Boron Monoxide Dimer as a Building Block for Boroxine Based Buckyballs and Related Cages: A Theoretical Study

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Theoretical Method:

Floppy Energy Surfaces:

Table S1-S15: Theoretical Cartesian coordinates for all compounds.

Theoretical Method:

The computations were performed using the popular B3LYP method, which is a hybrid HF/DFT method combining the three-parameter Becke functional (B3) with the Lee-Yang-Parr (LYP) generalized gradient correlation functional.[1,2] All computations were performed using double-ζ plus polarization (DZP) basis sets. The DZP basis sets used for boron and oxygen add one set of pure spherical harmonic d functions with orbital exponents $\alpha_d(B) = 0.70$ and $\alpha_d(O) = 0.85$ to the standard Huzinaga-Dunning contracted DZ sets.[3,4,5]

The geometries of all structures were fully optimized using the B3LYP/DZP method. Vibrational frequencies were determined by evaluating analytically the second derivatives of the energy with respect to the nuclear coordinates. All of the computations were carried out with the Gaussian 09 program,[6] exercising the fine grid option (75 radial shells, 302 angular points) for evaluating integrals numerically,[7] while the tight (10^{-8} hartree) designation is the default for the self-consistent field (SCF) convergence. The reported free energies (ΔG) were obtained by applying zero point energy corrections to the initially obtained ΔH values. An analytical frequency calculation was carried out for the polymer c-B_{30}. However, the basis sets are too larger for the larger polymers for such frequency calculations.
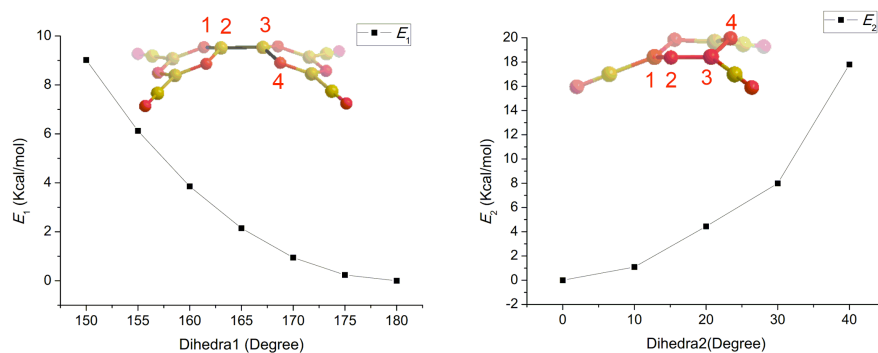
Floppy Energy Surfaces:

Figure S2. Potential energy surfaces around two B_3O_3 rings and in a single B_3O_3 ring.

The intrinsicly rippled graphene[8] leads to low-dimensional materials, such as nanotubes, by coupling reactive boundary carbon atoms.[9] In our earlier reported largest planar $(B_2O_2)_{84}$ structure[10], 34 vibrational frequencies less than 50 cm^{-1} in all were found for the bending around B_3O_3 rings or in a single B_3O_3 ring, suggesting the wrinkled surface of planar polymers. Furthermore, the energy surfaces around the OBBO dihedral angle in $(B_2O_2)_5$ and the BOBO dihedral angle in $(B_2O_2)_6$ are predicted in Figure S2. The data indicate that bending the OBBO or BOBO dihedral angle by 20° only increases the electronic energies by less than 4 kcal/mol. This is the direct indication of a wrinkled surface in the planar $(B_2O_2)_x$ polymers.

Table S1: Theoretical Cartesian coordinates for *c*-B$_6$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.617658	-0.617658	2.276000
2	5	0	0.617658	0.617658	2.276000
3	5	0	0.617658	2.276000	0.617658
4	5	0	-0.617658	2.276000	-0.617658
5	5	0	-0.617658	0.617658	-2.276000
6	5	0	0.617658	-0.617658	-2.276000
7	5	0	2.276000	-0.617658	-0.617658
8	5	0	2.276000	0.617658	0.617658
9	5	0	-2.276000	0.617658	-0.617658
10	5	0	-2.276000	-0.617658	0.617658
11	5	0	-0.617658	-2.276000	0.617658
12	5	0	0.617658	-2.276000	-0.617658
13	8	0	1.887989	-1.887989	-0.203296
14	8	0	0.203296	-1.887989	-1.887989
15	8	0	1.887989	-0.203296	-1.887989
16	8	0	-1.887989	1.887989	-0.203296
17	8	0	-0.203296	1.887989	-1.887989
18	8	0	-1.887989	0.203296	-1.887989
19	8	0	1.887989	0.203296	1.887989
20	8	0	0.203296	1.887989	1.887989
21	8	0	1.887989	1.887989	0.203296
22	8	0	-1.887989	-0.203296	1.887989
23	8	0	-1.887989	-1.887989	0.203296
24	8	0	-0.203296	-1.887989	1.887989

SCF Done: E(RB3LYP) =   -1202.03625749

Table S2: Theoretical Cartesian coordinates for *c*-B₉.

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	0.000000	2.752562	0.865004
2	5	0	0.000000	2.752562	-0.865004
3	5	0	-2.383789	-1.376281	0.865004
4	5	0	-2.383789	-1.376281	-0.865004
5	5	0	2.383789	-1.376281	0.865004
6	5	0	2.383789	-1.376281	-0.865004
7	5	0	-2.038253	0.171245	2.651612
8	5	0	-1.167429	1.679556	2.651612
9	5	0	2.038253	0.171245	2.651612
10	5	0	1.167429	1.679556	2.651612
11	5	0	0.870824	-1.850801	2.651612
12	5	0	-0.870824	-1.850801	2.651612
13	5	0	-0.870824	-1.850801	-2.651612
14	5	0	0.870824	-1.850801	-2.651612
15	5	0	2.038253	0.171245	-2.651612
16	5	0	1.167429	1.679556	-2.651612
17	5	0	-1.167429	1.679556	-2.651612
18	5	0	-2.038253	0.171245	-2.651612
19	8	0	-2.748688	-0.207527	1.522517
20	8	0	-1.554068	-2.276670	1.522517
21	8	0	-1.442259	-0.832689	3.403167
22	8	0	1.554068	-2.276670	1.522517
23	8	0	1.442259	-0.832689	3.403167
24	8	0	2.748688	-0.207527	1.522517
25	8	0	-1.194620	2.484197	1.522517
26	8	0	0.000000	1.665377	3.403167
27	8	0	1.194620	2.484197	1.522517
28	8	0	-1.194620	2.484197	-1.522517
29	8	0	1.194620	2.484197	-1.522517
30	8	0	0.000000	1.665377	-3.403167
31	8	0	2.748688	-0.207527	-1.522517
32	8	0	1.554068	-2.276670	-1.522517
33	8	0	1.442259	-0.832689	-3.403167
34	8	0	-2.748688	-0.207527	-1.522517
35	8	0	-1.442259	-0.832689	-3.403167
36	8	0	-1.554068	-2.276670	-1.522517

SCF Done: E(RB3LYP) =   -1803.19584768

Table S3: Theoretical Cartesian coordinates for *c*-B₁₂.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.557417	-0.865756	2.557250
2	5	0	-2.557417	0.865756	2.557250
3	5	0	-2.557250	2.557417	0.865756
4	5	0	-0.865756	2.557250	2.557417
5	5	0	-2.557250	-2.557417	0.865756
6	5	0	-2.557250	-2.557417	-0.865756
7	5	0	-0.865756	-2.557250	2.557417
8	5	0	0.865756	-2.557250	2.557417
9	5	0	2.557417	-0.865756	2.557250
10	5	0	2.557417	0.865756	2.557250
11	5	0	0.865756	2.557250	2.557417
12	5	0	2.557250	2.557417	0.865756
13	5	0	2.557250	2.557417	-0.865756
14	5	0	2.557250	-2.557417	0.865756
15	5	0	2.557250	-2.557417	-0.865756
16	5	0	0.865756	-2.557250	-2.557417
17	5	0	2.557417	-0.865756	-2.557250
18	5	0	-2.557417	-0.865756	-2.557250
19	5	0	-2.557417	0.865756	-2.557250
20	5	0	-0.865756	2.557250	-2.557417
21	5	0	0.865756	2.557250	-2.557417
22	5	0	2.557417	0.865756	-2.557250
23	8	0	-3.204062	-1.520312	1.521184
24	8	0	-1.521184	-3.204062	1.520312
25	8	0	-1.520312	-1.521184	3.204062
26	8	0	1.520312	-1.521184	3.204062
27	8	0	3.204062	1.520312	1.521184
28	8	0	1.520312	1.521184	3.204062
29	8	0	-1.520312	1.521184	3.204062
30	8	0	1.521184	3.204062	1.520312
31	8	0	-3.204062	1.520312	1.521184
32	8	0	-1.521184	3.204062	1.520312
33	8	0	-3.204062	1.520312	-1.521184
34	8	0	-1.521184	3.204062	-1.520312
35	8	0	-1.520312	1.521184	-3.204062
36	8	0	-3.204062	-1.520312	-1.521184
37	8	0	-1.521184	-3.204062	-1.520312
38	8	0	-1.520312	-1.521184	-3.204062
39	8	0	1.520312	-1.521184	-3.204062
40	8	0	1.521184	-3.204062	-1.520312
41	8	0	3.204062	-1.520312	-1.521184
42	8	0	1.521184	-3.204062	1.520312
43	8	0	3.204062	-1.520312	1.521184
44	8	0	1.521184	3.204062	-1.520312
45	8	0	3.204062	1.520312	-1.521184
46	8	0	1.520312	1.521184	-3.204062
47	5	0	-0.865756	-2.557250	-2.557417
48	5	0	-2.557250	2.557417	-0.865756

SCF Done: E(RB3LYP) = -2404.39165428

Table S4: Theoretical Cartesian coordinates for *c*-B$_{15}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	0.000000	4.403407	0.865971
2	5	0	0.000000	4.403407	-0.865971
3	5	0	-4.187889	1.360728	0.865971
4	5	0	-4.187889	1.360728	-0.865971
5	5	0	-2.588258	-3.562431	0.865971
6	5	0	-2.588258	-3.562431	-0.865971
7	5	0	2.588258	-3.562431	0.865971
8	5	0	2.588258	-3.562431	-0.865971
9	5	0	4.187889	1.360728	0.865971
10	5	0	4.187889	1.360728	-0.865971
11	5	0	-0.864625	-3.238506	-2.488483
12	5	0	0.864625	-3.238506	-2.488483
13	5	0	1.204050	3.128220	-2.488483
14	5	0	2.603042	2.111793	-2.488483
15	5	0	-1.204050	3.128220	-2.488483
16	5	0	-2.603042	2.111793	-2.488483
17	5	0	-3.347186	-0.178446	-2.488483
18	5	0	-2.812818	-1.823060	-2.488483
19	5	0	2.812818	-1.823060	-2.488483
20	5	0	3.347186	-0.178446	-2.488483
21	5	0	-1.204050	3.128220	2.488483
22	5	0	-2.603042	2.111793	2.488483
23	5	0	1.204050	3.128220	2.488483
24	5	0	2.603042	2.111793	2.488483
25	5	0	3.347186	-0.178446	2.488483
26	5	0	2.812818	-1.823060	2.488483
27	5	0	0.864625	-3.238506	2.488483
28	5	0	-0.864625	-3.238506	2.488483
29	5	0	-2.812818	-1.823060	2.488483
30	5	0	-3.347186	-0.178446	2.488483
31	8	0	-1.604083	-2.207831	-3.049933
32	8	0	-3.381725	-2.638471	-1.522660
33	8	0	-1.464324	-4.031544	-1.522660
34	8	0	3.381725	-2.638471	-1.522660
35	8	0	1.604083	-2.207831	-3.049933
36	8	0	1.464324	-4.031544	-1.522660
37	8	0	3.554345	2.400879	-1.522660
38	8	0	4.286727	0.146840	-1.522660
39	8	0	2.595461	0.843316	-3.049933
40	8	0	-2.595461	0.843316	-3.049933
41	8	0	-3.554345	2.400879	-1.522660
42	8	0	-4.286727	0.146840	-1.522660
43	8	0	1.185019	4.122296	-1.522660
44	8	0	-1.185019	4.122296	-1.522660
45	8	0	0.000000	2.729029	-3.049933
46	8	0	2.595461	0.843316	3.049933
47	8	0	4.286727	0.146840	1.522660
48	8	0	3.554345	2.400879	1.522660
49	8	0	0.000000	2.729029	3.049933
50	8	0	-1.185019	4.122296	1.522660
51	8	0	1.185019	4.122296	1.522660

52	8	0	-2.595461	0.843316	3.049933
53	8	0	-4.286727	0.146840	1.522660
54	8	0	-3.554345	2.400879	1.522660
55	8	0	-1.604083	-2.207831	3.049933
56	8	0	-1.464324	-4.031544	1.522660
57	8	0	-3.381725	-2.638471	1.522660
58	8	0	3.381725	-2.638471	1.522660
59	8	0	1.464324	-4.031544	1.522660
60	8	0	1.604083	-2.207831	3.049933

SCF Done: E(RB3LYP) =   -3005.53814743

Table S5: Theoretical Cartesian coordinates for *c*-B$_{18}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	0.000000	5.137205	0.865965
2	5	0	0.000000	5.137205	-0.865965
3	5	0	4.448950	2.568603	0.865965
4	5	0	4.448950	2.568603	-0.865965
5	5	0	-4.448950	2.568603	0.865965
6	5	0	-4.448950	2.568603	-0.865965
7	5	0	4.448950	-2.568603	0.865965
8	5	0	4.448950	-2.568603	-0.865965
9	5	0	-4.448950	-2.568603	0.865965
10	5	0	-4.448950	-2.568603	-0.865965
11	5	0	0.000000	-5.137205	0.865965
12	5	0	0.000000	-5.137205	-0.865965
13	5	0	3.912669	0.865849	2.451123
14	5	0	3.912669	-0.865849	2.451123
15	5	0	2.706182	-2.955546	2.451123
16	5	0	1.206487	-3.821395	2.451123
17	5	0	-1.206487	-3.821395	2.451123
18	5	0	-2.706182	-2.955546	2.451123
19	5	0	-3.912669	-0.865849	2.451123
20	5	0	-3.912669	0.865849	2.451123
21	5	0	-2.706182	2.955546	2.451123
22	5	0	-1.206487	3.821395	2.451123
23	5	0	1.206487	3.821395	2.451123
24	5	0	2.706182	2.955546	2.451123
25	5	0	-1.206487	-3.821395	-2.451123
26	5	0	-2.706182	-2.955546	-2.451123
27	5	0	-3.912669	-0.865849	-2.451123
28	5	0	-3.912669	0.865849	-2.451123
29	5	0	-2.706182	2.955546	-2.451123
30	5	0	-1.206487	3.821395	-2.451123
31	5	0	1.206487	3.821395	-2.451123
32	5	0	2.706182	2.955546	-2.451123
33	5	0	3.912669	0.865849	-2.451123
34	5	0	3.912669	-0.865849	-2.451123
35	5	0	2.706182	-2.955546	-2.451123
36	5	0	1.206487	-3.821395	-2.451123
37	8	0	2.908531	-1.679241	2.960446
38	8	0	1.179873	-4.853628	1.525887
39	8	0	4.793302	-1.405014	1.525887
40	8	0	2.908531	1.679241	2.960446
41	8	0	3.613429	3.448614	1.525887
42	8	0	4.793302	1.405014	1.525887
43	8	0	-1.179873	4.853628	1.525887
44	8	0	1.179873	4.853628	1.525887
45	8	0	0.000000	3.358483	2.960446
46	8	0	-2.908531	1.679241	2.960446
47	8	0	-4.793302	1.405014	1.525887
48	8	0	-3.613429	3.448614	1.525887
49	8	0	0.000000	-3.358483	2.960446
50	8	0	3.613429	-3.448614	1.525887
51	8	0	-1.179873	-4.853628	1.525887

52	8	0	-4.793302	-1.405014	1.525887
53	8	0	-3.613429	-3.448614	1.525887
54	8	0	-2.908531	-1.679241	2.960446
55	8	0	-1.179873	4.853628	-1.525887
56	8	0	0.000000	3.358483	-2.960446
57	8	0	1.179873	4.853628	-1.525887
58	8	0	2.908531	1.679241	-2.960446
59	8	0	4.793302	1.405014	-1.525887
60	8	0	3.613429	3.448614	-1.525887
61	8	0	2.908531	-1.679241	-2.960446
62	8	0	3.613429	-3.448614	-1.525887
63	8	0	4.793302	-1.405014	-1.525887
64	8	0	1.179873	-4.853628	-1.525887
65	8	0	-1.179873	-4.853628	-1.525887
66	8	0	0.000000	-3.358483	-2.960446
67	8	0	-4.793302	-1.405014	-1.525887
68	8	0	-3.613429	-3.448614	-1.525887
69	8	0	-2.908531	-1.679241	-2.960446
70	8	0	-2.908531	1.679241	-2.960446
71	8	0	-3.613429	3.448614	-1.525887
72	8	0	-4.793302	1.405014	-1.525887

SCF Done: E(RB3LYP) =   -3606.65495566

Table S6: Theoretical Cartesian coordinates for *t*-B$_{18}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-3.516638	1.037024	-5.162021
2	5	0	-2.656408	2.526986	-5.162021
3	5	0	2.656408	2.526986	-5.162021
4	5	0	3.516638	1.037024	-5.162021
5	5	0	0.000000	5.054110	-0.859278
6	5	0	0.000000	5.054110	0.859278
7	5	0	-0.868495	3.827929	-6.083610
8	5	0	0.868495	3.827929	-6.083610
9	5	0	-2.029267	4.651279	-4.242534
10	5	0	-1.167413	5.380719	-2.917467
11	5	0	1.167413	5.380719	-2.917467
12	5	0	2.029267	4.651279	-4.242534
13	8	0	1.193749	5.048793	-1.574929
14	8	0	0.000000	5.972010	-3.379303
15	8	0	-1.193749	5.048793	-1.574929
16	8	0	-1.422341	4.934669	-5.458944
17	8	0	-1.629933	2.673080	-6.086838
18	8	0	-2.799533	3.500359	-4.177846
19	8	0	1.422341	4.934669	-5.458944
20	8	0	2.799533	3.500359	-4.177846
21	8	0	1.629933	2.673080	-6.086838
22	5	0	4.376988	-2.527055	-0.859278
23	5	0	4.376988	-2.527055	0.859278
24	5	0	0.860230	-3.564010	-5.162021
25	5	0	-0.860230	-3.564010	-5.162021
26	5	0	3.749331	-1.161826	-6.083610
27	5	0	2.880836	-2.666103	-6.083610
28	5	0	5.042759	-0.568242	-4.242534
29	5	0	5.243546	-1.679350	-2.917467
30	5	0	4.076133	-3.701369	-2.917467
31	5	0	3.013492	-4.083036	-4.242534
32	8	0	5.171913	-2.986005	-3.379303
33	8	0	4.969258	-1.490579	-1.574929
34	8	0	3.775509	-3.558214	-1.574929
35	8	0	3.129922	0.075023	-6.086838
36	8	0	4.431167	0.674287	-4.177846
37	8	0	4.984719	-1.235551	-5.458944
38	8	0	3.562378	-3.699118	-5.458944
39	8	0	1.631634	-4.174646	-4.177846
40	8	0	1.499989	-2.748103	-6.086838
41	5	0	-2.880836	-2.666103	-6.083610
42	5	0	-3.749331	-1.161826	-6.083610
43	5	0	-3.013492	-4.083036	-4.242534
44	5	0	-4.076133	-3.701369	-2.917467
45	5	0	-5.243546	-1.679350	-2.917467
46	5	0	-5.042759	-0.568242	-4.242534
47	5	0	-4.376988	-2.527055	-0.859278
48	5	0	-4.376988	-2.527055	0.859278
49	8	0	-5.171913	-2.986005	-3.379303
50	8	0	-3.775509	-3.558214	-1.574929
51	8	0	-4.969258	-1.490579	-1.574929

52	8	0	-3.562378	-3.699118	-5.458944
53	8	0	-1.499989	-2.748103	-6.086838
54	8	0	-1.631634	-4.174646	-4.177846
55	8	0	-4.984719	-1.235551	-5.458944
56	8	0	-4.431167	0.674287	-4.177846
57	8	0	-3.129922	0.075023	-6.086838
58	5	0	3.516638	1.037024	5.162021
59	5	0	2.656408	2.526986	5.162021
60	5	0	0.860230	-3.564010	5.162021
61	5	0	-0.860230	-3.564010	5.162021
62	5	0	-2.656408	2.526986	5.162021
63	5	0	-3.516638	1.037024	5.162021
64	5	0	2.029267	4.651279	4.242534
65	5	0	1.167413	5.380719	2.917467
66	5	0	-1.167413	5.380719	2.917467
67	5	0	-2.029267	4.651279	4.242534
68	5	0	0.868495	3.827929	6.083610
69	5	0	-0.868495	3.827929	6.083610
70	8	0	0.000000	5.972010	3.379303
71	8	0	1.193749	5.048793	1.574929
72	8	0	-1.193749	5.048793	1.574929
73	8	0	1.422341	4.934669	5.458944
74	8	0	1.629933	2.673080	6.086838
75	8	0	2.799533	3.500359	4.177846
76	8	0	-1.422341	4.934669	5.458944
77	8	0	-2.799533	3.500359	4.177846
78	8	0	-1.629933	2.673080	6.086838
79	5	0	-3.749331	-1.161826	6.083610
80	5	0	-2.880836	-2.666103	6.083610
81	5	0	-5.042759	-0.568242	4.242534
82	5	0	-5.243546	-1.679350	2.917467
83	5	0	-4.076133	-3.701369	2.917467
84	5	0	-3.013492	-4.083036	4.242534
85	8	0	-5.171913	-2.986005	3.379303
86	8	0	-4.969258	-1.490579	1.574929
87	8	0	-3.775509	-3.558214	1.574929
88	8	0	-4.984719	-1.235551	5.458944
89	8	0	-3.129922	0.075023	6.086838
90	8	0	-4.431167	0.674287	4.177846
91	8	0	-3.562378	-3.699118	5.458944
92	8	0	-1.631634	-4.174646	4.177846
93	8	0	-1.499989	-2.748103	6.086838
94	5	0	2.880836	-2.666103	6.083610
95	5	0	3.749331	-1.161826	6.083610
96	5	0	3.013492	-4.083036	4.242534
97	5	0	4.076133	-3.701369	2.917467
98	5	0	5.243546	-1.679350	2.917467
99	5	0	5.042759	-0.568242	4.242534
100	8	0	5.171913	-2.986005	3.379303
101	8	0	3.775509	-3.558214	1.574929
102	8	0	4.969258	-1.490579	1.574929
103	8	0	3.562378	-3.699118	5.458944
104	8	0	1.499989	-2.748103	6.086838
105	8	0	1.631634	-4.174646	4.177846
106	8	0	4.984719	-1.235551	5.458944
107	8	0	4.431167	0.674287	4.177846
108	8	0	3.129922	0.075023	6.086838

SCF Done: E(RB3LYP) =   -3606.54865628

Table S7: Theoretical Cartesian coordinates for *c*-B$_{30}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	-2.599018	-2.110392	5.234352
2	5	0	-1.203961	-3.123960	5.234352
3	5	0	3.343107	0.179678	5.234352
4	5	0	2.810243	1.819666	5.234352
5	5	0	-3.343107	0.179678	5.234352
6	5	0	-2.810243	1.819666	5.234352
7	5	0	0.862193	3.235008	5.234352
8	5	0	-0.862193	3.235008	5.234352
9	5	0	3.343107	4.601392	2.501583
10	5	0	2.810243	3.867967	3.968433
11	5	0	-2.810243	3.867967	3.968433
12	5	0	-3.343107	4.601392	2.501583
13	5	0	-4.547068	-1.477432	3.968433
14	5	0	-5.409261	-1.757576	2.501583
15	5	0	-5.409261	-3.023495	0.453282
16	5	0	-4.547068	-4.210202	-0.453282
17	5	0	-2.599018	-5.625543	-0.453282
18	5	0	-1.203961	-6.078825	0.453282
19	5	0	0.000000	-5.687634	2.501583
20	5	0	0.000000	-4.781071	3.968433
21	5	0	1.203961	-6.078825	0.453282
22	5	0	2.599018	-5.625543	-0.453282
23	5	0	4.547068	-4.210202	-0.453282
24	5	0	5.409261	-3.023495	0.453282
25	5	0	5.409261	-1.757576	2.501583
26	5	0	4.547068	-1.477432	3.968433
27	5	0	2.599018	-2.110392	5.234352
28	5	0	1.203961	-3.123960	5.234352
29	5	0	2.810243	-1.819666	-5.234352
30	5	0	3.343107	-0.179678	-5.234352
31	5	0	4.547068	1.477432	-3.968433
32	5	0	5.409261	1.757576	-2.501583
33	5	0	6.153350	0.733425	-0.453282
34	5	0	6.153350	-0.733425	0.453282
35	5	0	3.343107	-4.601392	-2.501583
36	5	0	2.810243	-3.867967	-3.968433
37	5	0	0.862193	-3.235008	-5.234352
38	5	0	-0.862193	-3.235008	-5.234352
39	5	0	-2.810243	-1.819666	-5.234352
40	5	0	-3.343107	-0.179678	-5.234352
41	5	0	-2.599018	2.110392	-5.234352
42	5	0	-1.203961	3.123960	-5.234352
43	5	0	1.203961	3.123960	-5.234352
44	5	0	2.599018	2.110392	-5.234352
45	5	0	5.409261	3.023495	-0.453282
46	5	0	4.547068	4.210202	0.453282
47	5	0	2.599018	5.625543	0.453282
48	5	0	1.203961	6.078825	-0.453282
49	5	0	-1.203961	6.078825	-0.453282
50	5	0	-2.599018	5.625543	0.453282
51	5	0	0.000000	4.781071	-3.968433

52	5	0	0.000000	5.687634	-2.501583
53	5	0	-6.153350	-0.733425	0.453282
54	5	0	-6.153350	0.733425	-0.453282
55	5	0	-5.409261	1.757576	-2.501583
56	5	0	-4.547068	1.477432	-3.968433
57	5	0	-3.343107	-4.601392	-2.501583
58	5	0	-2.810243	-3.867967	-3.968433
59	5	0	-5.409261	3.023495	-0.453282
60	5	0	-4.547068	4.210202	0.453282
61	8	0	3.696597	-5.087930	0.196963
62	8	0	4.431601	-4.076284	-1.826329
63	8	0	2.507336	-5.474344	-1.826329
64	8	0	1.189261	-5.902613	1.826329
65	8	0	-1.189261	-5.902613	1.826329
66	8	0	0.000000	-6.289027	-0.196963
67	8	0	-3.696597	-5.087930	0.196963
68	8	0	-2.507336	-5.474344	-1.826329
69	8	0	-4.431601	-4.076284	-1.826329
70	8	0	-5.981220	-1.943416	-0.196963
71	8	0	-5.981220	-0.692953	1.826329
72	8	0	-5.246216	-2.955062	1.826329
73	8	0	-3.473884	-2.758099	-4.462698
74	8	0	-1.549619	-4.156160	-4.462698
75	8	0	-1.549619	-2.132868	-5.713161
76	8	0	1.549619	-2.132868	-5.713161
77	8	0	3.473884	-2.758099	-4.462698
78	8	0	1.549619	-4.156160	-4.462698
79	8	0	3.696597	2.451561	-4.462698
80	8	0	2.507336	0.814683	-5.713161
81	8	0	4.431601	0.189451	-4.462698
82	8	0	5.981220	1.943416	0.196963
83	8	0	5.246216	2.955062	-1.826329
84	8	0	5.981220	0.692953	-1.826329
85	8	0	1.189261	5.902613	-1.826329
86	8	0	0.000000	6.289027	0.196963
87	8	0	-1.189261	5.902613	-1.826329
88	8	0	0.000000	2.636369	-5.713161
89	8	0	1.189261	4.273247	-4.462698
90	8	0	-1.189261	4.273247	-4.462698
91	8	0	3.696597	5.087930	-0.196963
92	8	0	2.507336	5.474344	1.826329
93	8	0	4.431601	4.076284	1.826329
94	8	0	5.246216	-2.955062	1.826329
95	8	0	5.981220	-0.692953	1.826329
96	8	0	5.981220	-1.943416	-0.196963
97	8	0	1.549619	2.132868	5.713161
98	8	0	3.473884	2.758099	4.462698
99	8	0	1.549619	4.156160	4.462698
100	8	0	-4.431601	0.189451	-4.462698
101	8	0	-2.507336	0.814683	-5.713161
102	8	0	-3.696597	2.451561	-4.462698
103	8	0	-5.981220	0.692953	-1.826329
104	8	0	-5.246216	2.955062	-1.826329
105	8	0	-5.981220	1.943416	0.196963
106	8	0	-3.696597	-2.451561	4.462698
107	8	0	-2.507336	-0.814683	5.713161
108	8	0	-4.431601	-0.189451	4.462698
109	8	0	-3.473884	2.758099	4.462698

110	8	0	-1.549619	2.132868	5.713161
111	8	0	-1.549619	4.156160	4.462698
112	8	0	-4.431601	4.076284	1.826329
113	8	0	-2.507336	5.474344	1.826329
114	8	0	-3.696597	5.087930	-0.196963
115	8	0	-1.189261	-4.273247	4.462698
116	8	0	1.189261	-4.273247	4.462698
117	8	0	0.000000	-2.636369	5.713161
118	8	0	2.507336	-0.814683	5.713161
119	8	0	3.696597	-2.451561	4.462698
120	8	0	4.431601	-0.189451	4.462698

SCF Done: E(RB3LYP) =   -6011.35441125

Table S8: Theoretical Cartesian coordinates for *c*-B$_{30}$-2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-0.933478	-4.864340	2.991843
2	5	0	-1.949406	-3.451205	3.145131
3	5	0	-1.429910	-5.023665	0.643747
4	5	0	-2.664713	-5.111641	-0.564985
5	5	0	4.687948	-3.110548	-0.980836
6	5	0	3.704025	-3.359247	-2.379802
7	5	0	2.842441	-4.386506	2.017701
8	5	0	4.297433	-3.704834	1.403966
9	5	0	1.454008	-4.552871	-1.631388
10	5	0	0.990859	-4.328540	0.040685
11	5	0	-0.334756	-4.683919	-3.390642
12	5	0	-2.018676	-4.797014	-2.960082
13	5	0	-4.468037	-3.404747	0.062742
14	5	0	-3.743123	-2.620589	1.438359
15	5	0	5.522654	2.126306	1.485952
16	5	0	6.006588	0.500710	1.191965
17	5	0	3.183674	-1.025386	3.094248
18	5	0	4.738383	-1.398442	2.371099
19	5	0	0.842274	-2.697207	-4.338909
20	5	0	-0.056901	-1.431908	-3.559588
21	5	0	0.393660	1.611412	5.020673
22	5	0	-0.771713	2.900711	4.860234
23	5	0	2.665557	1.527855	3.762516
24	5	0	3.731783	2.759607	3.153162
25	5	0	-3.523367	-2.778756	-2.968354
26	5	0	-2.393683	-1.490149	-2.619251
27	5	0	-4.872735	1.545195	-2.373058
28	5	0	-3.240013	1.042459	-2.738369
29	5	0	-5.582012	-2.108052	-1.754552
30	5	0	-6.051748	-0.463544	-1.504293
31	5	0	1.877666	3.533796	-3.359996
32	5	0	0.877628	4.943887	-3.186953
33	5	0	2.157824	1.535382	-4.730779
34	5	0	0.522684	1.028685	-4.441721
35	5	0	-1.461162	4.334061	-3.689524
36	5	0	-1.403300	2.615988	-3.985254
37	5	0	-3.099874	4.495445	-2.035928
38	5	0	-4.554098	3.835245	-1.404188
39	5	0	1.303606	-4.414398	3.746330
40	5	0	1.401041	-2.703593	4.079887
41	5	0	-1.863710	-1.274559	4.582633
42	5	0	-0.217238	-0.898649	5.008213
43	5	0	-5.592907	0.563756	0.787203
44	5	0	-4.700818	-0.207966	2.064488
45	5	0	-1.064387	4.256078	-0.218887
46	5	0	-1.167751	3.353960	1.266617
47	5	0	-4.806336	3.029718	0.910829
48	5	0	-3.627456	3.073009	2.175659
49	5	0	-3.528611	0.700327	4.174658
50	5	0	-3.117066	2.381340	4.412324
51	5	0	2.076447	4.578459	2.664190
52	5	0	0.533429	3.906113	3.062667

53	5	0	2.471528	5.309601	0.347368
54	5	0	1.300601	5.444344	-0.910536
55	5	0	4.142305	3.421560	-0.248174
56	5	0	3.357469	2.498833	-1.513120
57	5	0	5.504590	-0.606501	-1.012737
58	5	0	4.656496	0.269326	-2.254367
59	5	0	3.236128	-1.947313	-4.448874
60	5	0	3.787529	-0.296421	-4.530492
61	8	0	3.191355	0.755179	-5.173519
62	8	0	5.397245	-1.952831	-0.776465
63	8	0	6.235697	0.139669	-0.116947
64	8	0	5.676365	-0.428813	2.146468
65	8	0	5.009910	-2.684484	1.986934
66	8	0	4.535060	-3.990403	0.067648
67	8	0	4.763712	-0.037666	-3.582204
68	8	0	3.732898	1.255776	-1.929708
69	8	0	2.252691	3.096270	-2.098058
70	8	0	2.370706	2.867895	-4.453500
71	8	0	-1.052878	-1.826785	-2.685747
72	8	0	-0.376536	2.047936	-4.694350
73	8	0	0.064324	-0.105400	-3.843374
74	8	0	-2.392432	1.864483	-3.418364
75	8	0	-2.806283	-0.211342	-2.373766
76	8	0	-2.074956	4.374918	-1.121003
77	8	0	-2.731614	4.785240	-3.322875
78	8	0	-0.398142	5.198870	-3.639845
79	8	0	1.431398	5.800163	-2.235098
80	8	0	0.124575	4.824426	-0.553092
81	8	0	0.255619	-3.928826	-4.386940
82	8	0	2.057817	-2.447235	-4.928583
83	8	0	3.979948	-2.654242	-3.523358
84	8	0	2.520116	-4.043217	-2.321009
85	8	0	0.470866	-5.163742	-2.378360
86	8	0	0.192452	-5.213434	3.705663
87	8	0	2.518171	-4.894580	3.251052
88	8	0	1.758629	-4.222009	1.156532
89	8	0	-0.379774	-4.231984	0.185937
90	8	0	-1.270289	-5.614756	1.883525
91	8	0	-3.913713	-4.519987	-0.505080
92	8	0	-5.532322	-2.815323	-0.570921
93	8	0	-4.871569	-2.573240	-2.837450
94	8	0	-3.020857	-3.967900	-3.417064
95	8	0	-2.243216	-5.531966	-1.810188
96	8	0	-6.231920	-0.183355	-0.162450
97	8	0	-5.584315	1.930147	0.632491
98	8	0	-4.763651	4.026961	-0.048333
99	8	0	-5.227116	2.822063	-2.054477
100	8	0	-5.827246	0.553041	-2.393224
101	8	0	-4.075594	-1.424445	1.998501
102	8	0	-4.480834	0.562344	3.181819
103	8	0	-2.899123	-0.392673	4.691628
104	8	0	-2.088671	-2.557437	4.156826
105	8	0	-2.664615	-3.297570	1.968625
106	8	0	0.017931	3.210735	1.967265
107	8	0	-2.309799	2.799866	1.780135
108	8	0	-3.777340	3.223980	3.527461
109	8	0	-2.100885	2.842389	5.207328
110	8	0	-0.281129	3.989268	4.171646

111	8	0	5.238969	2.882070	0.376140
112	8	0	3.658538	4.625736	0.170958
113	8	0	2.037599	5.520398	1.644911
114	8	0	4.984167	2.424908	2.713724
115	8	0	3.305606	4.058316	3.007734
116	8	0	2.689486	0.190947	3.471325
117	8	0	2.383625	-2.130993	3.285907
118	8	0	1.617697	2.009025	4.513910
119	8	0	0.222289	0.322699	5.427196
120	8	0	0.663062	-1.946988	4.931409

SCF Done: E(RB3LYP) =   -6011.05205759

Table S9: Theoretical Cartesian coordinates for *t*-B₃₆.

Standard orientation:

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

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	4.854302	0.859319	4.854302
2	5	0	4.854302	-0.859319	4.854302
3	5	0	5.816036	2.939025	4.168971
4	5	0	5.816036	4.168971	2.939025
5	5	0	2.939025	4.168971	5.816036
6	5	0	4.168971	2.939025	5.816036
7	5	0	4.854302	4.854302	0.859319
8	5	0	4.854302	4.854302	-0.859319
9	5	0	0.859319	4.854302	4.854302
10	5	0	-0.859319	4.854302	4.854302
11	5	0	2.939025	5.816036	4.168971
12	5	0	4.168971	5.816036	2.939025
13	8	0	5.386652	3.447040	5.386652
14	8	0	3.987768	1.574149	5.675012
15	8	0	5.675012	1.574149	3.987768
16	8	0	5.386652	5.386652	3.447040
17	8	0	3.987768	5.675012	1.574149
18	8	0	5.675012	3.987768	1.574149
19	8	0	3.447040	5.386652	5.386652
20	8	0	1.574149	5.675012	3.987768
21	8	0	1.574149	3.987768	5.675012
22	5	0	0.859319	4.854302	-4.854302
23	5	0	-0.859319	4.854302	-4.854302
24	5	0	4.854302	0.859319	-4.854302
25	5	0	4.854302	-0.859319	-4.854302
26	5	0	4.168971	2.939025	-5.816036
27	5	0	2.939025	4.168971	-5.816036
28	5	0	5.816036	4.168971	-2.939025
29	5	0	5.816036	2.939025	-4.168971
30	5	0	4.168971	5.816036	-2.939025
31	5	0	2.939025	5.816036	-4.168971
32	8	0	5.386652	3.447040	-5.386652
33	8	0	5.675012	1.574149	-3.987768
34	8	0	3.987768	1.574149	-5.675012
35	8	0	3.447040	5.386652	-5.386652
36	8	0	1.574149	5.675012	-3.987768
37	8	0	1.574149	3.987768	-5.675012
38	8	0	5.386652	5.386652	-3.447040
39	8	0	3.987768	5.675012	-1.574149
40	8	0	5.675012	3.987768	-1.574149
41	5	0	0.859319	-4.854302	-4.854302
42	5	0	-0.859319	-4.854302	-4.854302
43	5	0	4.854302	-4.854302	-0.859319
44	5	0	4.854302	-4.854302	0.859319
45	5	0	4.168971	-5.816036	-2.939025
46	5	0	2.939025	-5.816036	-4.168971
47	5	0	4.168971	-2.939025	-5.816036
48	5	0	2.939025	-4.168971	-5.816036
49	5	0	5.816036	-2.939025	-4.168971
50	5	0	5.816036	-4.168971	-2.939025
51	8	0	5.386652	-5.386652	-3.447040

52	8	0	5.675012	-3.987768	-1.574149
53	8	0	3.987768	-5.675012	-1.574149
54	8	0	3.447040	-5.386652	-5.386652
55	8	0	1.574149	-5.675012	-3.987768
56	8	0	1.574149	-3.987768	-5.675012
57	8	0	5.386652	-3.447040	-5.386652
58	8	0	3.987768	-1.574149	-5.675012
59	8	0	5.675012	-1.574149	-3.987768
60	5	0	0.859319	-4.854302	4.854302
61	5	0	-0.859319	-4.854302	4.854302
62	5	0	4.168971	-2.939025	5.816036
63	5	0	2.939025	-4.168971	5.816036
64	5	0	4.168971	-5.816036	2.939025
65	5	0	2.939025	-5.816036	4.168971
66	5	0	5.816036	-4.168971	2.939025
67	5	0	5.816036	-2.939025	4.168971
68	8	0	5.386652	-3.447040	5.386652
69	8	0	3.987768	-1.574149	5.675012
70	8	0	5.675012	-1.574149	3.987768
71	8	0	3.447040	-5.386652	5.386652
72	8	0	1.574149	-3.987768	5.675012
73	8	0	1.574149	-5.675012	3.987768
74	8	0	5.386652	-5.386652	3.447040
75	8	0	3.987768	-5.675012	1.574149
76	8	0	5.675012	-3.987768	1.574149
77	5	0	-4.854302	4.854302	0.859319
78	5	0	-4.854302	4.854302	-0.859319
79	5	0	-4.854302	-0.859319	4.854302
80	5	0	-4.854302	0.859319	4.854302
81	5	0	-4.168971	2.939025	5.816036
82	5	0	-2.939025	4.168971	5.816036
83	5	0	-4.168971	5.816036	2.939025
84	5	0	-2.939025	5.816036	4.168971
85	5	0	-5.816036	4.168971	2.939025
86	5	0	-5.816036	2.939025	4.168971
87	8	0	-5.386652	3.447040	5.386652
88	8	0	-5.675012	1.574149	3.987768
89	8	0	-3.987768	1.574149	5.675012
90	8	0	-3.447040	5.386652	5.386652
91	8	0	-1.574149	3.987768	5.675012
92	8	0	-1.574149	5.675012	3.987768
93	8	0	-5.386652	5.386652	3.447040
94	8	0	-3.987768	5.675012	1.574149
95	8	0	-5.675012	3.987768	1.574149
96	5	0	-4.854302	0.859319	-4.854302
97	5	0	-4.854302	-0.859319	-4.854302
98	5	0	-2.939025	4.168971	-5.816036
99	5	0	-4.168971	2.939025	-5.816036
100	5	0	-5.816036	4.168971	-2.939025
101	5	0	-5.816036	2.939025	-4.168971
102	5	0	-4.168971	5.816036	-2.939025
103	5	0	-2.939025	5.816036	-4.168971
104	8	0	-3.447040	5.386652	-5.386652
105	8	0	-1.574149	5.675012	-3.987768
106	8	0	-1.574149	3.987768	-5.675012
107	8	0	-5.386652	5.386652	-3.447040
108	8	0	-3.987768	5.675012	-1.574149
109	8	0	-5.675012	3.987768	-1.574149

110	8	0	-5.386652	3.447040	-5.386652
111	8	0	-5.675012	1.574149	-3.987768
112	8	0	-3.987768	1.574149	-5.675012
113	5	0	-4.854302	-4.854302	0.859319
114	5	0	-4.854302	-4.854302	-0.859319
115	5	0	-5.816036	-4.168971	-2.939025
116	5	0	-5.816036	-2.939025	-4.168971
117	5	0	-2.939025	-4.168971	-5.816036
118	5	0	-4.168971	-2.939025	-5.816036
119	5	0	-2.939025	-5.816036	-4.168971
120	5	0	-4.168971	-5.816036	-2.939025
121	8	0	-5.386652	-3.447040	-5.386652
122	8	0	-5.675012	-1.574149	-3.987768
123	8	0	-3.987768	-1.574149	-5.675012
124	8	0	-3.447040	-5.386652	-5.386652
125	8	0	-1.574149	-3.987768	-5.675012
126	8	0	-1.574149	-5.675012	-3.987768
127	8	0	-5.386652	-5.386652	-3.447040
128	8	0	-3.987768	-5.675012	-1.574149
129	8	0	-5.675012	-3.987768	-1.574149
130	5	0	-2.939025	-4.168971	5.816036
131	5	0	-4.168971	-2.939025	5.816036
132	5	0	-5.816036	-4.168971	2.939025
133	5	0	-5.816036	-2.939025	4.168971
134	5	0	-4.168971	-5.816036	2.939025
135	5	0	-2.939025	-5.816036	4.168971
136	8	0	-3.447040	-5.386652	5.386652
137	8	0	-1.574149	-5.675012	3.987768
138	8	0	-1.574149	-3.987768	5.675012
139	8	0	-5.386652	-3.447040	5.386652
140	8	0	-3.987768	-1.574149	5.675012
141	8	0	-5.675012	-1.574149	3.987768
142	8	0	-5.386652	-5.386652	3.447040
143	8	0	-5.675012	-3.987768	1.574149
144	8	0	-3.987768	-5.675012	1.574149

SCF Done: E(RB3LYP) =   -7213.15920077

Table S10: Theoretical Cartesian coordinates for *t*-B$_{36}$-2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-4.107433	0.000000	5.324543
2	5	0	-5.324543	0.000000	4.107433
3	5	0	-4.107433	5.324543	0.000000
4	5	0	-5.324543	4.107433	0.000000
5	5	0	-4.107433	0.000000	-5.324543
6	5	0	-5.324543	0.000000	-4.107433
7	5	0	-4.107433	-5.324543	0.000000
8	5	0	-5.324543	-4.107433	0.000000
9	5	0	-6.556530	-1.197189	-2.419731
10	5	0	-6.556530	-2.419731	-1.197189
11	5	0	-6.556530	1.197189	-2.419731
12	5	0	-6.556530	2.419731	-1.197189
13	5	0	-6.556530	-2.419731	1.197189
14	5	0	-6.556530	-1.197189	2.419731
15	5	0	-6.556530	2.419731	1.197189
16	5	0	-6.556530	1.197189	2.419731
17	8	0	-7.134675	-2.038643	0.000000
18	8	0	-5.742142	-3.538340	-1.194278
19	8	0	-5.742142	-3.538340	1.194278
20	8	0	-7.134675	0.000000	-2.038643
21	8	0	-5.742142	1.194278	-3.538340
22	8	0	-5.742142	-1.194278	-3.538340
23	8	0	-7.134675	2.038643	0.000000
24	8	0	-5.742142	3.538340	-1.194278
25	8	0	-5.742142	3.538340	1.194278
26	8	0	-7.134675	0.000000	2.038643
27	8	0	-5.742142	-1.194278	3.538340
28	8	0	-5.742142	1.194278	3.538340
29	5	0	5.324543	0.000000	-4.107433
30	5	0	4.107433	0.000000	-5.324543
31	5	0	5.324543	4.107433	0.000000
32	5	0	4.107433	5.324543	0.000000
33	5	0	5.324543	0.000000	4.107433
34	5	0	4.107433	0.000000	5.324543
35	5	0	6.556530	1.197189	-2.419731
36	5	0	6.556530	2.419731	-1.197189
37	5	0	6.556530	2.419731	1.197189
38	5	0	6.556530	1.197189	2.419731
39	5	0	6.556530	-1.197189	2.419731
40	5	0	6.556530	-2.419731	1.197189
41	5	0	6.556530	-2.419731	-1.197189
42	5	0	6.556530	-1.197189	-2.419731
43	5	0	5.324543	-4.107433	0.000000
44	5	0	4.107433	-5.324543	0.000000
45	8	0	7.134675	0.000000	2.038643
46	8	0	5.742142	1.194278	3.538340
47	8	0	5.742142	-1.194278	3.538340
48	8	0	7.134675	2.038643	0.000000
49	8	0	5.742142	3.538340	1.194278
50	8	0	5.742142	3.538340	-1.194278
51	8	0	7.134675	0.000000	-2.038643

52	8	0	5.742142	1.194278	-3.538340
53	8	0	5.742142	-1.194278	-3.538340
54	8	0	7.134675	-2.038643	0.000000
55	8	0	5.742142	-3.538340	-1.194278
56	8	0	5.742142	-3.538340	1.194278
57	5	0	0.000000	-5.324543	4.107433
58	5	0	0.000000	-4.107433	5.324543
59	5	0	0.000000	5.324543	4.107433
60	5	0	0.000000	4.107433	5.324543
61	5	0	2.419731	1.197189	6.556530
62	5	0	1.197189	2.419731	6.556530
63	5	0	-2.419731	1.197189	6.556530
64	5	0	-1.197189	2.419731	6.556530
65	5	0	-1.197189	-2.419731	6.556530
66	5	0	-2.419731	-1.197189	6.556530
67	5	0	1.197189	-2.419731	6.556530
68	5	0	2.419731	-1.197189	6.556530
69	8	0	0.000000	-2.038643	7.134675
70	8	0	1.194278	-3.538340	5.742142
71	8	0	-1.194278	-3.538340	5.742142
72	8	0	-2.038643	0.000000	7.134675
73	8	0	-3.538340	-1.194278	5.742142
74	8	0	-3.538340	1.194278	5.742142
75	8	0	0.000000	2.038643	7.134675
76	8	0	-1.194278	3.538340	5.742142
77	8	0	1.194278	3.538340	5.742142
78	8	0	2.038643	0.000000	7.134675
79	8	0	3.538340	1.194278	5.742142
80	8	0	3.538340	-1.194278	5.742142
81	5	0	0.000000	4.107433	-5.324543
82	5	0	0.000000	5.324543	-4.107433
83	5	0	-2.419731	6.556530	1.197189
84	5	0	-1.197189	6.556530	2.419731
85	5	0	1.197189	6.556530	2.419731
86	5	0	2.419731	6.556530	1.197189
87	5	0	2.419731	6.556530	-1.197189
88	5	0	1.197189	6.556530	-2.419731
89	5	0	-1.197189	6.556530	-2.419731
90	5	0	-2.419731	6.556530	-1.197189
91	8	0	2.038643	7.134675	0.000000
92	8	0	3.538340	5.742142	-1.194278
93	8	0	3.538340	5.742142	1.194278
94	8	0	0.000000	7.134675	2.038643
95	8	0	1.194278	5.742142	3.538340
96	8	0	-1.194278	5.742142	3.538340
97	8	0	-2.038643	7.134675	0.000000
98	8	0	-3.538340	5.742142	1.194278
99	8	0	-3.538340	5.742142	-1.194278
100	8	0	0.000000	7.134675	-2.038643
101	8	0	-1.194278	5.742142	-3.538340
102	8	0	1.194278	5.742142	-3.538340
103	5	0	0.000000	-5.324543	-4.107433
104	5	0	0.000000	-4.107433	-5.324543
105	5	0	-1.197189	-2.419731	-6.556530
106	5	0	-2.419731	-1.197189	-6.556530
107	5	0	2.419731	1.197189	-6.556530
108	5	0	1.197189	2.419731	-6.556530
109	5	0	-2.419731	1.197189	-6.556530

110	5	0	-1.197189	2.419731	-6.556530
111	5	0	1.197189	-2.419731	-6.556530
112	5	0	2.419731	-1.197189	-6.556530
113	8	0	0.000000	2.038643	-7.134675
114	8	0	1.194278	3.538340	-5.742142
115	8	0	-1.194278	3.538340	-5.742142
116	8	0	-2.038643	0.000000	-7.134675
117	8	0	-3.538340	1.194278	-5.742142
118	8	0	-3.538340	-1.194278	-5.742142
119	8	0	0.000000	-2.038643	-7.134675
120	8	0	-1.194278	-3.538340	-5.742142
121	8	0	1.194278	-3.538340	-5.742142
122	8	0	2.038643	0.000000	-7.134675
123	8	0	3.538340	-1.194278	-5.742142
124	8	0	3.538340	1.194278	-5.742142
125	5	0	2.419731	-6.556530	1.197189
126	5	0	1.197189	-6.556530	2.419731
127	5	0	-1.197189	-6.556530	-2.419731
128	5	0	-2.419731	-6.556530	-1.197189
129	5	0	2.419731	-6.556530	-1.197189
130	5	0	1.197189	-6.556530	-2.419731
131	5	0	-1.197189	-6.556530	2.419731
132	5	0	-2.419731	-6.556530	1.197189
133	8	0	0.000000	-7.134675	2.038643
134	8	0	-1.194278	-5.742142	3.538340
135	8	0	1.194278	-5.742142	3.538340
136	8	0	3.538340	-5.742142	1.194278
137	8	0	2.038643	-7.134675	0.000000
138	8	0	3.538340	-5.742142	-1.194278
139	8	0	0.000000	-7.134675	-2.038643
140	8	0	1.194278	-5.742142	-3.538340
141	8	0	-1.194278	-5.742142	-3.538340
142	8	0	-2.038643	-7.134675	0.000000
143	8	0	-3.538340	-5.742142	-1.194278
144	8	0	-3.538340	-5.742142	1.194278

SCF Done: E(RB3LYP) = -7213.57604891

Table S11: Theoretical Cartesian coordinates for *t*-B$_{27}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	-3.516638	1.037024	-5.162021
2	5	0	-2.656408	2.526986	-5.162021
3	5	0	2.656408	2.526986	-5.162021
4	5	0	3.516638	1.037024	-5.162021
5	5	0	0.000000	5.054110	-0.859278
6	5	0	0.000000	5.054110	0.859278
7	5	0	-0.868495	3.827929	-6.083610
8	5	0	0.868495	3.827929	-6.083610
9	5	0	-2.029267	4.651279	-4.242534
10	5	0	-1.167413	5.380719	-2.917467
11	5	0	1.167413	5.380719	-2.917467
12	5	0	2.029267	4.651279	-4.242534
13	8	0	1.193749	5.048793	-1.574929
14	8	0	0.000000	5.972010	-3.379303
15	8	0	-1.193749	5.048793	-1.574929
16	8	0	-1.422341	4.934669	-5.458944
17	8	0	-1.629933	2.673080	-6.086838
18	8	0	-2.799533	3.500359	-4.177846
19	8	0	1.422341	4.934669	-5.458944
20	8	0	2.799533	3.500359	-4.177846
21	8	0	1.629933	2.673080	-6.086838
22	5	0	4.376988	-2.527055	-0.859278
23	5	0	4.376988	-2.527055	0.859278
24	5	0	0.860230	-3.564010	-5.162021
25	5	0	-0.860230	-3.564010	-5.162021
26	5	0	3.749331	-1.161826	-6.083610
27	5	0	2.880836	-2.666103	-6.083610
28	5	0	5.042759	-0.568242	-4.242534
29	5	0	5.243546	-1.679350	-2.917467
30	5	0	4.076133	-3.701369	-2.917467
31	5	0	3.013492	-4.083036	-4.242534
32	8	0	5.171913	-2.986005	-3.379303
33	8	0	4.969258	-1.490579	-1.574929
34	8	0	3.775509	-3.558214	-1.574929
35	8	0	3.129922	0.075023	-6.086838
36	8	0	4.431167	0.674287	-4.177846
37	8	0	4.984719	-1.235551	-5.458944
38	8	0	3.562378	-3.699118	-5.458944
39	8	0	1.631634	-4.174646	-4.177846
40	8	0	1.499989	-2.748103	-6.086838
41	5	0	-2.880836	-2.666103	-6.083610
42	5	0	-3.749331	-1.161826	-6.083610
43	5	0	-3.013492	-4.083036	-4.242534
44	5	0	-4.076133	-3.701369	-2.917467
45	5	0	-5.243546	-1.679350	-2.917467
46	5	0	-5.042759	-0.568242	-4.242534
47	5	0	-4.376988	-2.527055	-0.859278
48	5	0	-4.376988	-2.527055	0.859278
49	8	0	-5.171913	-2.986005	-3.379303
50	8	0	-3.775509	-3.558214	-1.574929
51	8	0	-4.969258	-1.490579	-1.574929
52	8	0	-3.562378	-3.699118	-5.458944

53	8	0	-1.499989	-2.748103	-6.086838
54	8	0	-1.631634	-4.174646	-4.177846
55	8	0	-4.984719	-1.235551	-5.458944
56	8	0	-4.431167	0.674287	-4.177846
57	8	0	-3.129922	0.075023	-6.086838
58	5	0	3.516638	1.037024	5.162021
59	5	0	2.656408	2.526986	5.162021
60	5	0	0.860230	-3.564010	5.162021
61	5	0	-0.860230	-3.564010	5.162021
62	5	0	-2.656408	2.526986	5.162021
63	5	0	-3.516638	1.037024	5.162021
64	5	0	2.029267	4.651279	4.242534
65	5	0	1.167413	5.380719	2.917467
66	5	0	-1.167413	5.380719	2.917467
67	5	0	-2.029267	4.651279	4.242534
68	5	0	0.868495	3.827929	6.083610
69	5	0	-0.868495	3.827929	6.083610
70	8	0	0.000000	5.972010	3.379303
71	8	0	1.193749	5.048793	1.574929
72	8	0	-1.193749	5.048793	1.574929
73	8	0	1.422341	4.934669	5.458944
74	8	0	1.629933	2.673080	6.086838
75	8	0	2.799533	3.500359	4.177846
76	8	0	-1.422341	4.934669	5.458944
77	8	0	-2.799533	3.500359	4.177846
78	8	0	-1.629933	2.673080	6.086838
79	5	0	-3.749331	-1.161826	6.083610
80	5	0	-2.880836	-2.666103	6.083610
81	5	0	-5.042759	-0.568242	4.242534
82	5	0	-5.243546	-1.679350	2.917467
83	5	0	-4.076133	-3.701369	2.917467
84	5	0	-3.013492	-4.083036	4.242534
85	8	0	-5.171913	-2.986005	3.379303
86	8	0	-4.969258	-1.490579	1.574929
87	8	0	-3.775509	-3.558214	1.574929
88	8	0	-4.984719	-1.235551	5.458944
89	8	0	-3.129922	0.075023	6.086838
90	8	0	-4.431167	0.674287	4.177846
91	8	0	-3.562378	-3.699118	5.458944
92	8	0	-1.631634	-4.174646	4.177846
93	8	0	-1.499989	-2.748103	6.086838
94	5	0	2.880836	-2.666103	6.083610
95	5	0	3.749331	-1.161826	6.083610
96	5	0	3.013492	-4.083036	4.242534
97	5	0	4.076133	-3.701369	2.917467
98	5	0	5.243546	-1.679350	2.917467
99	5	0	5.042759	-0.568242	4.242534
100	8	0	5.171913	-2.986005	3.379303
101	8	0	3.775509	-3.558214	1.574929
102	8	0	4.969258	-1.490579	1.574929
103	8	0	3.562378	-3.699118	5.458944
104	8	0	1.499989	-2.748103	6.086838
105	8	0	1.631634	-4.174646	4.177846
106	8	0	4.984719	-1.235551	5.458944
107	8	0	4.431167	0.674287	4.177846
108	8	0	3.129922	0.075023	6.086838

SCF Done: E(RB3LYP) =   -5409.84449056

Table S12: Theoretical Cartesian coordinates for *t*-B$_{45}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	4.295171	4.449266	4.637952
2	5	0	2.904223	5.459849	4.637952
3	5	0	-2.904223	5.459849	4.637952
4	5	0	-4.295171	4.449266	4.637952
5	5	0	0.000000	8.488925	0.859368
6	5	0	0.000000	8.488925	-0.859368
7	5	0	0.872314	6.256158	5.604566
8	5	0	-0.872314	6.256158	5.604566
9	5	0	2.027352	7.616404	4.103644
10	5	0	1.161629	8.584456	2.949341
11	5	0	-1.161629	8.584456	2.949341
12	5	0	-2.027352	7.616404	4.103644
13	8	0	0.000000	9.116963	3.489866
14	8	0	1.192538	8.436402	1.573191
15	8	0	-1.192538	8.436402	1.573191
16	8	0	1.339467	7.528393	5.304926
17	8	0	1.756720	5.212182	5.386132
18	8	0	2.932656	6.604559	3.847016
19	8	0	-1.339467	7.528393	5.304926
20	8	0	-2.932656	6.604559	3.847016
21	8	0	-1.756720	5.212182	5.386132
22	5	0	-6.090079	-1.074894	4.637952
23	5	0	-5.558784	-2.710052	4.637952
24	5	0	-8.073448	2.623222	0.859368
25	5	0	-8.073448	2.623222	-0.859368
26	5	0	-5.680400	2.762879	5.604566
27	5	0	-6.219520	1.103639	5.604566
28	5	0	-6.617145	4.281725	4.103644
29	5	0	-7.805340	3.757517	2.949341
30	5	0	-8.523266	1.547968	2.949341
31	5	0	-7.870117	0.425472	4.103644
32	8	0	-8.670747	2.817297	3.489866
33	8	0	-7.654980	3.741163	1.573191
34	8	0	-8.392010	1.472820	1.573191
35	8	0	-6.746009	3.600310	5.304926
36	8	0	-4.414223	3.281393	5.386132
37	8	0	-5.375069	4.830043	3.847016
38	8	0	-7.573845	1.052492	5.304926
39	8	0	-7.187550	-0.748201	3.847016
40	8	0	-5.499936	-0.060087	5.386132
41	5	0	-0.859653	-6.124170	4.637952
42	5	0	0.859653	-6.124170	4.637952
43	5	0	-4.989665	-6.867685	0.859368
44	5	0	-4.989665	-6.867685	-0.859368
45	5	0	-4.382994	-4.548605	5.604566
46	5	0	-2.971561	-5.574071	5.604566
47	5	0	-6.116972	-4.970153	4.103644
48	5	0	-5.985594	-6.262183	2.949341
49	5	0	-4.106039	-7.627759	2.949341
50	5	0	-2.836648	-7.353448	4.103644
51	8	0	-5.358816	-7.375778	3.489866

52	8	0	-5.923576	-6.124236	1.573191
53	8	0	-3.994009	-7.526149	1.573191
54	8	0	-5.508730	-5.303279	5.304926
55	8	0	-4.484860	-3.184170	5.386132
56	8	0	-6.254631	-3.619429	3.847016
57	8	0	-3.341427	-6.877917	5.304926
58	8	0	-1.509494	-7.066973	3.847016
59	8	0	-1.642427	-5.249318	5.386132
60	5	0	5.558784	-2.710052	4.637952
61	5	0	6.090079	-1.074894	4.637952
62	5	0	4.989665	-6.867685	0.859368
63	5	0	4.989665	-6.867685	-0.859368
64	5	0	2.971561	-5.574071	5.604566
65	5	0	4.382994	-4.548605	5.604566
66	5	0	2.836648	-7.353448	4.103644
67	5	0	4.106039	-7.627759	2.949341
68	5	0	5.985594	-6.262183	2.949341
69	5	0	6.116972	-4.970153	4.103644
70	8	0	5.358816	-7.375778	3.489866
71	8	0	3.994009	-7.526149	1.573191
72	8	0	5.923576	-6.124236	1.573191
73	8	0	3.341427	-6.877917	5.304926
74	8	0	1.642427	-5.249318	5.386132
75	8	0	1.509494	-7.066973	3.847016
76	8	0	5.508730	-5.303279	5.304926
77	8	0	6.254631	-3.619429	3.847016
78	8	0	4.484860	-3.184170	5.386132
79	5	0	6.219520	1.103639	5.604566
80	5	0	5.680400	2.762879	5.604566
81	5	0	7.870117	0.425472	4.103644
82	5	0	8.523266	1.547968	2.949341
83	5	0	7.805340	3.757517	2.949341
84	5	0	6.617145	4.281725	4.103644
85	5	0	8.073448	2.623222	0.859368
86	5	0	8.073448	2.623222	-0.859368
87	8	0	8.670747	2.817297	3.489866
88	8	0	8.392010	1.472820	1.573191
89	8	0	7.654980	3.741163	1.573191
90	8	0	7.573845	1.052492	5.304926
91	8	0	5.499936	-0.060087	5.386132
92	8	0	7.187550	-0.748201	3.847016
93	5	0	-4.295171	4.449266	-4.637952
94	5	0	-2.904223	5.459849	-4.637952
95	5	0	2.904223	5.459849	-4.637952
96	5	0	4.295171	4.449266	-4.637952
97	5	0	-0.872314	6.256158	-5.604566
98	5	0	0.872314	6.256158	-5.604566
99	5	0	-2.027352	7.616404	-4.103644
100	5	0	-1.161629	8.584456	-2.949341
101	5	0	1.161629	8.584456	-2.949341
102	5	0	2.027352	7.616404	-4.103644
103	8	0	0.000000	9.116963	-3.489866
104	8	0	-1.192538	8.436402	-1.573191
105	8	0	1.192538	8.436402	-1.573191
106	8	0	-1.339467	7.528393	-5.304926
107	8	0	-1.756720	5.212182	-5.386132
108	8	0	-2.932656	6.604559	-3.847016
109	8	0	1.339467	7.528393	-5.304926

110	8	0	2.932656	6.604559	-3.847016
111	8	0	1.756720	5.212182	-5.386132
112	5	0	6.090079	-1.074894	-4.637952
113	5	0	5.558784	-2.710052	-4.637952
114	5	0	5.680400	2.762879	-5.604566
115	5	0	6.219520	1.103639	-5.604566
116	5	0	6.617145	4.281725	-4.103644
117	5	0	7.805340	3.757517	-2.949341
118	5	0	8.523266	1.547968	-2.949341
119	5	0	7.870117	0.425472	-4.103644
120	8	0	8.670747	2.817297	-3.489866
121	8	0	7.654980	3.741163	-1.573191
122	8	0	8.392010	1.472820	-1.573191
123	8	0	6.746009	3.600310	-5.304926
124	8	0	4.414223	3.281393	-5.386132
125	8	0	5.375069	4.830043	-3.847016
126	8	0	7.573845	1.052492	-5.304926
127	8	0	7.187550	-0.748201	-3.847016
128	8	0	5.499936	-0.060087	-5.386132
129	5	0	0.859653	-6.124170	-4.637952
130	5	0	-0.859653	-6.124170	-4.637952
131	5	0	4.382994	-4.548605	-5.604566
132	5	0	2.971561	-5.574071	-5.604566
133	5	0	6.116972	-4.970153	-4.103644
134	5	0	5.985594	-6.262183	-2.949341
135	5	0	4.106039	-7.627759	-2.949341
136	5	0	2.836648	-7.353448	-4.103644
137	8	0	5.358816	-7.375778	-3.489866
138	8	0	5.923576	-6.124236	-1.573191
139	8	0	3.994009	-7.526149	-1.573191
140	8	0	4.484860	-3.184170	-5.386132
141	8	0	6.254631	-3.619429	-3.847016
142	8	0	5.508730	-5.303279	-5.304926
143	8	0	3.341427	-6.877917	-5.304926
144	8	0	1.509494	-7.066973	-3.847016
145	8	0	1.642427	-5.249318	-5.386132
146	5	0	-5.558784	-2.710052	-4.637952
147	5	0	-6.090079	-1.074894	-4.637952
148	5	0	-2.971561	-5.574071	-5.604566
149	5	0	-4.382994	-4.548605	-5.604566
150	5	0	-2.836648	-7.353448	-4.103644
151	5	0	-4.106039	-7.627759	-2.949341
152	5	0	-5.985594	-6.262183	-2.949341
153	5	0	-6.116972	-4.970153	-4.103644
154	8	0	-5.358816	-7.375778	-3.489866
155	8	0	-3.994009	-7.526149	-1.573191
156	8	0	-5.923576	-6.124236	-1.573191
157	8	0	-3.341427	-6.877917	-5.304926
158	8	0	-1.642427	-5.249318	-5.386132
159	8	0	-1.509494	-7.066973	-3.847016
160	8	0	-5.508730	-5.303279	-5.304926
161	8	0	-6.254631	-3.619429	-3.847016
162	8	0	-4.484860	-3.184170	-5.386132
163	5	0	-6.219520	1.103639	-5.604566
164	5	0	-5.680400	2.762879	-5.604566
165	5	0	-7.870117	0.425472	-4.103644
166	5	0	-8.523266	1.547968	-2.949341
167	5	0	-7.805340	3.757517	-2.949341

168	5	0	-6.617145	4.281725	-4.103644
169	8	0	-8.670747	2.817297	-3.489866
170	8	0	-8.392010	1.472820	-1.573191
171	8	0	-7.654980	3.741163	-1.573191
172	8	0	-7.573845	1.052492	-5.304926
173	8	0	-5.499936	-0.060087	-5.386132
174	8	0	-7.187550	-0.748201	-3.847016
175	8	0	-6.746009	3.600310	-5.304926
176	8	0	-5.375069	4.830043	-3.847016
177	8	0	-4.414223	3.281393	-5.386132
178	8	0	6.746009	3.600310	5.304926
179	8	0	5.375069	4.830043	3.847016
180	8	0	4.414223	3.281393	5.386132

SCF Done: E(RB3LYP) =   -9016.43867671

Table S13: Theoretical Cartesian coordinates for *t*-B$_{54}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	2.941948	6.817145	4.494700
2	5	0	0.000000	9.986954	0.859423
3	5	0	-2.941948	6.817145	4.494700
4	5	0	-8.648956	4.993477	0.859423
5	5	0	-8.648956	4.993477	-0.859423
6	5	0	-7.374795	0.860771	4.494700
7	5	0	-7.374795	-0.860771	4.494700
8	5	0	-4.432847	5.956375	4.494700
9	5	0	-6.060957	4.509507	5.462132
10	5	0	-6.935826	2.994189	5.462132
11	5	0	-6.762177	6.231972	4.051657
12	5	0	-8.087465	6.007313	2.953488
13	5	0	-9.246218	4.000294	2.953488
14	5	0	-8.778134	2.740231	4.051657
15	8	0	-9.113056	5.261426	3.516272
16	8	0	-7.994073	5.992145	1.572072
17	8	0	-9.186386	3.926998	1.572072
18	8	0	-6.960288	5.543435	5.239320
19	8	0	-4.728319	4.794720	5.203190
20	8	0	-5.452056	6.534632	3.742664
21	8	0	-8.280899	3.256068	5.239320
22	8	0	-8.385185	1.454303	3.742664
23	8	0	-6.516509	1.697485	5.203190
24	5	0	-4.432847	-5.956375	4.494700
25	5	0	-2.941948	-6.817145	4.494700
26	5	0	-8.648956	-4.993477	-0.859423
27	5	0	-8.648956	-4.993477	0.859423
28	5	0	-6.935826	-2.994189	5.462132
29	5	0	-6.060957	-4.509507	5.462132
30	5	0	-8.778134	-2.740231	4.051657
31	5	0	-9.246218	-4.000294	2.953488
32	5	0	-8.087465	-6.007313	2.953488
33	5	0	-6.762177	-6.231972	4.051657
34	8	0	-9.113056	-5.261426	3.516272
35	8	0	-9.186386	-3.926998	1.572072
36	8	0	-7.994073	-5.992145	1.572072
37	8	0	-8.280899	-3.256068	5.239320
38	8	0	-6.516509	-1.697485	5.203190
39	8	0	-8.385185	-1.454303	3.742664
40	8	0	-6.960288	-5.543435	5.239320
41	8	0	-5.452056	-6.534632	3.742664
42	8	0	-4.728319	-4.794720	5.203190
43	5	0	2.941948	-6.817145	4.494700
44	5	0	4.432847	-5.956375	4.494700
45	5	0	0.000000	-9.986954	0.859423
46	5	0	0.000000	-9.986954	-0.859423
47	5	0	-0.874869	-7.503696	5.462132
48	5	0	0.874869	-7.503696	5.462132
49	5	0	-2.015957	-8.972203	4.051657
50	5	0	-1.158753	-10.007607	2.953488
51	5	0	1.158753	-10.007607	2.953488

52	5	0	2.015957	-8.972203	4.051657
53	8	0	0.000000	-10.522851	3.516272
54	8	0	-1.192313	-9.919143	1.572072
55	8	0	1.192313	-9.919143	1.572072
56	8	0	-1.320612	-8.799503	5.239320
57	8	0	-1.788190	-6.492205	5.203190
58	8	0	-2.933130	-7.988935	3.742664
59	8	0	1.320612	-8.799503	5.239320
60	8	0	2.933130	-7.988935	3.742664
61	8	0	1.788190	-6.492205	5.203190
62	5	0	6.060957	-4.509507	5.462132
63	5	0	6.935826	-2.994189	5.462132
64	5	0	6.762177	-6.231972	4.051657
65	5	0	8.087465	-6.007313	2.953488
66	5	0	9.246218	-4.000294	2.953488
67	5	0	8.778134	-2.740231	4.051657
68	5	0	7.374795	-0.860771	4.494700
69	5	0	7.374795	0.860771	4.494700
70	5	0	8.648956	-4.993477	0.859423
71	5	0	8.648956	-4.993477	-0.859423
72	8	0	9.113056	-5.261426	3.516272
73	8	0	7.994073	-5.992145	1.572072
74	8	0	9.186386	-3.926998	1.572072
75	8	0	6.960288	-5.543435	5.239320
76	8	0	4.728319	-4.794720	5.203190
77	8	0	5.452056	-6.534632	3.742664
78	8	0	8.280899	-3.256068	5.239320
79	8	0	8.385185	-1.454303	3.742664
80	8	0	6.516509	-1.697485	5.203190
81	5	0	4.432847	5.956375	4.494700
82	5	0	8.648956	4.993477	0.859423
83	5	0	8.648956	4.993477	-0.859423
84	5	0	6.935826	2.994189	5.462132
85	5	0	6.060957	4.509507	5.462132
86	5	0	8.778134	2.740231	4.051657
87	5	0	9.246218	4.000294	2.953488
88	5	0	8.087465	6.007313	2.953488
89	5	0	6.762177	6.231972	4.051657
90	8	0	9.113056	5.261426	3.516272
91	8	0	9.186386	3.926998	1.572072
92	8	0	7.994073	5.992145	1.572072
93	8	0	8.280899	3.256068	5.239320
94	8	0	6.516509	1.697485	5.203190
95	8	0	8.385185	1.454303	3.742664
96	8	0	6.960288	5.543435	5.239320
97	8	0	5.452056	6.534632	3.742664
98	8	0	4.728319	4.794720	5.203190
99	5	0	0.000000	9.986954	-0.859423
100	5	0	-4.432847	5.956375	-4.494700
101	5	0	-2.941948	6.817145	-4.494700
102	5	0	2.941948	6.817145	-4.494700
103	5	0	4.432847	5.956375	-4.494700
104	5	0	-2.015957	8.972203	-4.051657
105	5	0	-1.158753	10.007607	-2.953488
106	5	0	1.158753	10.007607	-2.953488
107	5	0	2.015957	8.972203	-4.051657
108	5	0	-0.874869	7.503696	-5.462132
109	5	0	0.874869	7.503696	-5.462132

110	8	0	0.000000	10.522851	-3.516272
111	8	0	-1.192313	9.919143	-1.572072
112	8	0	1.192313	9.919143	-1.572072
113	8	0	-1.320612	8.799503	-5.239320
114	8	0	-1.788190	6.492205	-5.203190
115	8	0	-2.933130	7.988935	-3.742664
116	8	0	1.320612	8.799503	-5.239320
117	8	0	2.933130	7.988935	-3.742664
118	8	0	1.788190	6.492205	-5.203190
119	5	0	7.374795	0.860771	-4.494700
120	5	0	7.374795	-0.860771	-4.494700
121	5	0	6.060957	4.509507	-5.462132
122	5	0	6.935826	2.994189	-5.462132
123	5	0	6.762177	6.231972	-4.051657
124	5	0	8.087465	6.007313	-2.953488
125	5	0	9.246218	4.000294	-2.953488
126	5	0	8.778134	2.740231	-4.051657
127	8	0	9.113056	5.261426	-3.516272
128	8	0	7.994073	5.992145	-1.572072
129	8	0	9.186386	3.926998	-1.572072
130	8	0	6.960288	5.543435	-5.239320
131	8	0	4.728319	4.794720	-5.203190
132	8	0	5.452056	6.534632	-3.742664
133	8	0	8.280899	3.256068	-5.239320
134	8	0	8.385185	1.454303	-3.742664
135	8	0	6.516509	1.697485	-5.203190
136	5	0	4.432847	-5.956375	-4.494700
137	5	0	2.941948	-6.817145	-4.494700
138	5	0	-2.941948	-6.817145	-4.494700
139	5	0	-4.432847	-5.956375	-4.494700
140	5	0	0.874869	-7.503696	-5.462132
141	5	0	-0.874869	-7.503696	-5.462132
142	5	0	2.015957	-8.972203	-4.051657
143	5	0	1.158753	-10.007607	-2.953488
144	5	0	-1.158753	-10.007607	-2.953488
145	5	0	-2.015957	-8.972203	-4.051657
146	8	0	0.000000	-10.522851	-3.516272
147	8	0	1.192313	-9.919143	-1.572072
148	8	0	-1.192313	-9.919143	-1.572072
149	8	0	1.320612	-8.799503	-5.239320
150	8	0	1.788190	-6.492205	-5.203190
151	8	0	2.933130	-7.988935	-3.742664
152	8	0	-1.320612	-8.799503	-5.239320
153	8	0	-2.933130	-7.988935	-3.742664
154	8	0	-1.788190	-6.492205	-5.203190
155	5	0	-7.374795	-0.860771	-4.494700
156	5	0	-7.374795	0.860771	-4.494700
157	5	0	-6.060957	-4.509507	-5.462132
158	5	0	-6.935826	-2.994189	-5.462132
159	5	0	-6.762177	-6.231972	-4.051657
160	5	0	-8.087465	-6.007313	-2.953488
161	5	0	-9.246218	-4.000294	-2.953488
162	5	0	-8.778134	-2.740231	-4.051657
163	8	0	-9.113056	-5.261426	-3.516272
164	8	0	-7.994073	-5.992145	-1.572072
165	8	0	-9.186386	-3.926998	-1.572072
166	8	0	-6.960288	-5.543435	-5.239320
167	8	0	-4.728319	-4.794720	-5.203190

168	8	0	-5.452056	-6.534632	-3.742664
169	8	0	-8.280899	-3.256068	-5.239320
170	8	0	-8.385185	-1.454303	-3.742664
171	8	0	-6.516509	-1.697485	-5.203190
172	5	0	-6.935826	2.994189	-5.462132
173	5	0	-6.060957	4.509507	-5.462132
174	5	0	-8.778134	2.740231	-4.051657
175	5	0	-9.246218	4.000294	-2.953488
176	5	0	-8.087465	6.007313	-2.953488
177	5	0	-6.762177	6.231972	-4.051657
178	8	0	-9.113056	5.261426	-3.516272
179	8	0	-9.186386	3.926998	-1.572072
180	8	0	-7.994073	5.992145	-1.572072
181	8	0	-8.280899	3.256068	-5.239320
182	8	0	-6.516509	1.697485	-5.203190
183	8	0	-8.385185	1.454303	-3.742664
184	8	0	-6.960288	5.543435	-5.239320
185	8	0	-5.452056	6.534632	-3.742664
186	8	0	-4.728319	4.794720	-5.203190
187	5	0	6.935826	-2.994189	-5.462132
188	5	0	6.060957	-4.509507	-5.462132
189	5	0	8.778134	-2.740231	-4.051657
190	5	0	9.246218	-4.000294	-2.953488
191	5	0	8.087465	-6.007313	-2.953488
192	5	0	6.762177	-6.231972	-4.051657
193	8	0	9.113056	-5.261426	-3.516272
194	8	0	9.186386	-3.926998	-1.572072
195	8	0	7.994073	-5.992145	-1.572072
196	8	0	8.280899	-3.256068	-5.239320
197	8	0	6.516509	-1.697485	-5.203190
198	8	0	8.385185	-1.454303	-3.742664
199	8	0	6.960288	-5.543435	-5.239320
200	8	0	5.452056	-6.534632	-3.742664
201	8	0	4.728319	-4.794720	-5.203190
202	5	0	0.874869	7.503696	5.462132
203	5	0	-0.874869	7.503696	5.462132
204	5	0	2.015957	8.972203	4.051657
205	5	0	1.158753	10.007607	2.953488
206	5	0	-1.158753	10.007607	2.953488
207	5	0	-2.015957	8.972203	4.051657
208	8	0	0.000000	10.522851	3.516272
209	8	0	1.192313	9.919143	1.572072
210	8	0	-1.192313	9.919143	1.572072
211	8	0	1.320612	8.799503	5.239320
212	8	0	1.788190	6.492205	5.203190
213	8	0	2.933130	7.988935	3.742664
214	8	0	-1.320612	8.799503	5.239320
215	8	0	-2.933130	7.988935	3.742664
216	8	0	-1.788190	6.492205	5.203190

SCF Done: E(RB3LYP) =   -10819.6977504

Table S14: Theoretical Cartesian coordinates for *t*-B$_{90}$.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	5.461228	7.830306	7.057878
2	8	0	7.060811	6.086813	7.352653
3	8	0	4.245435	3.288765	10.591891
4	8	0	5.647820	5.158758	10.834175
5	8	0	6.337753	3.387533	9.452268
6	8	0	3.834809	7.134167	10.498851
7	8	0	1.899085	5.844600	10.163609
8	8	0	2.391860	7.682951	8.727220
9	8	0	8.017669	-2.616974	8.365155
10	8	0	6.846980	-4.687785	8.526531
11	8	0	7.397265	-3.475266	10.462992
12	8	0	3.782559	-4.831238	10.195259
13	8	0	5.022804	-3.587496	11.756515
14	8	0	2.865394	-2.859854	11.174405
15	8	0	4.589085	0.173537	10.952311
16	8	0	6.680778	0.272313	9.811961
17	8	0	-2.484596	-7.989017	10.309306
18	8	0	-1.170475	-8.341303	8.393165
19	8	0	-3.500723	-7.876559	8.193375
20	8	0	-3.520031	-5.753686	11.429047
21	8	0	-4.835025	-4.988539	9.638080
22	8	0	-3.418060	-3.484163	10.827557
23	8	0	-0.002372	-4.168798	11.128813
24	8	0	0.910423	-6.138373	10.141768
25	8	0	-9.416512	-1.426815	7.100991
26	8	0	-9.776700	-0.051862	8.972346
27	8	0	-9.684947	0.928246	6.838620
28	8	0	-7.604294	3.125642	8.582471
29	8	0	-5.920718	2.271497	10.038871
30	8	0	-7.871503	-1.016891	10.623922
31	8	0	-5.534941	-1.179396	10.437027
32	8	0	-6.951302	-2.681730	9.244091
33	8	0	-4.406657	9.365726	8.287591
34	8	0	-5.309208	8.559665	6.273238
35	8	0	-3.143496	9.556859	6.315426
36	8	0	-2.506737	8.400275	9.953773
37	8	0	-0.690512	8.303514	8.465541
38	8	0	-1.182894	6.459387	9.894833
39	8	0	-4.362710	5.005801	9.844255
40	8	0	-6.034802	5.855824	8.372000
41	5	0	0.237082	-7.219400	-9.212057
42	5	0	-1.442051	-6.882755	-9.356366
43	8	0	2.094692	-11.688807	-0.448144
44	8	0	3.208766	-11.340988	1.631508
45	8	0	6.697915	-11.463575	-0.037506
46	8	0	6.390027	-9.892426	1.682646
47	8	0	7.443670	-9.258507	-0.360343
48	8	0	5.434394	-11.865212	-2.394080
49	8	0	5.814886	-9.780302	-3.408875
50	8	0	3.643430	-10.765328	-3.444984
51	8	0	2.506737	-8.400275	-9.953773

52	8	0	1.182895	-6.459387	-9.894833
53	8	0	0.690513	-8.303513	-8.465541
54	8	0	4.406657	-9.365725	-8.287591
55	8	0	3.143496	-9.556859	-6.315426
56	8	0	5.309209	-8.559665	-6.273238
57	8	0	6.034803	-5.855824	-8.372000
58	8	0	4.362711	-5.005801	-9.844255
59	8	0	7.871503	1.016891	-10.623921
60	8	0	6.951302	2.681730	-9.244090
61	8	0	5.534941	1.179396	-10.437026
62	8	0	8.170217	-1.654367	-10.325635
63	8	0	5.920718	-2.271497	-10.038871
64	8	0	7.604294	-3.125642	-8.582471
65	8	0	9.684948	-0.928246	-6.838619
66	8	0	9.416512	1.426815	-7.100990
67	8	0	12.950008	2.646422	-1.160137
68	8	0	11.449394	3.088374	0.593486
69	8	0	11.079462	4.007162	-1.575643
70	8	0	12.808784	1.013032	-3.311776
71	8	0	10.898783	1.898802	-4.355527
72	8	0	11.146907	-0.457475	-4.085030
73	8	0	11.698449	-1.805690	-0.904291
74	8	0	11.820010	-0.365583	0.992536
75	8	0	10.697397	-5.741625	5.356081
76	8	0	8.449795	-5.787311	6.040682
77	8	0	9.625265	-3.718503	5.885258
78	8	0	11.892002	-5.031651	3.036471
79	8	0	11.168387	-2.800891	2.886091
80	8	0	11.044265	-4.243126	0.991479
81	8	0	9.316332	-7.273813	1.216443
82	8	0	8.265973	-7.903407	3.262544
83	5	0	-5.539593	-0.926517	-10.268255
84	5	0	-5.3352654	-2.623647	-10.072232
85	8	0	-6.680778	-0.272313	-9.811961
86	8	0	-6.356234	1.243610	-11.577595
87	8	0	-4.589085	-0.173537	-10.952311
88	8	0	-5.022804	3.587496	-11.756514
89	8	0	-2.865394	2.859854	-11.174404
90	8	0	-3.782559	4.831238	-10.195258
91	8	0	-6.846980	4.687785	-8.526530
92	8	0	-8.017669	2.616974	-8.365155
93	8	0	-11.892003	5.031651	-3.036471
94	8	0	-11.044266	4.243126	-0.991478
95	8	0	-11.168388	2.800891	-2.886090
96	8	0	-10.697397	5.741624	-5.356081
97	8	0	-9.625266	3.718502	-5.885258
98	8	0	-8.449796	5.787311	-6.040682
99	8	0	-8.265974	7.903407	-3.262544
100	8	0	-9.316333	7.273813	-1.216443
101	8	0	-5.434393	11.865211	2.394080
102	8	0	-3.643430	10.765328	3.444983
103	8	0	-5.814885	9.780301	3.408875
104	8	0	-7.443670	9.258507	0.360343
105	8	0	-6.390027	9.892426	-1.682646
106	8	0	-4.237205	12.580764	0.079478
107	8	0	-3.208766	11.340987	-1.631508
108	8	0	-2.094692	11.688807	0.448144
109	8	0	4.096649	12.308765	-2.791620

110	8	0	5.306290	10.300069	-2.636754
111	8	0	4.088677	11.127115	-0.760641
112	8	0	0.673665	11.821597	-1.056344
113	8	0	-0.438235	11.467884	-3.135972
114	8	0	2.838101	11.907933	-5.147450
115	8	0	1.341484	10.253978	-5.886984
116	8	0	3.668812	9.775959	-5.683547
117	8	0	10.468472	8.003599	1.526295
118	8	0	9.866881	6.608957	-0.266693
119	8	0	10.247370	5.694504	1.902319
120	8	0	9.087971	8.945676	3.650553
121	8	0	8.460328	6.913128	4.649017
122	8	0	6.864928	8.661260	4.357578
123	8	0	6.306349	9.999104	1.177154
124	8	0	7.522436	9.166517	-0.697376
125	8	0	0.880610	6.283586	-11.656036
126	8	0	-0.910423	6.138373	-10.141768
127	8	0	0.002372	4.168798	-11.128812
128	8	0	3.520031	5.753686	-11.429047
129	8	0	3.418060	3.484163	-10.827556
130	8	0	4.835025	4.988539	-9.638080
131	8	0	3.500724	7.876560	-8.193375
132	8	0	1.170476	8.341303	-8.393165
133	8	0	-13.231412	0.025336	0.855028
134	8	0	-11.820011	0.365583	-0.992536
135	8	0	-11.698449	1.805690	0.904291
136	8	0	-12.808784	-1.013032	3.311776
137	8	0	-11.146907	0.457475	4.085031
138	8	0	-10.898782	-1.898802	4.355527
139	8	0	-11.079462	-4.007162	1.575643
140	8	0	-11.449394	-3.088374	-0.593486
141	5	0	-4.360880	-4.640679	-10.863635
142	5	0	-3.192931	-5.913170	-10.649366
143	8	0	-2.391860	-7.682950	-8.727219
144	8	0	-1.899085	-5.844600	-10.163609
145	8	0	-5.647820	-5.158758	-10.834175
146	8	0	-4.245435	-3.288765	-10.591891
147	8	0	-6.337753	-3.387533	-9.452268
148	8	0	-7.060812	-6.086814	-7.352653
149	8	0	-6.206574	-7.247534	-9.208842
150	8	0	-5.461228	-7.830306	-7.057878
151	8	0	-2.838101	-11.907932	5.147449
152	8	0	-3.668812	-9.775959	5.683546
153	8	0	-1.341484	-10.253978	5.886984
154	8	0	0.438235	-11.467884	3.135972
155	8	0	-0.673665	-11.821597	1.056343
156	8	0	-4.096649	-12.308764	2.791620
157	8	0	-4.088677	-11.127115	0.760641
158	8	0	-5.306290	-10.300068	2.636754
159	8	0	-10.247371	-5.694504	-1.902320
160	8	0	-9.866881	-6.608957	0.266693
161	8	0	-10.468472	-8.003599	-1.526296
162	8	0	-7.522436	-9.166516	0.697376
163	8	0	-6.306349	-9.999104	-1.177155
164	8	0	-9.087971	-8.945676	-3.650554
165	8	0	-6.864929	-8.661260	-4.357579
166	8	0	-8.460328	-6.913128	-4.649018
167	5	0	-6.764758	-6.081515	-8.704474

168	5	0	-6.404879	-4.737301	-9.750201
169	5	0	-5.201624	-7.783800	-8.416238
170	5	0	-3.674056	-7.710367	-9.246957
171	5	0	-6.558554	-7.124415	-6.572063
172	5	0	-7.322121	-7.576002	-5.100102
173	5	0	-7.752111	-9.290393	-3.502088
174	5	0	-9.311665	-7.583257	-3.788085
175	5	0	-10.201228	-6.976670	-2.420612
176	5	0	-9.829091	-7.869950	-0.302058
177	5	0	-8.662105	-9.143512	-0.087265
178	5	0	-7.474024	-9.957117	-1.918548
179	5	0	-6.391808	-9.808343	0.199277
180	5	0	-5.184268	-10.424729	1.255489
181	5	0	-10.299164	-5.544151	-0.519167
182	5	0	-10.956827	-4.125577	0.193884
183	5	0	-12.029069	-3.134065	2.076556
184	5	0	-11.938502	-2.083240	3.461167
185	5	0	-12.180735	0.218986	3.196711
186	5	0	-12.454440	0.889103	1.613690
187	5	0	-12.573899	-0.517422	-0.239660
188	5	0	-12.390697	-2.236997	-0.042041
189	5	0	-10.656717	-0.612254	4.829197
190	5	0	-9.854896	-0.355458	6.327361
191	5	0	-8.022220	-1.852047	9.526052
192	5	0	-9.249195	-1.228692	8.460296
193	5	0	-9.510271	1.072214	8.203729
194	5	0	-8.474888	2.168323	9.073153
195	5	0	-6.830594	1.334609	10.496315
196	5	0	-6.638500	-0.384225	10.691444
197	5	0	-5.745074	-2.445780	9.898082
198	5	0	-4.592110	-3.702126	10.111785
199	5	0	-6.388656	3.308070	9.235915
200	5	0	-5.536421	4.796351	9.125335
201	5	0	-2.414049	7.031628	10.162831
202	5	0	-3.996770	6.308004	10.135728
203	5	0	-1.932721	8.833668	8.767058
204	5	0	-3.154933	9.456729	7.695550
205	5	0	-5.271093	8.484023	7.654468
206	5	0	-5.631094	7.138603	8.698324
207	5	0	-4.326788	9.304694	5.626551
208	5	0	-4.600701	9.966238	4.064265
209	5	0	-0.237082	7.219401	9.212058
210	5	0	1.442052	6.882756	9.356367
211	5	0	3.674057	7.710368	9.246957
212	5	0	5.201625	7.783800	8.416238
213	5	0	4.360881	4.640680	10.863635
214	5	0	3.192931	5.913170	10.649367
215	5	0	6.404879	4.737301	9.750200
216	5	0	6.764758	6.081515	8.704473
217	5	0	6.558554	7.124415	6.572062
218	5	0	7.322121	7.576001	5.100102
219	5	0	5.352654	2.623647	10.072232
220	5	0	5.539593	0.926517	10.268255
221	5	0	7.030791	-0.926915	10.407010
222	5	0	7.698359	-2.364455	9.687743
223	5	0	6.552683	-4.386376	9.844645
224	5	0	5.025372	-4.458162	10.676156
225	5	0	4.129028	-2.533065	11.634098

226	5	0	4.987458	-1.023201	11.521520
227	5	0	2.665363	-4.130112	10.640804
228	5	0	1.101730	-4.842660	10.613812
229	5	0	-1.088456	-4.915921	11.549501
230	5	0	-2.788686	-4.574659	11.401521
231	5	0	-0.196746	-6.840395	10.584746
232	5	0	-1.231482	-7.937554	9.715388
233	5	0	-2.365949	-8.515344	7.700997
234	5	0	-3.507530	-7.482839	9.519944
235	5	0	-4.172765	-6.044326	10.239601
236	5	0	-2.458397	-9.553876	6.334802
237	5	0	-1.543098	-11.409602	5.152898
238	5	0	-3.816895	-10.943214	4.955264
239	5	0	-4.630085	-11.203065	3.438205
240	5	0	-3.442020	-12.012601	1.604668
241	5	0	-1.742679	-12.359326	1.751305
242	5	0	-0.656221	-12.014611	3.782701
243	5	0	0.508973	-11.579779	1.750064
244	5	0	2.017819	-11.509267	0.930375
245	5	0	4.382437	-11.779589	1.044098
246	5	0	5.966780	-11.059003	1.070306
247	5	0	6.997245	-10.440146	-0.925397
248	5	0	6.185377	-10.699404	-2.443026
249	5	0	4.064398	-11.661621	-2.478366
250	5	0	3.293421	-12.121727	-0.987108
251	5	0	7.319077	-9.097485	1.016887
252	5	0	8.340186	-8.015103	1.876752
253	5	0	4.600701	-9.966239	-4.064266
254	5	0	4.326789	-9.304694	-5.626551
255	5	0	3.154933	-9.456728	-7.695550
256	5	0	1.932721	-8.833668	-8.767058
257	5	0	5.271093	-8.484023	-7.654468
258	5	0	5.631094	-7.138603	-8.698324
259	5	0	3.996771	-6.308003	-10.135728
260	5	0	2.414050	-7.031627	-10.162830
261	5	0	5.536421	-4.796351	-9.125334
262	5	0	6.388657	-3.308070	-9.235915
263	5	0	8.474889	-2.168323	-9.073153
264	5	0	9.510271	-1.072214	-8.203729
265	5	0	9.854896	0.355458	-6.327361
266	5	0	9.249195	1.228693	-8.460296
267	5	0	8.022220	1.852047	-9.526051
268	5	0	5.745073	2.445780	-9.898081
269	5	0	6.638500	0.384225	-10.691444
270	5	0	6.830595	-1.334609	-10.496314
271	5	0	11.574747	-1.633273	0.471706
272	5	0	11.218634	-2.960428	1.503906
273	5	0	12.454440	-0.889103	-1.613689
274	5	0	12.180735	-0.218986	-3.196711
275	5	0	10.656717	0.612254	-4.829197
276	5	0	11.938503	2.083240	-3.461167
277	5	0	12.029070	3.134065	-2.076556
278	5	0	12.390696	2.236997	0.042041
279	5	0	12.573899	0.517422	0.239660
280	5	0	10.956827	4.125577	-0.193884
281	5	0	10.299164	5.544151	0.519167
282	5	0	10.201228	6.976670	2.420612
283	5	0	9.311664	7.583257	3.788085

284	5	0	7.752111	9.290393	3.502087
285	5	0	7.474024	9.957118	1.918548
286	5	0	8.662104	9.143512	0.087265
287	5	0	9.829091	7.869950	0.302058
288	5	0	6.391808	9.808343	-0.199278
289	5	0	5.184268	10.424729	-1.255490
290	5	0	3.442019	12.012601	-1.604668
291	5	0	4.630085	11.203066	-3.438205
292	5	0	3.816895	10.943215	-4.955265
293	5	0	2.458397	9.553877	-6.334802
294	5	0	2.365950	8.515344	-7.700998
295	5	0	1.543098	11.409602	-5.152898
296	5	0	0.656221	12.014611	-3.782702
297	5	0	1.742679	12.359326	-1.751306
298	5	0	-0.508973	11.579778	-1.750064
299	5	0	-2.017819	11.509266	-0.930376
300	5	0	-4.064398	11.661620	2.478366
301	5	0	-3.293421	12.121726	0.987108
302	5	0	-4.382437	11.779588	-1.044099
303	5	0	-5.966780	11.059002	-1.070307
304	5	0	-6.185376	10.699404	2.443025
305	5	0	-6.997245	10.440146	0.925397
306	5	0	-7.319078	9.097485	-1.016887
307	5	0	-8.340186	8.015103	-1.876752
308	5	0	-10.406056	6.828836	-1.944073
309	5	0	-11.266414	5.319891	-1.831816
310	5	0	-9.379143	7.442628	-3.943289
311	5	0	-9.470535	6.389292	-5.326090
312	5	0	-10.619588	4.368149	-5.175144
313	5	0	-11.388194	3.911259	-3.682079
314	5	0	-11.218634	2.960428	-1.503906
315	5	0	-11.574747	1.633273	-0.471706
316	5	0	-8.646661	4.489995	-6.505989
317	5	0	-7.772284	3.890433	-7.858663
318	5	0	-6.552683	4.386376	-9.844644
319	5	0	-7.698359	2.364455	-9.687743
320	5	0	-7.030791	0.926915	-10.407009
321	5	0	-4.987458	1.023201	-11.521519
322	5	0	-4.129028	2.533066	-11.634097
323	5	0	-5.025372	4.458162	-10.676155
324	5	0	-2.665363	4.130112	-10.640804
325	5	0	-1.101730	4.842660	-10.613812
326	5	0	0.196746	6.840395	-10.584746
327	5	0	1.231482	7.937555	-9.715389
328	5	0	3.507530	7.482840	-9.519944
329	5	0	4.172765	6.044327	-10.239602
330	5	0	2.788686	4.574659	-11.401521
331	5	0	1.088456	4.915921	-11.549501
332	5	0	4.592110	3.702126	-10.111785
333	5	0	7.772283	-3.890433	7.858663
334	5	0	8.646660	-4.489996	6.505989
335	5	0	10.619587	-4.368149	5.175144
336	5	0	11.388193	-3.911259	3.682080
337	5	0	11.266414	-5.319891	1.831816
338	5	0	10.406055	-6.828836	1.944073
339	5	0	9.379142	-7.442628	3.943289
340	5	0	9.470534	-6.389292	5.326090
341	8	0	1.459386	12.849020	-3.018384

342	8	0	8.656251	9.982600	1.192378
343	8	0	-6.697915	11.463574	0.037506
344	8	0	-10.555560	7.376123	-3.210348
345	8	0	-7.397265	3.475266	-10.462991
346	8	0	-4.963540	7.276631	9.906911
347	8	0	2.484596	7.989017	-10.309306
348	8	0	6.206575	7.247534	9.208842
349	8	0	13.231412	-0.025337	-0.855027
350	8	0	9.776700	0.051862	-8.972345
351	8	0	6.356234	-1.243609	11.577596
352	8	0	10.555560	-7.376123	3.210348
353	8	0	4.963541	-7.276631	-9.906911
354	8	0	-0.880610	-6.283586	11.656036
355	8	0	4.237205	-12.580765	-0.079479
356	8	0	-1.459386	-12.849020	3.018383
357	8	0	-8.656251	-9.982600	-1.192379
358	8	0	-3.834808	-7.134166	-10.498851
359	8	0	-8.170216	1.654368	10.325635
360	8	0	-12.950008	-2.646422	1.160138

SCF Done: E(RB3LYP) =   -18032.8749915

Table S15: Theoretical Cartesian coordinates for *t*-B$_{90}$-2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	5	0	2.970907	4.089103	9.815112
2	5	0	3.831480	5.273579	8.910253
3	5	0	8.075867	-1.354610	7.545994
4	5	0	8.937328	-0.168911	6.640201
5	5	0	-2.970907	-4.089103	-9.815112
6	5	0	-3.831480	-5.273579	-8.910253
7	5	0	-8.075867	1.354610	-7.545994
8	5	0	-8.937328	0.168911	-6.640201
9	5	0	-4.807029	1.561898	-9.815112
10	5	0	-6.199464	2.014328	-8.910253
11	5	0	-7.131166	-5.389882	-6.640201
12	5	0	-5.737294	-5.842778	-7.545994
13	5	0	7.131166	5.389882	6.640201
14	5	0	5.737294	5.842778	7.545994
15	5	0	4.807029	-1.561898	9.815112
16	5	0	6.199464	-2.014328	8.910253
17	5	0	-2.814864	-1.820398	-10.618819
18	5	0	-3.347276	-0.181803	-10.618819
19	5	0	-9.170372	-2.074775	-5.786456
20	5	0	-8.638509	-3.711681	-5.786456
21	5	0	8.638509	3.711681	5.786456
22	5	0	9.170372	2.074775	5.786456
23	5	0	3.347276	0.181803	10.618819
24	5	0	2.814864	1.820398	10.618819
25	5	0	-7.131166	-8.349604	-1.851269
26	5	0	-5.737294	-9.362312	-1.851269
27	5	0	-6.199464	-7.068738	5.786456
28	5	0	-4.807029	-8.080401	5.786456
29	5	0	6.199464	7.068738	-5.786456
30	5	0	4.807029	8.080401	-5.786456
31	5	0	7.131166	8.349604	1.851269
32	5	0	5.737294	9.362312	1.851269
33	5	0	-3.831480	-10.327989	-0.732047
34	5	0	-2.970907	-10.607606	0.732047
35	5	0	-8.937328	-5.863637	3.120667
36	5	0	-8.075867	-6.143542	4.586271
37	5	0	8.075867	6.143542	-4.586271
38	5	0	8.937328	5.863637	-3.120667
39	5	0	2.970907	10.607606	-0.732047
40	5	0	3.831480	10.327989	0.732047
41	5	0	-2.814864	-10.311867	3.120667
42	5	0	-3.347276	-9.579065	4.586271
43	5	0	-8.638509	-6.835478	-0.732047
44	5	0	-9.170372	-6.103431	0.732047
45	5	0	3.347276	9.579065	-4.586271
46	5	0	2.814864	10.311867	-3.120667
47	5	0	9.170372	6.103431	-0.732047
48	5	0	8.638509	6.835478	0.732047
49	5	0	-10.144597	4.201973	-1.851269
50	5	0	-10.677009	2.563377	-1.851269
51	5	0	-9.170372	2.074775	5.786456

52	5	0	-8.638509	3.711681	5.786456
53	5	0	10.677009	-2.563377	1.851269
54	5	0	10.144597	-4.201973	1.851269
55	5	0	9.170372	-2.074775	-5.786456
56	5	0	8.638509	-3.711681	-5.786456
57	5	0	-8.338436	5.782147	4.586271
58	5	0	-8.338436	6.687940	3.120667
59	5	0	-11.006494	-0.452430	0.732047
60	5	0	-11.006494	0.452430	-0.732047
61	5	0	11.006494	-0.452430	0.732047
62	5	0	11.006494	0.452430	-0.732047
63	5	0	8.338436	-5.782147	-4.586271
64	5	0	8.338436	-6.687940	-3.120667
65	5	0	-8.638509	6.835478	0.732047
66	5	0	-9.170372	6.103431	-0.732047
67	5	0	-10.677009	-0.509448	3.120667
68	5	0	-10.144597	0.223354	4.586271
69	5	0	10.144597	-0.223354	-4.586271
70	5	0	10.677009	0.509448	-3.120667
71	5	0	8.638509	-6.835478	-0.732047
72	5	0	9.170372	-6.103431	0.732047
73	5	0	2.601142	8.552100	-6.640201
74	5	0	1.207270	8.099204	-7.545994
75	5	0	6.199464	2.014328	-8.910253
76	5	0	4.807029	1.561898	-9.815112
77	5	0	-4.807029	-1.561898	9.815112
78	5	0	-6.199464	-2.014328	8.910253
79	5	0	-1.207270	-8.099204	7.545994
80	5	0	-2.601142	-8.552100	6.640201
81	5	0	2.601142	2.114561	-10.618819
82	5	0	1.207270	3.127268	-10.618819
83	5	0	-1.207270	-3.127268	10.618819
84	5	0	-2.601142	-2.114561	10.618819
85	5	0	7.329734	3.650973	-7.545994
86	5	0	7.329734	5.116577	-6.640201
87	5	0	0.000000	5.054410	-9.815112
88	5	0	0.000000	6.518503	-8.910253
89	5	0	-7.329734	-5.116577	6.640201
90	5	0	-7.329734	-3.650973	7.545994
91	5	0	0.000000	-6.518503	8.910253
92	5	0	0.000000	-5.054410	9.815112
93	5	0	-8.075867	-1.354610	7.545994
94	5	0	-8.937328	-0.168911	6.640201
95	5	0	-2.970907	4.089103	9.815112
96	5	0	-3.831480	5.273579	8.910253
97	5	0	3.831480	-5.273579	-8.910253
98	5	0	2.970907	-4.089103	-9.815112
99	5	0	8.937328	0.168911	-6.640201
100	5	0	8.075867	1.354610	-7.545994
101	5	0	-7.131166	5.389882	6.640201
102	5	0	-5.737294	5.842778	7.545994
103	5	0	5.737294	-5.842778	-7.545994
104	5	0	7.131166	-5.389882	-6.640201
105	5	0	-3.347276	0.181803	10.618819
106	5	0	-2.814864	1.820398	10.618819
107	5	0	2.814864	-1.820398	-10.618819
108	5	0	3.347276	-0.181803	-10.618819
109	5	0	-0.861461	3.239628	10.618819

110	5	0	0.861461	3.239628	10.618819
111	5	0	0.860572	9.362683	5.786456
112	5	0	-0.860572	9.362683	5.786456
113	5	0	0.861461	-3.239628	-10.618819
114	5	0	-0.861461	-3.239628	-10.618819
115	5	0	-0.860572	-9.362683	-5.786456
116	5	0	0.860572	-9.362683	-5.786456
117	5	0	3.783891	-7.262009	-7.545994
118	5	0	2.922430	-8.447707	-6.640201
119	5	0	-2.922430	8.447707	6.640201
120	5	0	-3.783891	7.262009	7.545994
121	5	0	2.922430	8.447707	6.640201
122	5	0	3.783891	7.262009	7.545994
123	5	0	-3.783891	-7.262009	-7.545994
124	5	0	-2.922430	-8.447707	-6.640201
125	5	0	-10.677009	-2.563377	1.851269
126	5	0	-10.144597	-4.201973	1.851269
127	5	0	10.144597	4.201973	-1.851269
128	5	0	10.677009	2.563377	-1.851269
129	5	0	-8.338436	-5.782147	-4.586271
130	5	0	-8.338436	-6.687940	-3.120667
131	5	0	8.338436	6.687940	3.120667
132	5	0	8.338436	5.782147	4.586271
133	5	0	-3.783891	-9.997011	-3.120667
134	5	0	-2.922430	-9.717106	-4.586271
135	5	0	2.922430	9.717106	4.586271
136	5	0	3.783891	9.997011	3.120667
137	5	0	3.831480	-10.327989	-0.732047
138	5	0	2.970907	-10.607606	0.732047
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161	5	0	-1.207270	8.099204	-7.545994
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