4.542952	-1.371531
35	6	0	1.996461	3.084572	3.439621
36	6	0	4.033070	2.489781	-2.612564
37	6	0	5.562926	-5.140077	-1.295143
38	6	0	-5.229017	4.889019	0.740054
39	6	0	-3.377347	-1.909646	-0.793036
40	6	0	-3.997502	-1.979920	-2.027538
41	6	0	-5.024979	-2.916614	-2.287129
42	6	0	-5.434490	-3.783851	-1.302684
43	6	0	-4.840013	-3.745810	-0.013356
44	6	0	-3.798277	-2.795728	0.255009
45	6	0	-5.258916	-4.623395	1.023089
46	6	0	-4.686452	-4.568639	2.272661
47	6	0	-3.666838	-3.625168	2.542773
48	6	0	-3.235702	-2.761508	1.561065
49	1	0	-3.717294	0.679561	-0.422471
50	1	0	1.116700	-3.947398	-0.806685
51	1	0	-1.242466	-3.349625	-0.881577
52	1	0	3.027739	-4.214777	-1.165923
53	1	0	7.025022	-3.174154	-0.076375
54	1	0	6.229957	-1.096699	0.922881
55	1	0	-0.830540	6.043566	-0.277154
56	1	0	-3.120102	6.590773	0.359455
57	1	0	-4.163091	2.449044	0.283148
58	1	0	5.457848	0.216818	2.222663
59	1	0	4.568001	2.140016	3.427969
60	1	0	0.721038	1.462495	1.692324
61	1	0	2.130266	0.852270	-1.607842

62	1	0	2.973134	4.991446	-2.261692
63	1	0	0.782118	5.585001	-1.372636
64	1	0	2.092108	2.898267	4.515930
65	1	0	2.525389	4.021368	3.228777
66	1	0	0.937954	3.242918	3.218219
67	1	0	4.088184	2.821472	-3.656229
68	1	0	4.868241	2.961931	-2.082128
69	1	0	4.195096	1.409096	-2.593860
70	1	0	6.059624	-5.777813	-0.554385
71	1	0	4.746687	-5.717277	-1.737768
72	1	0	6.296168	-4.936772	-2.084240
73	1	0	-5.710104	5.533698	-0.005016
74	1	0	-5.845134	3.992948	0.852776
75	1	0	-5.248896	5.431764	1.692226
76	1	0	-3.678458	-1.304303	-2.815586
77	1	0	-5.484740	-2.945882	-3.270587
78	1	0	-6.221563	-4.508385	-1.494767
79	1	0	-6.046945	-5.340800	0.808769
80	1	0	-5.017097	-5.245034	3.055409
81	1	0	-3.223266	-3.581759	3.533159
82	1	0	-2.457428	-2.038125	1.777691

Radical cation of **S2'** (UB3LYP/6-31G(d,p), gas phase) $E = -1849.521422$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.693031	0.468521	-0.443295
2	6	0	-1.746083	1.501726	-0.374264
3	6	0	-0.351549	1.163150	-0.468514
4	6	0	0.034677	-0.206798	-0.233941
5	6	0	-0.945475	-1.223679	-0.458457
6	6	0	-2.335925	-0.873634	-0.541284
7	6	0	1.359042	-0.624774	0.170469
8	6	0	1.803154	-1.937098	-0.195266

9	6	0	0.836634	-2.876403	-0.611906
10	6	0	-0.502524	-2.552592	-0.662024
11	6	0	3.221796	-2.263774	-0.122133
12	6	0	-2.135747	2.898158	-0.216454
13	6	0	3.738952	-3.431071	-0.728179
14	6	0	5.095979	-3.726095	-0.734303
15	6	0	5.968659	-2.810541	-0.115331
16	6	0	5.489335	-1.661370	0.490574
17	6	0	4.113568	-1.362488	0.515333
18	6	0	-1.170861	3.916793	-0.422906
19	6	0	-1.551028	5.249309	-0.180907
20	6	0	-2.835590	5.571372	0.228421
21	6	0	-3.810312	4.574890	0.421336
22	6	0	-3.437838	3.254376	0.198743
23	6	0	3.573888	-0.199304	1.217471
24	6	0	4.357732	0.568578	2.099470
25	6	0	3.821764	1.625179	2.816092
26	6	0	2.455238	1.955297	2.715023
27	6	0	1.676357	1.211127	1.843724
28	6	0	2.205913	0.160651	1.053580
29	6	0	0.151584	3.553155	-0.932612
30	6	0	0.553882	2.186048	-0.962940
31	6	0	1.785463	1.849651	-1.579239
32	6	0	2.651955	2.805018	-2.085506
33	6	0	2.265494	4.156476	-1.985894
34	6	0	1.043493	4.514896	-1.439007
35	6	0	1.867754	3.059680	3.557492
36	6	0	3.949711	2.424066	-2.752537
37	6	0	5.631395	-4.971790	-1.394148
38	6	0	-5.202067	4.937650	0.874269
39	6	0	-3.415492	-1.877853	-0.714506
40	6	0	-4.230680	-1.759341	-1.834675
41	6	0	-5.251934	-2.691478	-2.104357
42	6	0	-5.480616	-3.732410	-1.231835
43	6	0	-4.713872	-3.870321	-0.045734
44	6	0	-3.666135	-2.929949	0.236274

45	6	0	-4.983213	-4.911188	0.883382
46	6	0	-4.272274	-5.014247	2.056637
47	6	0	-3.264810	-4.068184	2.353906
48	6	0	-2.971451	-3.052289	1.469926
49	1	0	-3.748036	0.710842	-0.451979
50	1	0	1.132539	-3.894208	-0.831877
51	1	0	-1.230473	-3.315757	-0.909187
52	1	0	3.069469	-4.111158	-1.242611
53	1	0	7.037642	-3.004926	-0.118520
54	1	0	6.200527	-0.979988	0.942248
55	1	0	-0.830895	6.049870	-0.302305
56	1	0	-3.090724	6.611516	0.411338
57	1	0	-4.169964	2.478805	0.394155
58	1	0	5.399304	0.315233	2.255727
59	1	0	4.458064	2.182919	3.497885
60	1	0	0.614287	1.418927	1.795977
61	1	0	2.044417	0.804735	-1.695775
62	1	0	2.918465	4.930185	-2.380610
63	1	0	0.765618	5.561938	-1.438769
64	1	0	2.373212	4.012407	3.364789
65	1	0	0.802949	3.197035	3.354293
66	1	0	1.982419	2.846598	4.625970
67	1	0	4.801215	2.903064	-2.256962
68	1	0	4.111176	1.343764	-2.729188
69	1	0	3.965689	2.745227	-3.799816
70	1	0	6.365205	-4.725116	-2.169041
71	1	0	6.137873	-5.614758	-0.665803
72	1	0	4.833915	-5.556162	-1.859322
73	1	0	-5.179171	5.489981	1.819806
74	1	0	-5.698462	5.580573	0.139001
75	1	0	-5.823501	4.050447	1.017311
76	1	0	-4.045732	-0.954963	-2.540235
77	1	0	-5.847842	-2.587132	-3.005107
78	1	0	-6.264988	-4.456401	-1.433325
79	1	0	-5.773992	-5.619650	0.653932
80	1	0	-4.490590	-5.810519	2.760959

81	1	0	-2.722056	-4.138782	3.291490
82	1	0	-2.207044	-2.327119	1.725735

Radical cation of **S2'**-INT-5ring (UB3LYP/6-31G(d,p), gas phase) $E = -1849.467041$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.646131	-0.154685	-0.066490
2	6	0	1.850818	-1.290658	0.191666
3	6	0	0.450241	-1.150502	0.457949
4	6	0	-0.162103	0.147623	0.230711
5	6	0	0.701711	1.241270	0.257559
6	6	0	2.095792	1.131732	0.017822
7	6	0	-1.518500	0.468873	-0.192878
8	6	0	-2.030810	1.822443	0.021442
9	6	0	-1.167297	2.868464	0.229796
10	6	0	0.276121	2.651482	0.387221
11	6	0	-3.490848	2.036639	-0.005845
12	6	0	2.433890	-2.639373	0.138561
13	6	0	-4.072590	3.180066	0.571682
14	6	0	-5.448946	3.384808	0.587801
15	6	0	-6.267830	2.394037	0.015702
16	6	0	-5.719680	1.255651	-0.547378
17	6	0	-4.325137	1.052442	-0.580815
18	6	0	1.650740	-3.759177	0.519398
19	6	0	2.212558	-5.047137	0.378817
20	6	0	3.498208	-5.230636	-0.089304
21	6	0	4.299662	-4.128831	-0.446308
22	6	0	3.749281	-2.860718	-0.326977
23	6	0	-3.716380	-0.119970	-1.206364
24	6	0	-4.457383	-0.975384	-2.041118
25	6	0	-3.880853	-2.074595	-2.653329
26	6	0	-2.514109	-2.373705	-2.478326
27	6	0	-1.775046	-1.547589	-1.649747

28	6	0	-2.335402	-0.423000	-0.986323
29	6	0	0.316893	-3.555593	1.076770
30	6	0	-0.278861	-2.264844	1.041382
31	6	0	-1.536692	-2.078466	1.665615
32	6	0	-2.230141	-3.110992	2.274725
33	6	0	-1.642040	-4.392588	2.266136
34	6	0	-0.401789	-4.601179	1.694699
35	6	0	-1.887285	-3.545291	-3.191389
36	6	0	-3.559054	-2.881838	2.950334
37	6	0	-6.055302	4.612885	1.218442
38	6	0	5.704572	-4.335464	-0.954562
39	6	0	2.597958	2.461941	-0.206441
40	6	0	1.420085	3.361234	-0.502361
41	6	0	1.657951	4.820981	-0.375295
42	6	0	2.906817	5.298538	-0.221262
43	6	0	4.064358	4.430694	-0.098079
44	6	0	3.905343	3.000300	-0.060826
45	6	0	5.345465	4.981060	0.043367
46	6	0	6.457662	4.169029	0.232137
47	6	0	6.306452	2.774305	0.312874
48	6	0	5.055145	2.201637	0.180847
49	1	0	3.677978	-0.280363	-0.355365
50	1	0	-1.549008	3.874453	0.361631
51	1	0	0.525126	2.990225	1.406213
52	1	0	-3.443339	3.915245	1.062147
53	1	0	-7.347222	2.516323	0.031287
54	1	0	-6.386951	0.502853	-0.949969
55	1	0	1.624653	-5.921843	0.629115
56	1	0	3.894737	-6.237477	-0.187405
57	1	0	4.365078	-2.022715	-0.632073
58	1	0	-5.499558	-0.759292	-2.241665
59	1	0	-4.487923	-2.703421	-3.299085
60	1	0	-0.718017	-1.747263	-1.540324
61	1	0	-1.964507	-1.083890	1.703525
62	1	0	-2.158214	-5.222485	2.741175
63	1	0	0.033481	-5.591004	1.756824

64	1	0	-2.395904	-4.480127	-2.931584
65	1	0	-0.831544	-3.654413	-2.932598
66	1	0	-1.959646	-3.431866	-4.278735
67	1	0	-3.509370	-3.130050	4.016380
68	1	0	-4.338965	-3.513942	2.511196
69	1	0	-3.881134	-1.841189	2.862454
70	1	0	-6.768138	4.343221	2.005096
71	1	0	-6.605115	5.203477	0.477059
72	1	0	-5.292662	5.257862	1.661734
73	1	0	6.328454	-4.826605	-0.199383
74	1	0	6.181779	-3.388287	-1.218752
75	1	0	5.714333	-4.976232	-1.843101
76	1	0	1.088839	3.159775	-1.533189
77	1	0	0.814353	5.494676	-0.493966
78	1	0	3.082096	6.370256	-0.190291
79	1	0	5.460726	6.060436	0.013774
80	1	0	7.441978	4.614247	0.335083
81	1	0	7.173105	2.144953	0.486376
82	1	0	4.951846	1.128939	0.274172

TS between radical cation of **S2'** and radical cation of **S2'**-INT-5ring

(UB3LYP/6-31G(d,p), gas phase) $E = -1849.464669$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.648663	0.156501	0.115600
2	6	0	1.856774	1.292374	-0.160064
3	6	0	0.460022	1.142770	-0.439692
4	6	0	-0.152040	-0.157098	-0.222392
5	6	0	0.717850	-1.249576	-0.271416
6	6	0	2.101323	-1.122623	0.018446
7	6	0	-1.517100	-0.476032	0.175913
8	6	0	-2.022520	-1.818771	-0.054694

9	6	0	-1.146760	-2.854696	-0.333452
10	6	0	0.273335	-2.636931	-0.420711
11	6	0	-3.478160	-2.042683	-0.025140
12	6	0	2.434642	2.641629	-0.099953
13	6	0	-4.054589	-3.205854	-0.573668
14	6	0	-5.428813	-3.413173	-0.602413
15	6	0	-6.257108	-2.407718	-0.069465
16	6	0	-5.717585	-1.255882	0.472298
17	6	0	-4.323695	-1.047834	0.519214
18	6	0	1.646187	3.760066	-0.473703
19	6	0	2.199983	5.049887	-0.320037
20	6	0	3.484159	5.236126	0.151228
21	6	0	4.292943	4.135572	0.495719
22	6	0	3.750160	2.865370	0.364399
23	6	0	-3.729559	0.132981	1.141378
24	6	0	-4.487903	1.000593	1.949883
25	6	0	-3.919594	2.096408	2.574056
26	6	0	-2.544087	2.376288	2.442098
27	6	0	-1.789249	1.537568	1.640172
28	6	0	-2.343554	0.423281	0.957801
29	6	0	0.319009	3.551544	-1.044398
30	6	0	-0.266745	2.255883	-1.029782
31	6	0	-1.510229	2.062382	-1.679951
32	6	0	-2.204471	3.094895	-2.287671
33	6	0	-1.630287	4.382542	-2.252945
34	6	0	-0.401096	4.597351	-1.660475
35	6	0	-1.924295	3.540597	3.173242
36	6	0	-3.518852	2.860228	-2.989161
37	6	0	-6.025528	-4.660544	-1.204089
38	6	0	5.697486	4.345636	1.003491
39	6	0	2.612194	-2.443976	0.320625
40	6	0	1.499053	-3.306603	0.762514
41	6	0	1.727153	-4.746589	0.824941
42	6	0	2.952292	-5.256228	0.552720
43	6	0	4.066499	-4.419539	0.178350
44	6	0	3.889958	-2.998132	0.038045

45	6	0	5.324596	-4.984280	-0.095973
46	6	0	6.385320	-4.193163	-0.509032
47	6	0	6.208441	-2.807058	-0.687843
48	6	0	4.984474	-2.222418	-0.432478
49	1	0	3.672345	0.275275	0.439184
50	1	0	-1.522648	-3.849309	-0.538684
51	1	0	0.702435	-3.141762	-1.288237
52	1	0	-3.422213	-3.959102	-1.030392
53	1	0	-7.336077	-2.532380	-0.095424
54	1	0	-6.391015	-0.495721	0.849761
55	1	0	1.607651	5.923464	-0.563732
56	1	0	3.874674	6.244244	0.259640
57	1	0	4.372574	2.027687	0.656741
58	1	0	-5.537325	0.795005	2.121622
59	1	0	-4.538672	2.734487	3.198950
60	1	0	-0.726050	1.722150	1.566978
61	1	0	-1.924541	1.063250	-1.737586
62	1	0	-2.147360	5.212699	-2.726608
63	1	0	0.025002	5.592061	-1.705121
64	1	0	-2.404274	4.483230	2.888004
65	1	0	-0.857068	3.628718	2.956556
66	1	0	-2.042208	3.435958	4.257484
67	1	0	-3.454533	3.125592	-4.050269
68	1	0	-4.313524	3.475949	-2.553245
69	1	0	-3.829413	1.814600	-2.922315
70	1	0	-6.718932	-4.415876	-2.015997
71	1	0	-6.594594	-5.223834	-0.456077
72	1	0	-5.255418	-5.322628	-1.607574
73	1	0	6.315088	4.854438	0.254926
74	1	0	6.183315	3.398363	1.251013
75	1	0	5.704097	4.971833	1.902406
76	1	0	0.986563	-2.928604	1.649007
77	1	0	0.916896	-5.389574	1.153965
78	1	0	3.130452	-6.324487	0.638792
79	1	0	5.454604	-6.056905	0.012394
80	1	0	7.350901	-4.644811	-0.712391

81	1	0	7.035828	-2.198597	-1.037933
82	1	0	4.851255	-1.161830	-0.605039

Radical cation of **S2'**-INT-6ring (UB3LYP/6-31G(d,p), gas phase) $E = -1849.479541$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.575059	1.386377	-0.013631
2	6	0	2.482469	-0.004409	-0.218948
3	6	0	1.197337	-0.587904	-0.348654
4	6	0	0.057311	0.198904	0.061441
5	6	0	0.186595	1.603004	0.167721
6	6	0	1.459977	2.208574	0.108443
7	6	0	-1.225254	-0.363284	0.448830
8	6	0	-2.421101	0.420514	0.204457
9	6	0	-2.304008	1.782157	0.167950
10	6	0	-1.017910	2.485090	0.337119
11	6	0	-3.723141	-0.261312	0.133339
12	6	0	3.678052	-0.845410	-0.317722
13	6	0	-4.836356	0.350507	-0.465676
14	6	0	-6.067405	-0.293194	-0.561887
15	6	0	-6.169453	-1.599059	-0.045869
16	6	0	-5.083247	-2.222666	0.542172
17	6	0	-3.838240	-1.570514	0.653756
18	6	0	3.544151	-2.198388	-0.720396
19	6	0	4.696485	-3.013889	-0.709034
20	6	0	5.931250	-2.514316	-0.344142
21	6	0	6.084377	-1.166409	0.037742
22	6	0	4.953043	-0.362707	0.048517
23	6	0	-2.682003	-2.177721	1.310537
24	6	0	-2.796635	-3.346028	2.084560
25	6	0	-1.699898	-3.908285	2.715137
26	6	0	-0.415365	-3.327325	2.625585
27	6	0	-0.282750	-2.183563	1.861045

28	6	0	-1.381063	-1.591020	1.179309
29	6	0	2.246720	-2.683781	-1.181843
30	6	0	1.084421	-1.880374	-1.017100
31	6	0	-0.126084	-2.309646	-1.611221
32	6	0	-0.248254	-3.520313	-2.273642
33	6	0	0.896521	-4.338412	-2.362144
34	6	0	2.108400	-3.920815	-1.847915
35	6	0	0.751968	-3.932017	3.363256
36	6	0	-1.545722	-3.943913	-2.916000
37	6	0	-7.252462	0.366697	-1.219297
38	6	0	7.436763	-0.632535	0.438313
39	6	0	1.562406	3.681898	0.215114
40	6	0	2.730037	4.322027	0.659100
41	6	0	2.788364	5.714591	0.760930
42	6	0	1.677212	6.483194	0.452101
43	6	0	0.479735	5.870298	0.019410
44	6	0	0.441409	4.459826	-0.122489
45	6	0	-0.700666	6.640195	-0.230785
46	6	0	-1.907832	6.017737	-0.582099
47	6	0	-1.994463	4.656032	-0.747014
48	6	0	-0.809605	3.759284	-0.609207
49	1	0	3.553217	1.848165	-0.039360
50	1	0	-3.201948	2.389285	0.149004
51	1	0	-1.027786	2.915794	1.353241
52	1	0	-4.732565	1.337264	-0.906397
53	1	0	-7.113387	-2.131213	-0.122392
54	1	0	-5.200129	-3.236976	0.905213
55	1	0	4.621180	-4.060239	-0.980028
56	1	0	6.796141	-3.172033	-0.344623
57	1	0	5.064704	0.661148	0.387885
58	1	0	-3.766113	-3.809071	2.221440
59	1	0	-1.836744	-4.804125	3.315065
60	1	0	0.683770	-1.698692	1.809264
61	1	0	-0.987460	-1.652036	-1.591340
62	1	0	0.835446	-5.291294	-2.880923
63	1	0	2.976865	-4.550563	-1.997952

64	1	0	0.919114	-4.968028	3.049045
65	1	0	1.673011	-3.373204	3.182917
66	1	0	0.571398	-3.948543	4.443629
67	1	0	-2.343972	-3.222004	-2.725421
68	1	0	-1.874335	-4.917754	-2.536381
69	1	0	-1.436039	-4.045053	-4.001549
70	1	0	-8.090015	0.454563	-0.518548
71	1	0	-7.609111	-0.221152	-2.072042
72	1	0	-7.008847	1.369047	-1.579454
73	1	0	7.382842	0.415809	0.742380
74	1	0	8.149189	-0.704843	-0.391102
75	1	0	7.857922	-1.204405	1.272423
76	1	0	3.592536	3.734899	0.955140
77	1	0	3.700559	6.190690	1.105539
78	1	0	1.708052	7.563196	0.560732
79	1	0	-0.656064	7.718589	-0.118333
80	1	0	-2.790241	6.629974	-0.742915
81	1	0	-2.930297	4.217517	-1.078397
82	1	0	-0.607767	3.319100	-1.600775

TS between radical cation of **S2'** and radical cation of **S2'**-INT-6ring

(UB3LYP/6-31G(d,p), gas phase) $E = -1849.473439$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.486045	1.571821	0.097500
2	6	0	2.482510	0.177943	-0.129259
3	6	0	1.239225	-0.484214	-0.285926
4	6	0	0.048652	0.196015	0.169756
5	6	0	0.089140	1.601536	0.347107
6	6	0	1.319301	2.301763	0.242594
7	6	0	-1.201137	-0.477533	0.505492
8	6	0	-2.431950	0.252139	0.342398

9	6	0	-2.389174	1.633141	0.418978
10	6	0	-1.160862	2.362010	0.538153
11	6	0	-3.700870	-0.478047	0.259061
12	6	0	3.730721	-0.576842	-0.244764
13	6	0	-4.863783	0.134599	-0.242949
14	6	0	-6.065194	-0.554815	-0.369422
15	6	0	-6.088750	-1.910194	0.012373
16	6	0	-4.956473	-2.534675	0.504062
17	6	0	-3.739684	-1.837156	0.648985
18	6	0	3.693980	-1.914390	-0.712246
19	6	0	4.897355	-2.651774	-0.715224
20	6	0	6.089470	-2.089559	-0.301206
21	6	0	6.145727	-0.754786	0.147688
22	6	0	4.963365	-0.028721	0.172221
23	6	0	-2.539654	-2.445857	1.217958
24	6	0	-2.580629	-3.686002	1.881251
25	6	0	-1.448520	-4.241443	2.451144
26	6	0	-0.203202	-3.577619	2.409346
27	6	0	-0.143816	-2.363662	1.749633
28	6	0	-1.278039	-1.776573	1.127249
29	6	0	2.437906	-2.457862	-1.221113
30	6	0	1.222235	-1.747546	-1.024005
31	6	0	0.051470	-2.223960	-1.658799
32	6	0	0.022878	-3.394585	-2.400258
33	6	0	1.222527	-4.123390	-2.525406
34	6	0	2.395626	-3.656245	-1.966163
35	6	0	1.005894	-4.174343	3.084092
36	6	0	-1.236978	-3.867353	-3.082284
37	6	0	-7.302749	0.108999	-0.918003
38	6	0	7.452025	-0.154097	0.603423
39	6	0	1.307372	3.782886	0.287814
40	6	0	2.342804	4.530031	0.850193
41	6	0	2.264516	5.930092	0.939809
42	6	0	1.127104	6.592541	0.521287
43	6	0	0.048241	5.867160	-0.041748
44	6	0	0.173459	4.461646	-0.217344

45	6	0	-1.177910	6.504832	-0.391949
46	6	0	-2.254952	5.779814	-0.902974
47	6	0	-2.136401	4.419465	-1.147681
48	6	0	-0.938512	3.693113	-0.814694
49	1	0	3.427678	2.104495	0.050012
50	1	0	-3.316809	2.187007	0.515223
51	1	0	-1.167840	3.089595	1.348837
52	1	0	-4.821450	1.164912	-0.582629
53	1	0	-7.008779	-2.478442	-0.092114
54	1	0	-5.014507	-3.584747	0.765334
55	1	0	4.895929	-3.687137	-1.034947
56	1	0	6.996059	-2.688471	-0.313325
57	1	0	4.996720	0.981478	0.565709
58	1	0	-3.522111	-4.212123	1.981884
59	1	0	-1.526750	-5.195566	2.965504
60	1	0	0.794491	-1.824284	1.737925
61	1	0	-0.857171	-1.636521	-1.601358
62	1	0	1.233794	-5.043567	-3.103357
63	1	0	3.309206	-4.211242	-2.142189
64	1	0	1.229134	-5.168134	2.680773
65	1	0	1.891150	-3.549255	2.946518
66	1	0	0.839662	-4.294210	4.160351
67	1	0	-2.084382	-3.213568	-2.860572
68	1	0	-1.501797	-4.881364	-2.762632
69	1	0	-1.111498	-3.898344	-4.170445
70	1	0	-8.111808	0.101551	-0.179179
71	1	0	-7.674165	-0.416526	-1.804420
72	1	0	-7.113571	1.148425	-1.197250
73	1	0	7.321460	0.869921	0.962410
74	1	0	8.181372	-0.132114	-0.214146
75	1	0	7.897751	-0.741104	1.413887
76	1	0	3.209001	4.021649	1.261136
77	1	0	3.086564	6.484237	1.380787
78	1	0	1.035900	7.667511	0.643357
79	1	0	-1.268215	7.576826	-0.243819
80	1	0	-3.173680	6.296229	-1.162090

81	1	0	-2.944703	3.886773	-1.639487
82	1	0	-0.648510	2.966305	-1.572587

Cation of **S2'** (B3LYP/6-31G(d,p), gas phase) $E = -1850.119715$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.542586	0.150417	0.259355
2	6	0	-1.638968	1.208590	-0.058962
3	6	0	-0.262470	0.920823	-0.345580
4	6	0	0.225094	-0.358180	0.027837
5	6	0	-0.742048	-1.447560	0.122098
6	6	0	-2.159372	-1.162760	0.305318
7	6	0	1.626435	-0.680439	0.320607
8	6	0	2.093678	-1.946200	-0.025205
9	6	0	1.117016	-3.007494	-0.442791
10	6	0	-0.301660	-2.707409	-0.163269
11	6	0	3.502140	-2.246505	-0.016982
12	6	0	-2.084788	2.588408	-0.030616
13	6	0	4.000904	-3.473472	-0.527102
14	6	0	5.354781	-3.750440	-0.594533
15	6	0	6.253175	-2.759929	-0.136077
16	6	0	5.799571	-1.562062	0.377316
17	6	0	4.419930	-1.270614	0.465969
18	6	0	-1.207472	3.621857	-0.472251
19	6	0	-1.637086	4.957490	-0.337373
20	6	0	-2.880460	5.269093	0.178663
21	6	0	-3.774970	4.260342	0.597197
22	6	0	-3.357763	2.945348	0.487197
23	6	0	3.911037	-0.048732	1.068405
24	6	0	4.754065	0.843846	1.770097
25	6	0	4.256155	1.963214	2.403003
26	6	0	2.874322	2.245752	2.392124
27	6	0	2.039970	1.385979	1.696236

28	6	0	2.521950	0.250321	1.005173
29	6	0	0.069380	3.276282	-1.086087
30	6	0	0.545566	1.942007	-1.020790
31	6	0	1.726357	1.608951	-1.717406
32	6	0	2.470345	2.548819	-2.418266
33	6	0	2.008157	3.878777	-2.434002
34	6	0	0.833047	4.226837	-1.796870
35	6	0	2.332697	3.441567	3.134489
36	6	0	3.724493	2.163923	-3.161584
37	6	0	5.873517	-5.054443	-1.145442
38	6	0	-3.119733	-2.251305	0.591691
39	6	0	-2.861580	-3.091001	1.671534
40	6	0	-3.778297	-4.084685	2.070426
41	6	0	-4.956654	-4.246935	1.379342
42	6	0	-5.259937	-3.436992	0.252994
43	6	0	-4.333063	-2.422712	-0.164728
44	6	0	-6.463037	-3.624618	-0.477939
45	6	0	-6.743083	-2.862181	-1.588453
46	6	0	-5.818644	-1.884882	-2.021346
47	6	0	-4.644707	-1.672245	-1.330872
48	6	0	-5.126198	4.621170	1.160145
49	1	0	-3.583139	0.380336	0.438689
50	1	0	1.369624	-3.960266	0.042489
51	1	0	1.201761	-3.235891	-1.520210
52	1	0	-1.019881	-3.515463	-0.259226
53	1	0	3.309868	-4.221629	-0.900268
54	1	0	7.322368	-2.945964	-0.190078
55	1	0	6.528618	-0.832318	0.707874
56	1	0	-0.980058	5.767540	-0.628858
57	1	0	-3.172803	6.311742	0.269730
58	1	0	-4.029673	2.175898	0.846502
59	1	0	5.814127	0.635086	1.847333
60	1	0	4.933690	2.620537	2.941042
61	1	0	0.975657	1.584623	1.710227
62	1	0	2.059501	0.579054	-1.733389
63	1	0	2.565917	4.634916	-2.979491

64	1	0	0.481515	5.247813	-1.882260
65	1	0	2.784595	4.370093	2.768052
66	1	0	1.249077	3.528120	3.022613
67	1	0	2.557329	3.377830	4.205012
68	1	0	4.585962	2.735932	-2.799592
69	1	0	3.953075	1.102039	-3.043198
70	1	0	3.629321	2.372509	-4.232981
71	1	0	6.458004	-5.594669	-0.392487
72	1	0	5.059901	-5.707451	-1.470728
73	1	0	6.534304	-4.886166	-2.002931
74	1	0	-1.956865	-2.943136	2.253019
75	1	0	-3.554676	-4.704802	2.932271
76	1	0	-5.673893	-5.003233	1.685318
77	1	0	-7.157616	-4.391063	-0.146275
78	1	0	-7.664955	-3.016211	-2.140011
79	1	0	-6.032206	-1.300850	-2.911240
80	1	0	-3.941447	-0.931033	-1.692720
81	1	0	-5.690432	3.732998	1.454335
82	1	0	-5.028139	5.265675	2.040475
83	1	0	-5.723661	5.171289	0.424823

Cation of **S2'**-INT-5ring (B3LYP/6-31G(d,p), gas phase) $E = -1850.113826$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.702624	0.183057	-0.087887
2	6	0	-1.876015	1.296560	-0.181019
3	6	0	-0.442080	1.127684	-0.352361
4	6	0	0.143578	-0.131160	0.034310
5	6	0	-0.724118	-1.201311	0.098684
6	6	0	-2.130652	-1.109115	-0.067550
7	6	0	1.574542	-0.457143	0.309175
8	6	0	2.039609	-1.703442	-0.087784
9	6	0	1.045904	-2.753304	-0.575436

10	6	0	-0.253449	-2.610947	0.227732
11	6	0	3.450450	-2.009317	-0.033097
12	6	0	-2.435743	2.655889	-0.142378
13	6	0	3.978781	-3.195486	-0.606010
14	6	0	5.334208	-3.475097	-0.622906
15	6	0	6.211042	-2.533417	-0.040475
16	6	0	5.731876	-1.372279	0.528604
17	6	0	4.349916	-1.073791	0.557131
18	6	0	-1.645788	3.747654	-0.570345
19	6	0	-2.188643	5.044894	-0.468813
20	6	0	-3.464347	5.256978	0.021459
21	6	0	-4.263213	4.180509	0.449594
22	6	0	-3.727102	2.900249	0.364946
23	6	0	3.823043	0.124446	1.185927
24	6	0	4.634259	0.992125	1.955643
25	6	0	4.113413	2.100479	2.588090
26	6	0	2.736836	2.402819	2.504208
27	6	0	1.933968	1.569825	1.744119
28	6	0	2.440036	0.437000	1.061341
29	6	0	-0.315113	3.495514	-1.120536
30	6	0	0.288658	2.209645	-0.984395
31	6	0	1.555357	1.983077	-1.581158
32	6	0	2.245722	2.970183	-2.264443
33	6	0	1.647057	4.242749	-2.357748
34	6	0	0.400955	4.491815	-1.809500
35	6	0	2.169999	3.591747	3.239421
36	6	0	3.584079	2.701322	-2.905122
37	6	0	5.875807	-4.735879	-1.249089
38	6	0	-5.644693	4.422189	1.003855
39	6	0	-2.657495	-2.422127	-0.143810
40	6	0	-1.508610	-3.401778	-0.236744
41	6	0	-1.787702	-4.759590	0.319877
42	6	0	-3.053423	-5.157364	0.533706
43	6	0	-4.188882	-4.292474	0.249158
44	6	0	-3.998334	-2.918137	-0.125223
45	6	0	-5.497147	-4.786350	0.360307

46	6	0	-6.592724	-3.977758	0.083655
47	6	0	-6.411243	-2.642535	-0.313603
48	6	0	-5.134452	-2.119400	-0.405604
49	1	0	-3.773737	0.319281	-0.063662
50	1	0	0.830967	-2.634680	-1.648492
51	1	0	1.457930	-3.754645	-0.442547
52	1	0	-0.049473	-2.846186	1.282019
53	1	0	3.310389	-3.905534	-1.080151
54	1	0	7.280656	-2.725192	-0.045461
55	1	0	6.443336	-0.672208	0.949860
56	1	0	-1.595784	5.904039	-0.759112
57	1	0	-3.848081	6.270861	0.093023
58	1	0	-4.318759	2.076299	0.750218
59	1	0	5.687911	0.773606	2.081157
60	1	0	4.766745	2.737925	3.177780
61	1	0	0.872699	1.783324	1.699401
62	1	0	1.987854	0.992896	-1.532803
63	1	0	2.162132	5.038159	-2.889878
64	1	0	-0.037233	5.472701	-1.947124
65	1	0	2.658405	4.520792	2.924384
66	1	0	1.096751	3.699957	3.063043
67	1	0	2.325906	3.500444	4.320299
68	1	0	4.351519	3.374078	-2.506907
69	1	0	3.914010	1.674997	-2.728398
70	1	0	3.545085	2.863570	-3.988002
71	1	0	6.577146	-4.506406	-2.059087
72	1	0	6.422529	-5.338038	-0.514711
73	1	0	5.076612	-5.356099	-1.663035
74	1	0	-5.616369	5.118591	1.848716
75	1	0	-6.300068	4.865500	0.245645
76	1	0	-6.109632	3.494915	1.348018
77	1	0	-1.382280	-3.553224	-1.329792
78	1	0	-0.950919	-5.434226	0.474392
79	1	0	-3.265108	-6.158321	0.897483
80	1	0	-5.647315	-5.819459	0.657935
81	1	0	-7.595870	-4.384239	0.165644

82	1	0	-7.270291	-2.025872	-0.555083
83	1	0	-5.000676	-1.102850	-0.752203

TS between cation of **S2'** and cation of **S2'**-INT-5ring

(B3LYP/6-31G(d,p), gas phase) $E = -1850.079638$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.676155	-0.270190	-0.251774
2	6	0	1.778920	-1.347135	-0.340158
3	6	0	0.357134	-1.104683	-0.460125
4	6	0	-0.140996	0.180064	-0.097902
5	6	0	0.794935	1.235747	-0.063449
6	6	0	2.190682	1.033569	-0.220916
7	6	0	-1.536375	0.538543	0.289475
8	6	0	-1.992591	1.806455	-0.023754
9	6	0	-1.015682	2.868278	-0.544302
10	6	0	0.353906	2.599641	-0.000192
11	6	0	-3.384093	2.159604	0.116525
12	6	0	2.268822	-2.727195	-0.321059
13	6	0	-3.904682	3.380231	-0.385898
14	6	0	-5.250816	3.695921	-0.320970
15	6	0	-6.122622	2.756038	0.272355
16	6	0	-5.648038	1.563417	0.776673
17	6	0	-4.275471	1.228105	0.724223
18	6	0	1.391134	-3.790963	-0.645763
19	6	0	1.871995	-5.110230	-0.526474
20	6	0	3.170161	-5.374261	-0.129199
21	6	0	4.060739	-4.329097	0.183139
22	6	0	3.587216	-3.027895	0.088161
23	6	0	-3.744113	0.004438	1.296947
24	6	0	-4.533948	-0.850049	2.102688
25	6	0	-4.007623	-1.976653	2.696371

26	6	0	-2.645016	-2.308747	2.536586
27	6	0	-1.864704	-1.490600	1.737751
28	6	0	-2.379191	-0.343235	1.086996
29	6	0	0.042448	-3.491171	-1.125836
30	6	0	-0.472360	-2.172192	-1.023503
31	6	0	-1.734180	-1.890252	-1.593937
32	6	0	-2.515560	-2.863192	-2.201348
33	6	0	-2.008243	-4.174625	-2.252871
34	6	0	-0.758273	-4.473464	-1.741125
35	6	0	-2.066233	-3.514295	3.234244
36	6	0	-3.857006	-2.532416	-2.806442
37	6	0	-5.788564	4.992472	-0.872473
38	6	0	5.470628	-4.628442	0.627274
39	6	0	2.867513	2.299836	-0.458751
40	6	0	2.061522	3.228328	-1.196121
41	6	0	2.466337	4.594403	-1.338710
42	6	0	3.653253	5.005459	-0.808552
43	6	0	4.510278	4.097822	-0.102160
44	6	0	4.112671	2.730189	0.094853
45	6	0	5.734146	4.541767	0.442631
46	6	0	6.539063	3.683435	1.167927
47	6	0	6.132733	2.352859	1.400706
48	6	0	4.939470	1.889750	0.887577
49	1	0	3.736804	-0.453460	-0.351446
50	1	0	-0.995119	2.848303	-1.644476
51	1	0	-1.349658	3.862858	-0.250040
52	1	0	0.739762	3.265931	0.763112
53	1	0	-3.242970	4.089632	-0.870766
54	1	0	-7.185434	2.975191	0.328012
55	1	0	-6.356211	0.867333	1.209779
56	1	0	1.213450	-5.945438	-0.732427
57	1	0	3.503545	-6.404978	-0.044577
58	1	0	4.255547	-2.225452	0.380399
59	1	0	-5.572231	-0.604269	2.290021
60	1	0	-4.643113	-2.603259	3.316322
61	1	0	-0.813836	-1.729358	1.635259

62	1	0	-2.101326	-0.872108	-1.584877
63	1	0	-2.592365	-4.958401	-2.727585
64	1	0	-0.381760	-5.482966	-1.853591
65	1	0	-2.588523	-4.430455	2.936361
66	1	0	-1.005745	-3.642414	3.003181
67	1	0	-2.166810	-3.429107	4.322139
68	1	0	-4.099891	-1.473432	-2.690323
69	1	0	-3.879966	-2.770155	-3.875710
70	1	0	-4.655598	-3.113167	-2.331627
71	1	0	-6.537999	4.811055	-1.650894
72	1	0	-6.278394	5.581180	-0.088790
73	1	0	-4.995330	5.606469	-1.306633
74	1	0	5.479325	-5.272723	1.513117
75	1	0	6.026677	-5.154337	-0.156839
76	1	0	6.019236	-3.714971	0.870539
77	1	0	1.429876	2.827013	-1.981357
78	1	0	1.850206	5.274216	-1.917783
79	1	0	3.987113	6.031004	-0.935919
80	1	0	6.032928	5.574340	0.289924
81	1	0	7.478993	4.038836	1.577907
82	1	0	6.756260	1.696216	1.998396
83	1	0	4.619666	0.878545	1.105171

Cation of **S2'**-INT-6ring (B3LYP/6-31G(d,p), gas phase) $E = -1850.101641$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.443862	1.609545	-0.094465
2	6	0	2.501745	0.225012	-0.313481
3	6	0	1.281875	-0.503242	-0.450398
4	6	0	0.056693	0.162048	-0.110167
5	6	0	0.033006	1.561268	-0.055168
6	6	0	1.236392	2.296854	-0.014483
7	6	0	-1.222576	-0.521795	0.244165

8	6	0	-2.402556	0.036249	-0.216120
9	6	0	-2.305559	1.391109	-0.876807
10	6	0	-1.321990	2.255000	-0.065030
11	6	0	-3.666703	-0.634750	-0.042244
12	6	0	3.788860	-0.480529	-0.358709
13	6	0	-4.856418	-0.171978	-0.661887
14	6	0	-6.062081	-0.843940	-0.554957
15	6	0	-6.089365	-2.033903	0.204381
16	6	0	-4.950770	-2.511534	0.821123
17	6	0	-3.714003	-1.834363	0.726191
18	6	0	3.817407	-1.857606	-0.688828
19	6	0	5.055927	-2.533219	-0.628289
20	6	0	6.223081	-1.878872	-0.287302
21	6	0	6.216251	-0.504442	0.019655
22	6	0	4.999378	0.161355	-0.016265
23	6	0	-2.511715	-2.300293	1.397243
24	6	0	-2.534549	-3.374092	2.316988
25	6	0	-1.265454	-1.651798	1.156471
26	6	0	2.589347	-2.521361	-1.120570
27	6	0	1.338219	-1.856051	-1.011395
28	6	0	0.193306	-2.480556	-1.558680
29	6	0	0.228088	-3.739889	-2.137572
30	6	0	1.466793	-4.407600	-2.186667
31	6	0	2.612753	-3.806009	-1.705118
32	6	0	1.173213	3.750193	0.222165
33	6	0	2.226108	4.488234	0.790556
34	6	0	2.132540	5.868360	1.037175
35	6	0	0.964516	6.545802	0.757941
36	6	0	-0.133705	5.831451	0.205802
37	6	0	-0.016133	4.434580	-0.072463
38	6	0	-1.358360	6.471653	-0.053381
39	6	0	-2.480449	5.794337	-0.574511
40	6	0	-2.392131	4.460212	-0.868884
41	6	0	-1.145644	3.684230	-0.699659
42	6	0	1.064105	-3.561706	3.543322
43	6	0	-1.011362	-4.376032	-2.716243

44	6	0	-7.312865	-0.342588	-1.232813
45	6	0	7.494470	0.204567	0.392500
46	6	0	-0.123258	-2.082121	1.876616
47	6	0	-1.397884	-3.783093	2.982758
48	6	0	-0.163383	-3.128875	2.781034
49	1	0	3.366795	2.172332	-0.053357
50	1	0	-1.943183	1.318744	-1.913877
51	1	0	-3.288590	1.860218	-0.904400
52	1	0	-1.713655	2.374975	0.956251
53	1	0	-4.829217	0.723212	-1.274232
54	1	0	-7.020361	-2.586332	0.298488
55	1	0	-5.016985	-3.438546	1.377828
56	1	0	5.102362	-3.594788	-0.838882
57	1	0	7.156788	-2.433323	-0.247779
58	1	0	4.996075	1.208989	0.263141
59	1	0	-3.467921	-3.880424	2.531576
60	1	0	-0.749999	-1.950846	-1.554035
61	1	0	1.528727	-5.394649	-2.637225
62	1	0	3.554220	-4.329931	-1.815654
63	1	0	3.138242	3.974259	1.073536
64	1	0	2.978826	6.390141	1.470802
65	1	0	0.864654	7.606553	0.963947
66	1	0	-1.442324	7.533548	0.166249
67	1	0	-3.403396	6.338396	-0.742815
68	1	0	-3.252209	3.951349	-1.291906
69	1	0	-0.824921	3.450189	-1.741188
70	1	0	1.303713	-4.611650	3.340691
71	1	0	1.936530	-2.961187	3.274135
72	1	0	0.912046	-3.471773	4.624895
73	1	0	-1.235703	-5.325721	-2.217551
74	1	0	-1.884139	-3.727437	-2.606904
75	1	0	-0.884858	-4.596742	-3.782119
76	1	0	-7.709185	-1.085978	-1.933348
77	1	0	-8.104052	-0.138962	-0.502422
78	1	0	-7.127292	0.578326	-1.791953
79	1	0	7.971800	-0.266206	1.259039

80	1	0	8.218890	0.170291	-0.429066
81	1	0	7.316513	1.255113	0.637007
82	1	0	0.815605	-1.562678	1.732699
83	1	0	-1.457938	-4.608399	3.687243

TS between cation of **S2'** and cation of **S2'**-INT-6ring

(B3LYP/6-31G(d,p), gas phase) $E = -1850.079659$ Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.504472	1.502414	0.106050
2	6	0	2.462039	0.115455	-0.184097
3	6	0	1.199783	-0.516130	-0.390736
4	6	0	0.023235	0.185698	0.025249
5	6	0	0.095622	1.597763	0.186969
6	6	0	1.360647	2.259741	0.223219
7	6	0	-1.259407	-0.468953	0.395461
8	6	0	-2.432447	0.213377	0.139756
9	6	0	-2.364730	1.668513	-0.304434
10	6	0	-1.132121	2.356252	0.216049
11	6	0	-3.714782	-0.435362	0.230866
12	6	0	3.687156	-0.669710	-0.260368
13	6	0	-4.907837	0.187120	-0.220475
14	6	0	-6.133499	-0.454623	-0.196812
15	6	0	-6.177675	-1.776887	0.300016
16	6	0	-5.038309	-2.406936	0.755349
17	6	0	-3.779289	-1.764090	0.744340
18	6	0	3.631479	-2.010463	-0.727116
19	6	0	4.818539	-2.772570	-0.700050
20	6	0	6.012776	-2.235973	-0.259553
21	6	0	6.090707	-0.900927	0.189488
22	6	0	4.926572	-0.149738	0.184722
23	6	0	-2.576573	-2.382045	1.273986

24	6	0	-2.617076	-3.597776	1.997172
25	6	0	-1.315955	-1.740561	1.108305
26	6	0	2.376701	-2.538633	-1.252223
27	6	0	1.170750	-1.807744	-1.083686
28	6	0	-0.003777	-2.290295	-1.703066
29	6	0	-0.039764	-3.478730	-2.417985
30	6	0	1.154807	-4.215247	-2.534105
31	6	0	2.329579	-3.748416	-1.978028
32	6	0	1.392864	3.732473	0.374207
33	6	0	2.333160	4.382566	1.166850
34	6	0	2.269665	5.772335	1.395027
35	6	0	1.221948	6.513870	0.893747
36	6	0	0.235921	5.888207	0.087648
37	6	0	0.372787	4.505764	-0.240564
38	6	0	-0.917634	6.582716	-0.363313
39	6	0	-1.902643	5.962230	-1.123082
40	6	0	-1.724698	4.642398	-1.541995
41	6	0	-0.611696	3.885404	-1.113450
42	6	0	0.990743	-4.078120	3.101409
43	6	0	-1.308891	-3.967000	-3.070453
44	6	0	-7.390478	0.215694	-0.691585
45	6	0	7.400302	-0.331654	0.674240
46	6	0	-0.177873	-2.314921	1.722788
47	6	0	-1.482722	-4.146333	2.555168
48	6	0	-0.234724	-3.497316	2.441316
49	1	0	3.462087	2.005452	0.133762
50	1	0	-2.371719	1.699521	-1.402898
51	1	0	-3.250158	2.212434	0.026583
52	1	0	-1.275919	3.091270	1.000950
53	1	0	-4.870090	1.191148	-0.629074
54	1	0	-7.125980	-2.306985	0.320681
55	1	0	-5.120222	-3.425049	1.116277
56	1	0	4.802056	-3.808736	-1.015334
57	1	0	6.905272	-2.855783	-0.249845
58	1	0	4.977714	0.860704	0.573701
59	1	0	-3.563702	-4.102008	2.149413

60	1	0	-0.912232	-1.704766	-1.642278
61	1	0	1.159866	-5.146983	-3.093186
62	1	0	3.238491	-4.315016	-2.139887
63	1	0	3.107881	3.801692	1.657228
64	1	0	3.023625	6.244142	2.016354
65	1	0	1.124216	7.569150	1.128778
66	1	0	-1.030640	7.628252	-0.089347
67	1	0	-2.774800	6.523363	-1.440917
68	1	0	-2.429571	4.199708	-2.239406
69	1	0	-0.278601	3.101728	-1.784133
70	1	0	1.877741	-3.469068	2.910155
71	1	0	0.859032	-4.151641	4.186839
72	1	0	1.192596	-5.090970	2.735095
73	1	0	-1.182944	-4.074035	-4.153642
74	1	0	-1.595951	-4.950965	-2.683085
75	1	0	-2.141735	-3.282157	-2.892866
76	1	0	-7.843922	-0.350001	-1.513112
77	1	0	-8.141543	0.281148	0.103544
78	1	0	-7.193127	1.229138	-1.050450
79	1	0	7.805863	-0.920962	1.503914
80	1	0	8.152339	-0.340919	-0.122634
81	1	0	7.289034	0.699975	1.017420
82	1	0	0.773685	-1.803100	1.656132
83	1	0	-1.554563	-5.076707	3.111954
