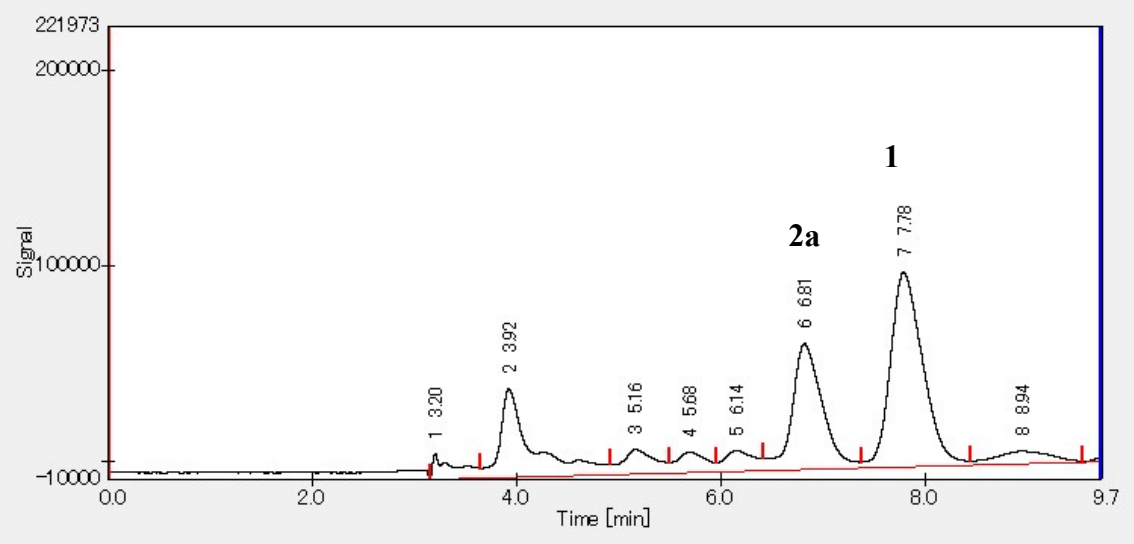
Supporting Information

for

Regioselective Addition of Grignard Reagents to Tosylazafulleroid and Derivatization to 1,2-Disubstituted [60]Fullerene

(a)



(b)

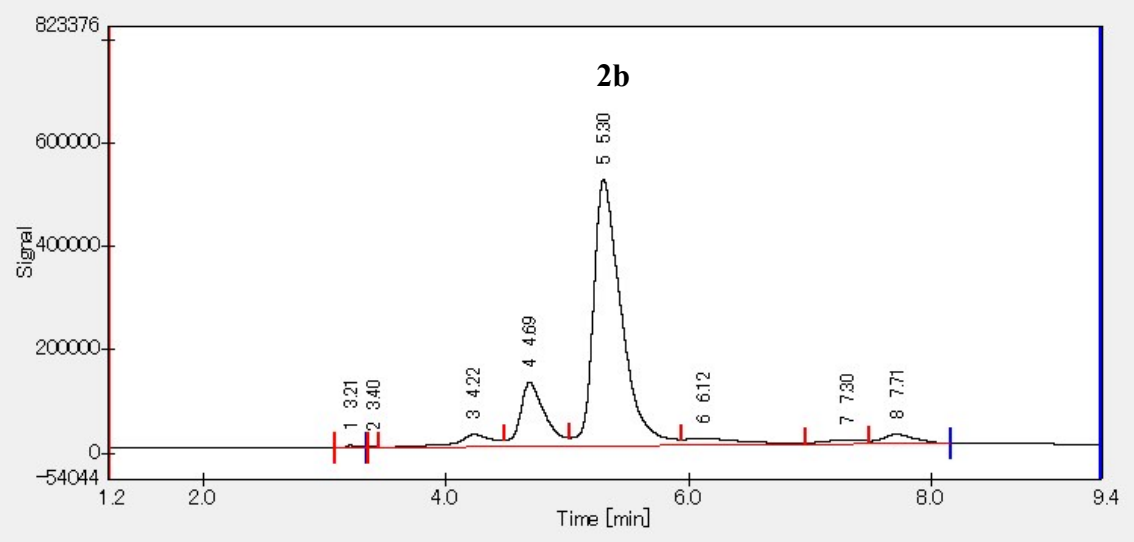
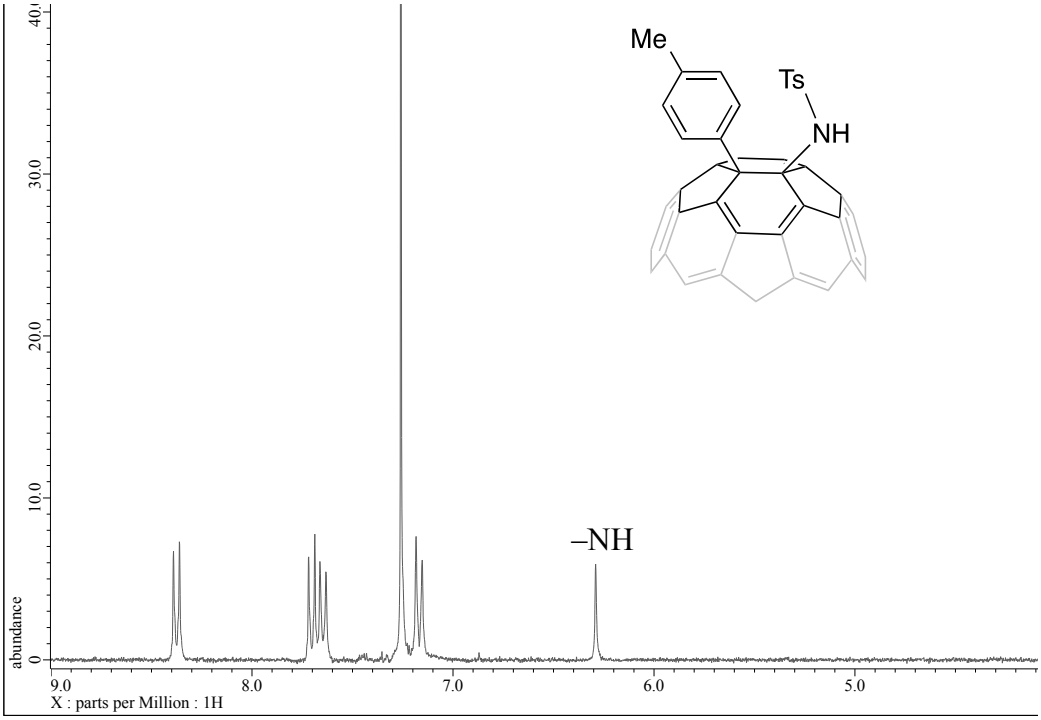


Fig. S1. HPLC charts (buckyprep, toluene) for (a) **1** + EtMgBr (–70 ºC, 3 equiv) and (b) **1** + TolMgBr (rt, 3 equiv).

(a)



(b)

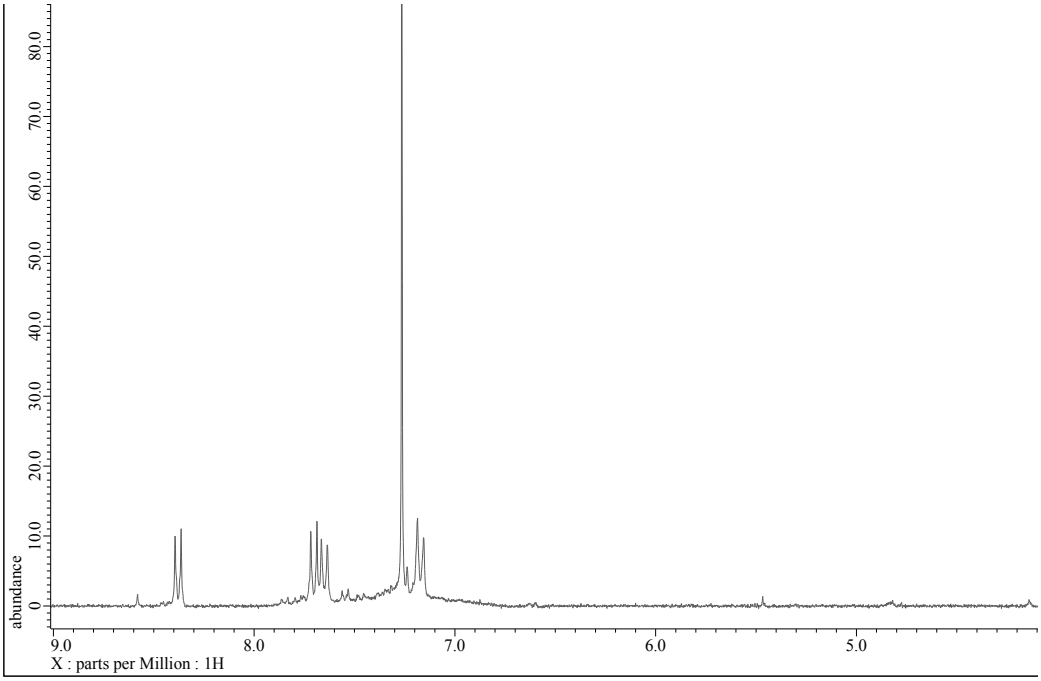


Fig. S2. ^{1}NMR spectrum of compound **2b** in $CDCl_3$ (a) without and (b) with D_2O addition.

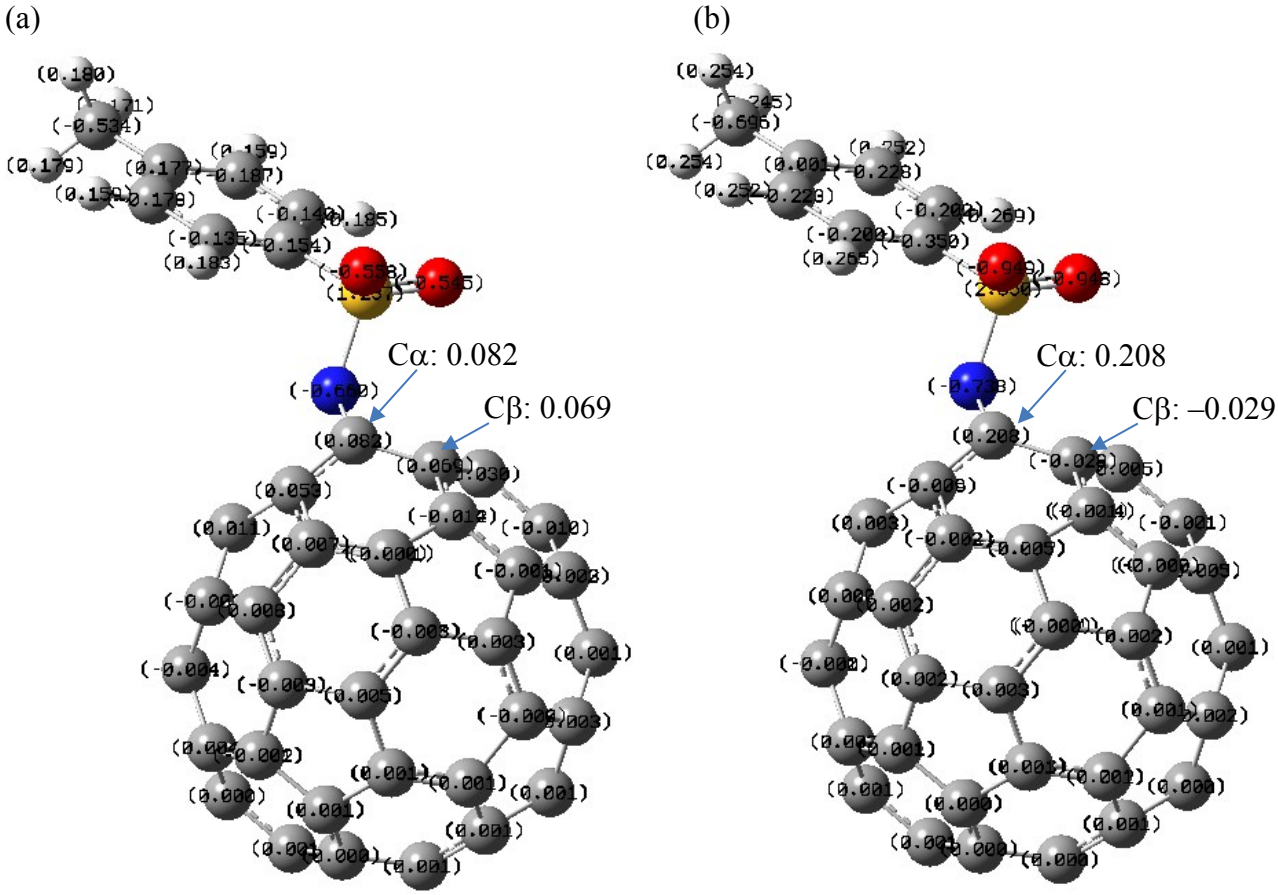
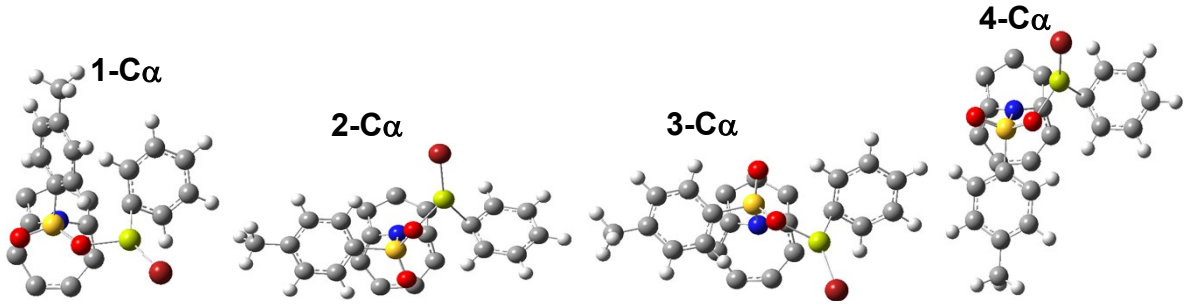


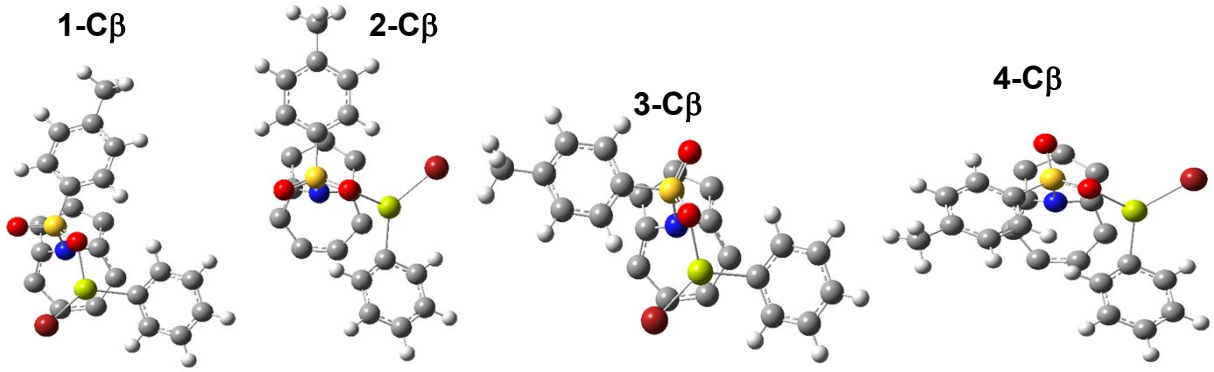
Fig. S3. (a) Mulliken and (b) NBO charge of Tosylazafulleroid **1**.

Table S1. TS structures for Cα-addition of PhMgBr to **1** (top view, only azepine linkage of **1** was illustrated for clarity)



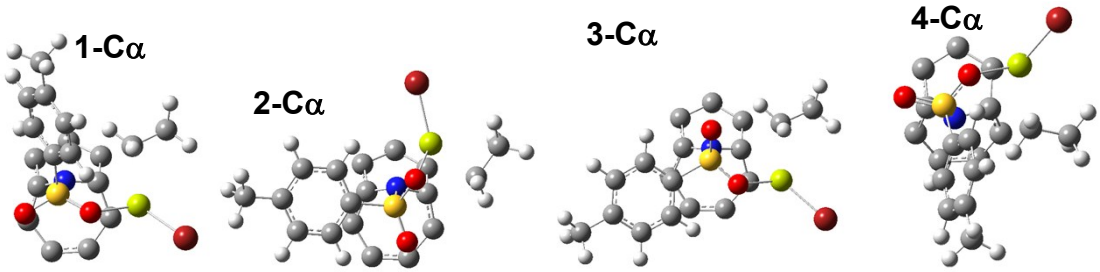
TS-configuration	1-Cα	2-Cα	3-Cα	4-Cα
E / au	–6163.970157	–6163.973306	–6163.975099	–6163.969697
ν_i / cm^{-1}	258.6i	239.6i	224.0i	222.0i
ΔE / kJ mol^{-1}	46.5	38.2	33.5	47.7
O•••Mg / Å	2.00	2.02	2.01	2.02
N•••Mg / Å	3.55	3.10	3.26	3.15
C_{ipso}•••C_α /Å	2.24	2.26	2.27	2.28

Table S2. TS structures for Cβ-addition of PhMgBr to **1** (top view, only azepine linkage of **1** was illustrated for clarity)



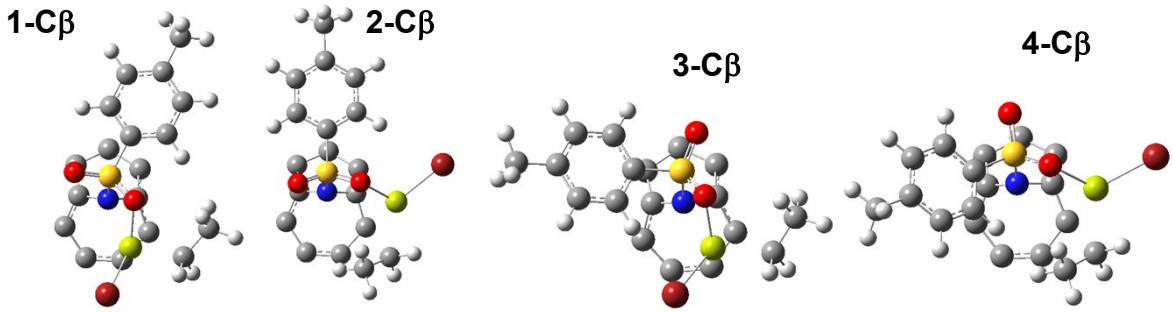
TS-configuration	1-Cβ	2-Cβ	3-Cβ	4-Cβ
E / au	–6163.977873	–6163.981783	–6163.977935	–6163.978702
ν_i / cm^{-1}	262.6i	240.9i	281.0i	253.7i
ΔE / kJ mol^{-1}	26.2	16.0	26.1	24.1
O•••Mg / Å	2.08	2.04	2.09	2.05
N•••Mg / Å	2.64	3.02	2.45	3.01
C_{ipso}•••C_β / Å	2.20	2.30	2.21	2.44

Table S3. TS structures for Cα-addition of EtMgBr to **1** (top view, only azepine linkage of **1** was illustrated for clarity)



TS-configuration	1-Cα	2-Cα	3-Cα	4-Cα
E / au	-6011.544788	-6011.533260	-6011.541835	-6011.540061
ν_i / cm^{-1}	227.7i	282.0i	237.8i	267.6i
ΔE / kJ mol^{-1}	33.5	63.8	41.2	45.9
O•••Mg / Å	2.06	2.06	2.05	2.05
N•••Mg / Å	3.17	2.34	3.16	3.27
C_{Et}•••C_α /Å	2.46	2.31	2.48	2.33

Table S4. TS structures for Cβ-addition of EtMgBr to **1** (top view, only azepine linkage of **1** was illustrated for clarity)



TS-configuration	1-Cβ	2-Cβ	3-Cβ	4-Cβ
E / au	-6011.53942	-6011.547790	-6011.539267	-6011.544735
ν_i / cm^{-1}	348.8i	274.0i	383.9i	287.8i
ΔE / kJ mol^{-1}	47.6	25.6	48.0	33.6
O•••Mg / Å	2.09	2.05	2.09	2.06
N•••Mg / Å	2.40	2.97	2.34	2.98
C_{Et}•••C_β / Å	2.25	2.39	2.22	2.44

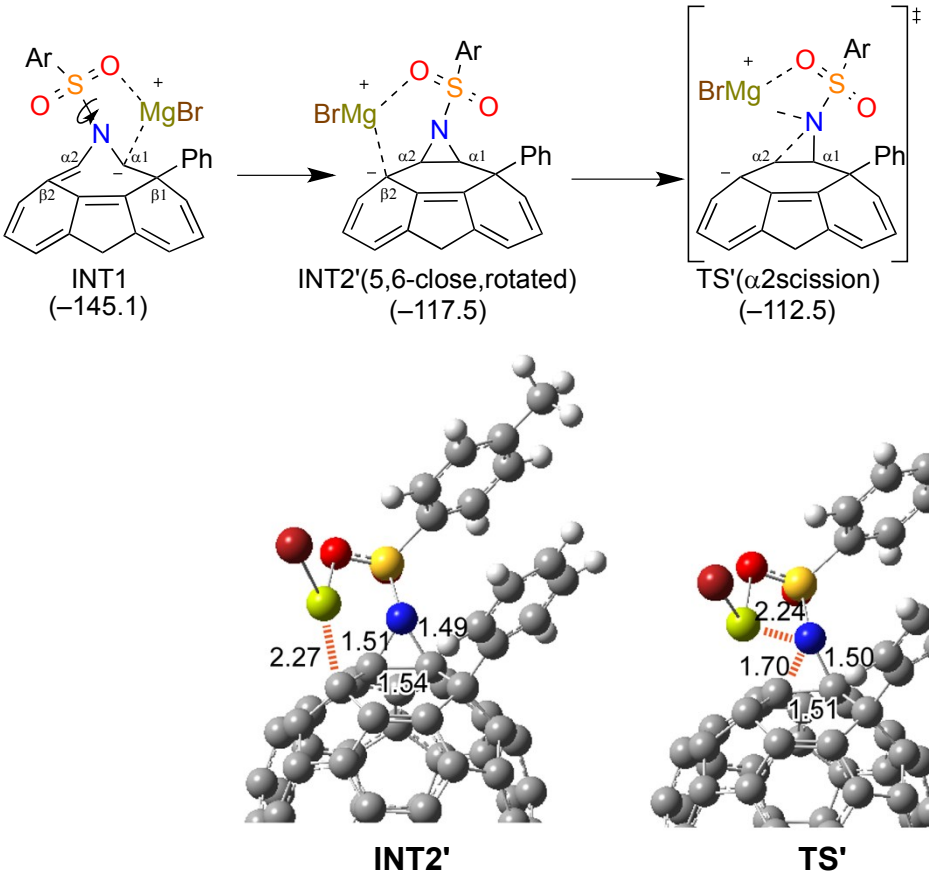
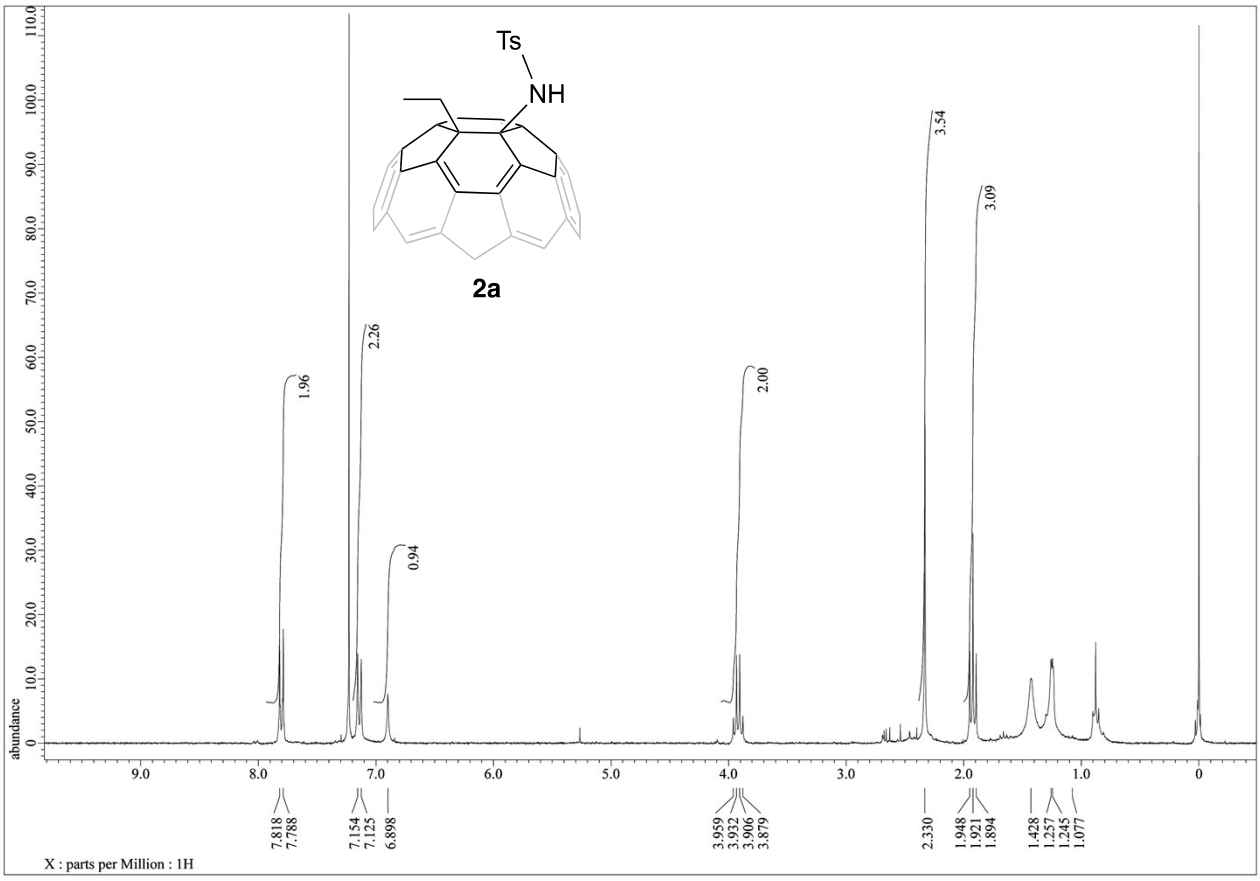
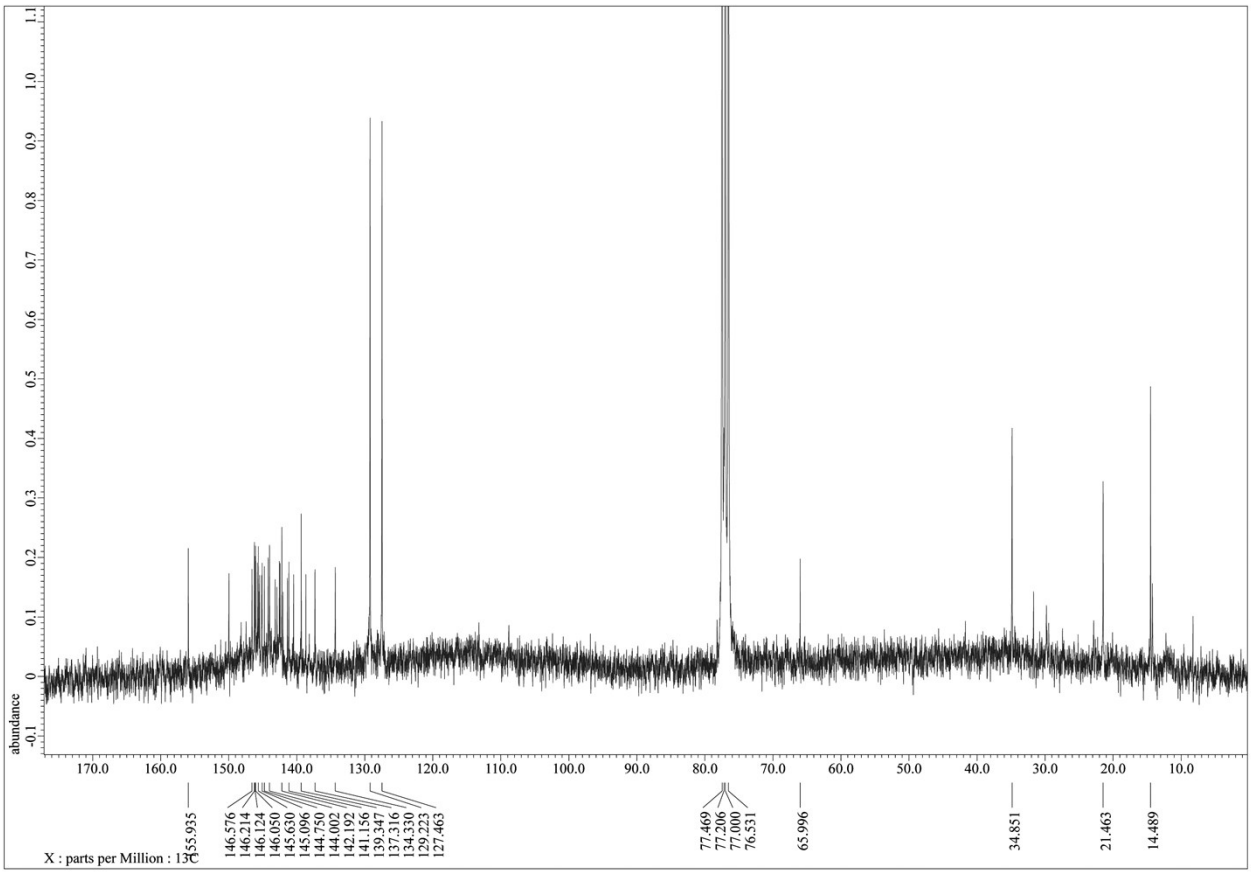
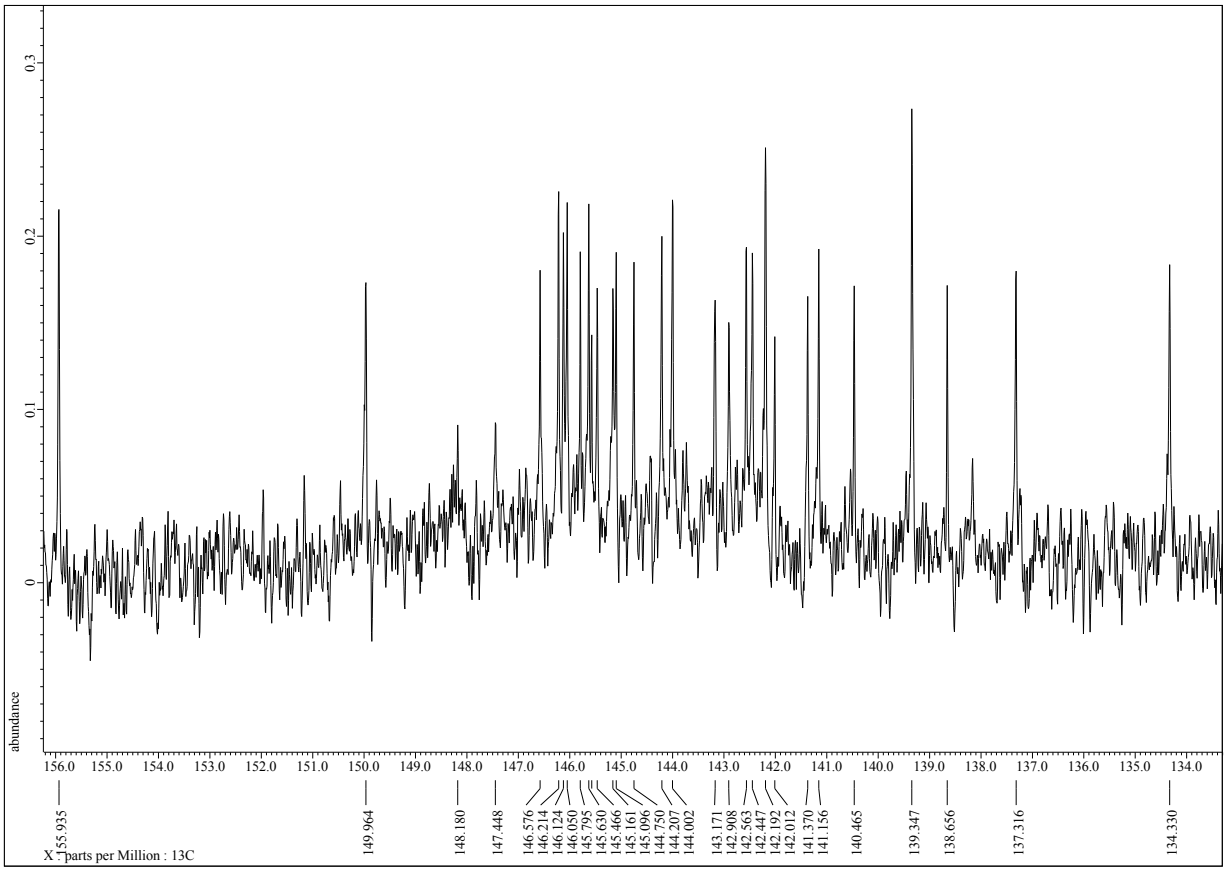


Fig. S4. CN scission along with rotation of tosyl group and Mg–Cβ2 coordination (kJ/mol and Å).

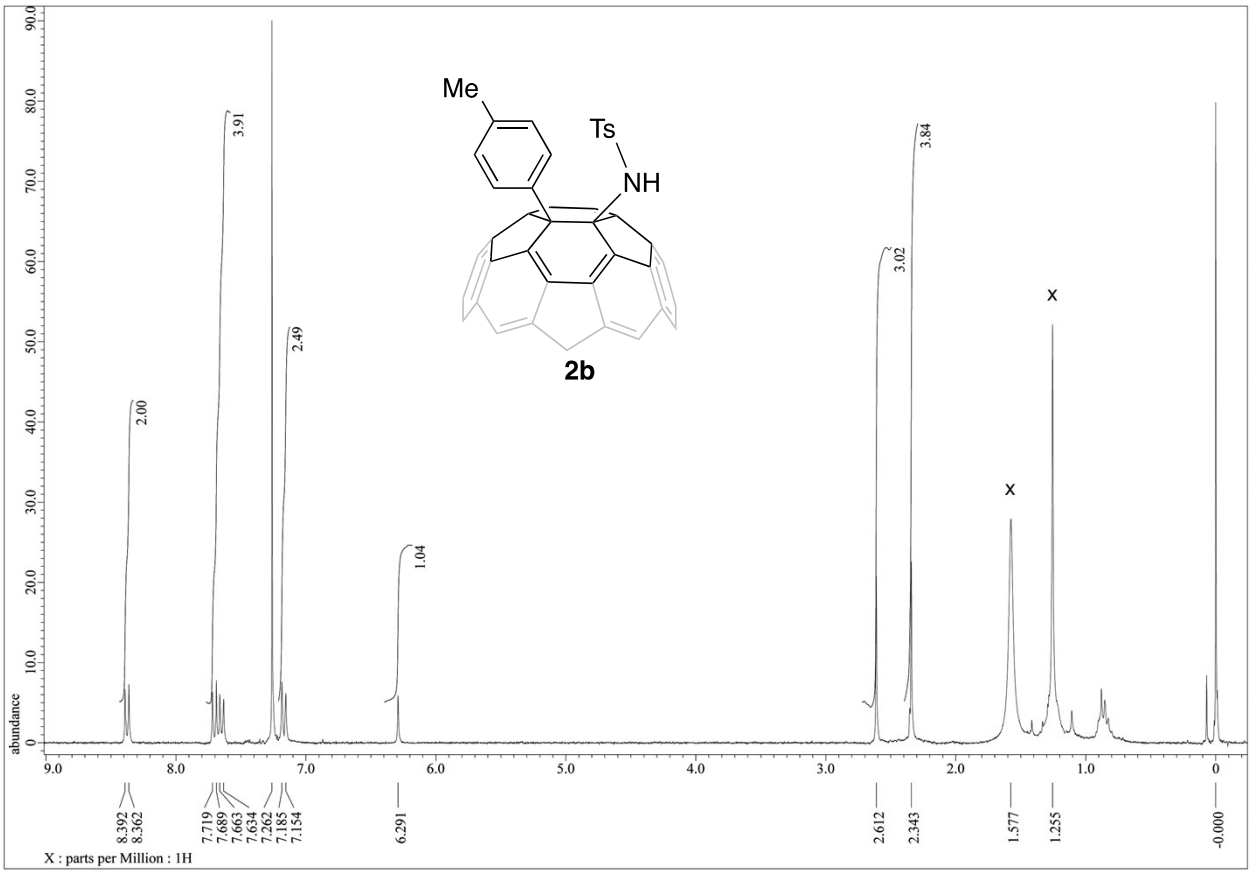
NMR Chart of **2a**

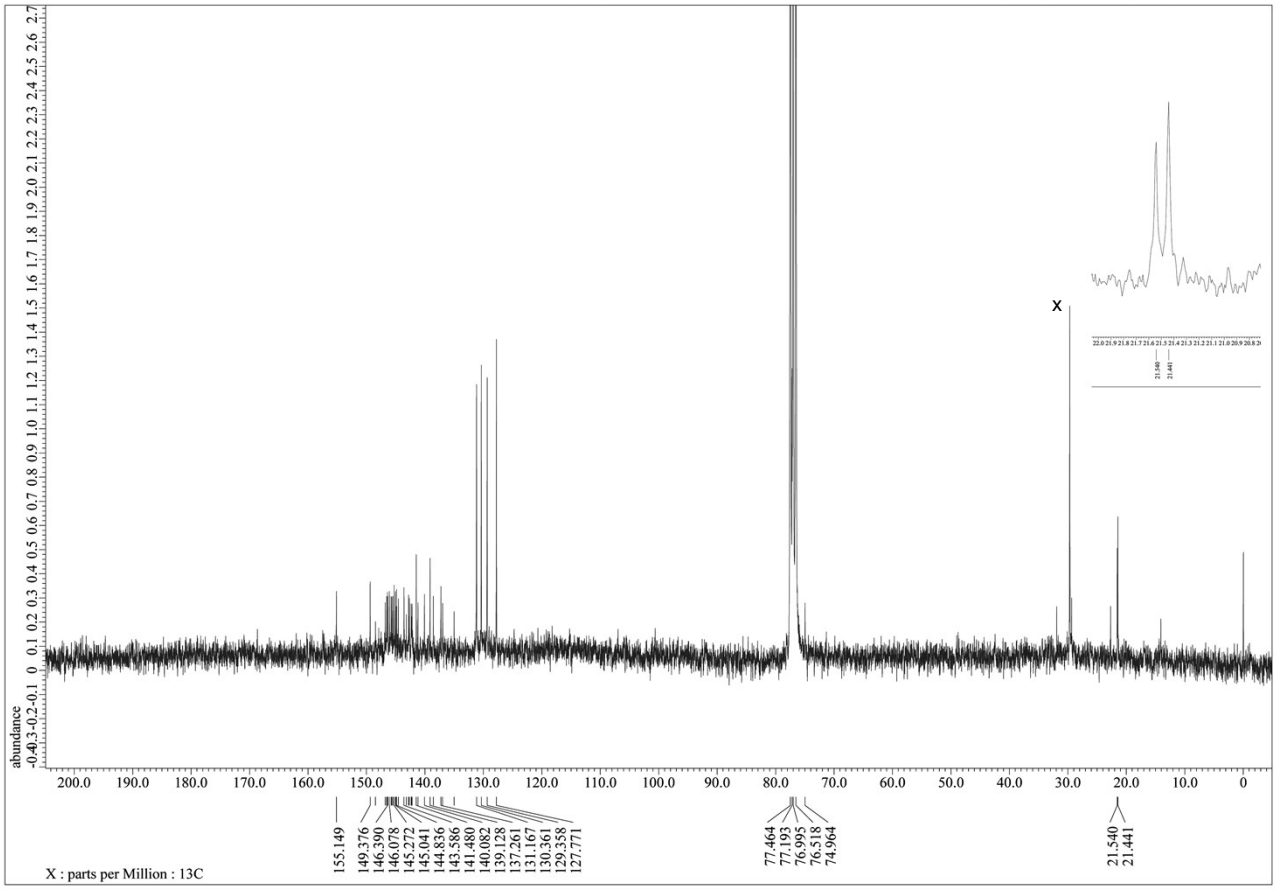




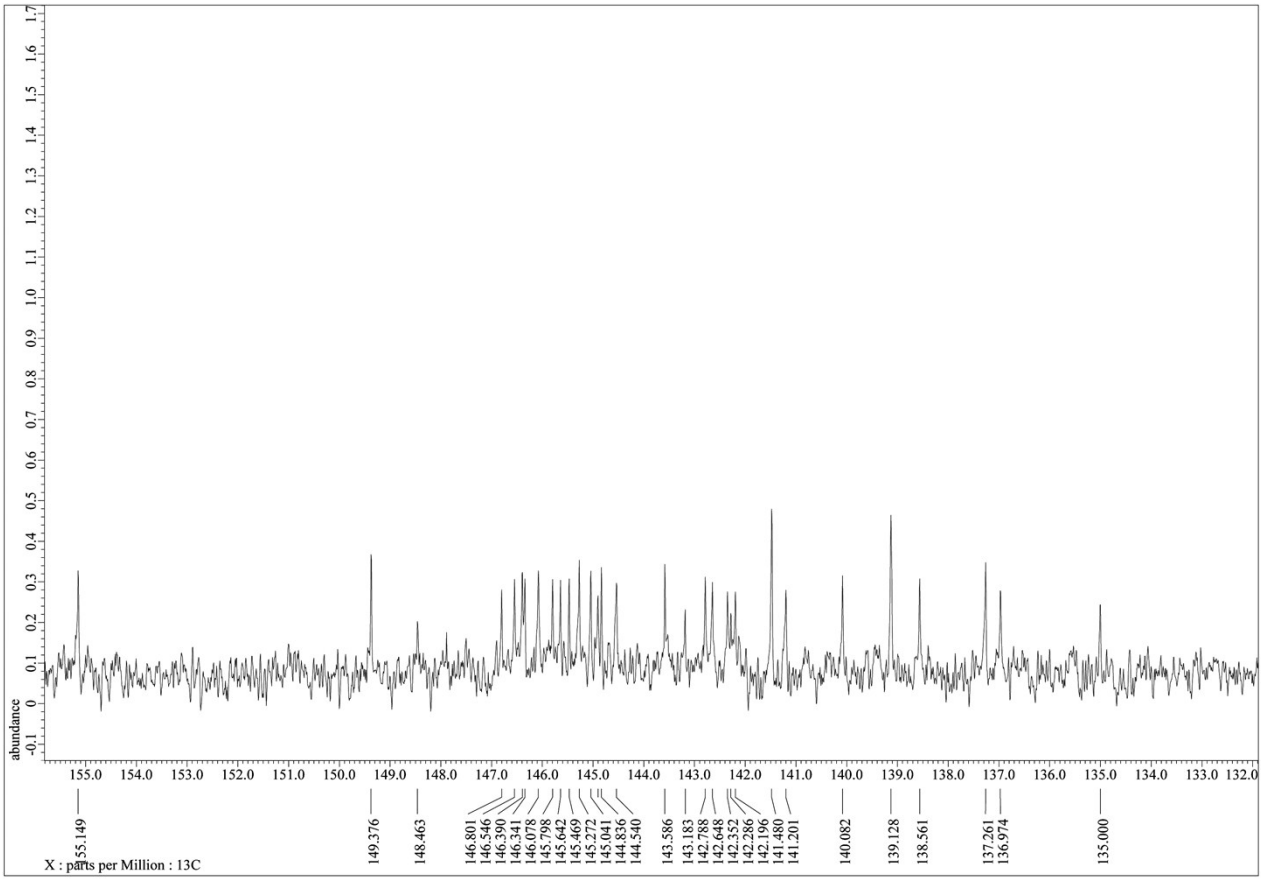


NMR Chart of **2b**

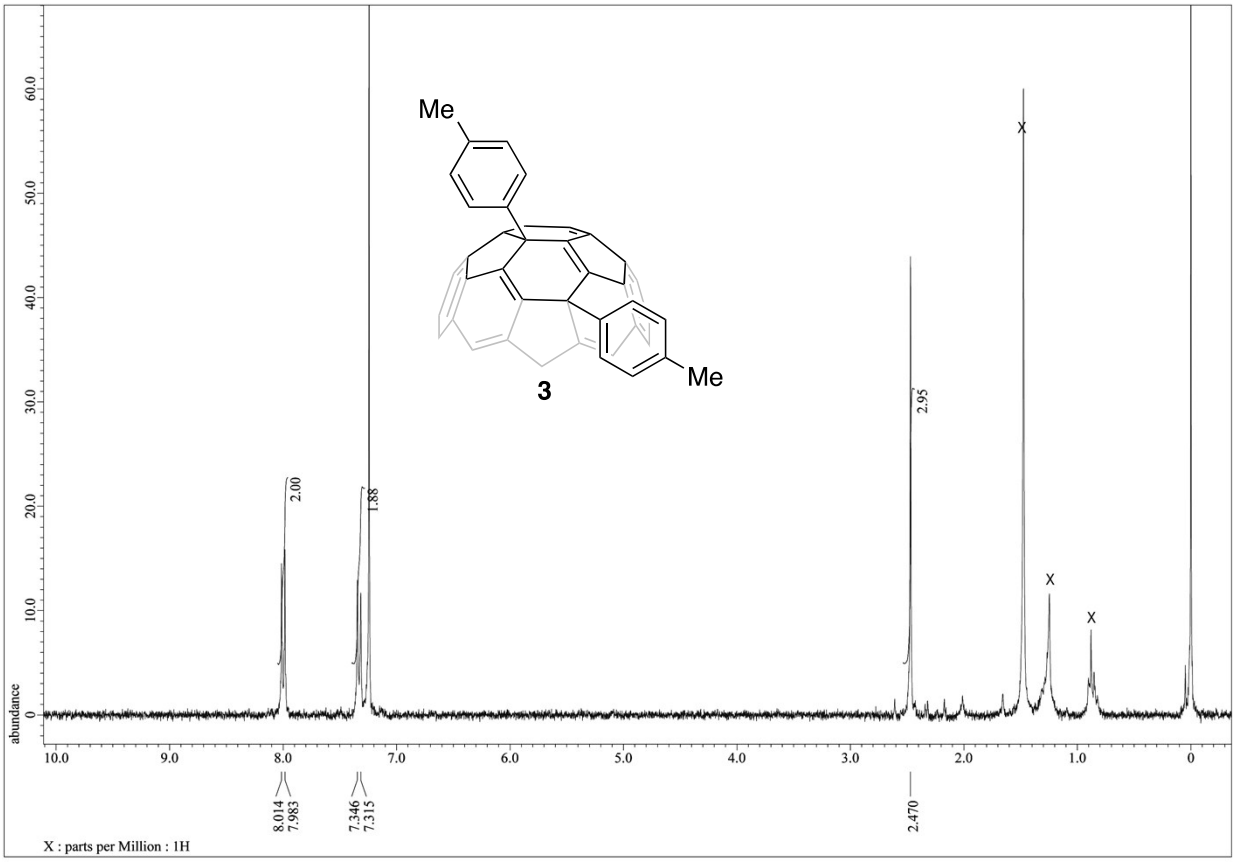


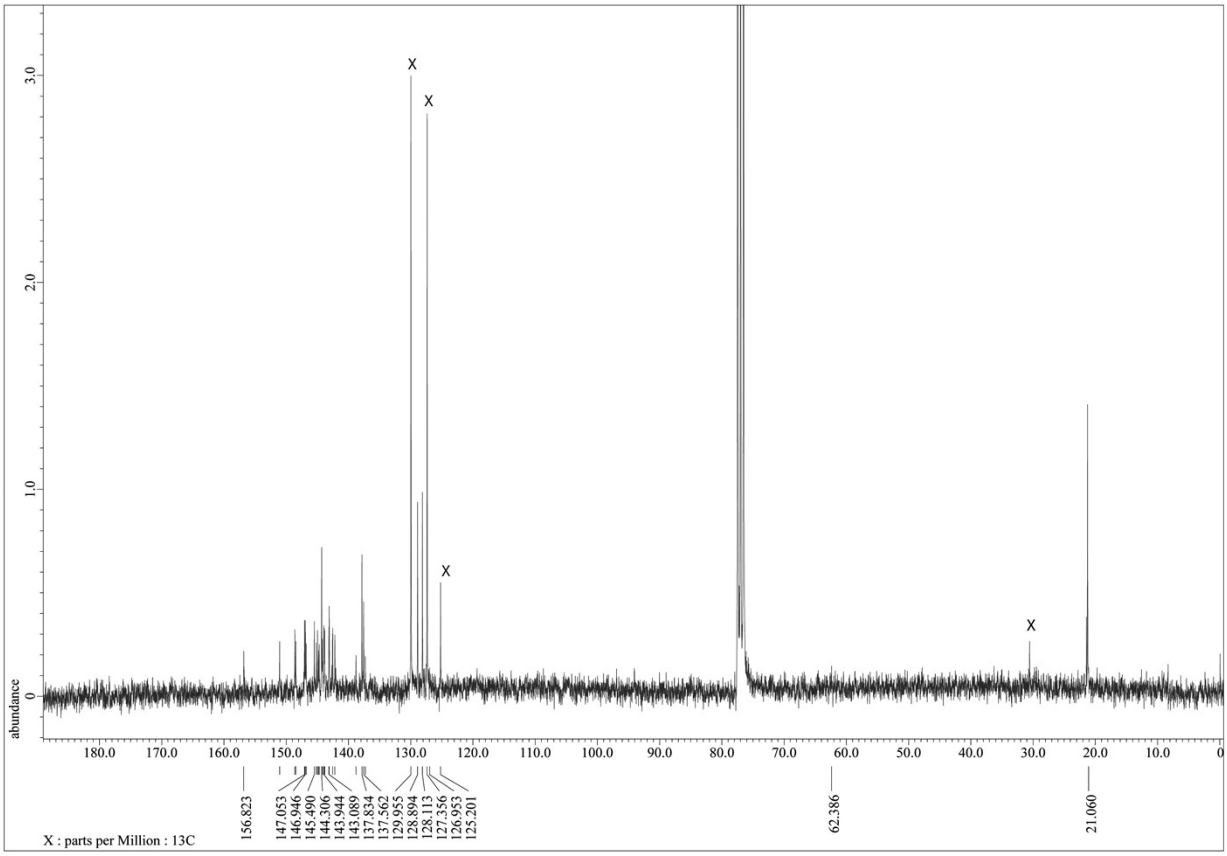


(**x**: remaining grease)

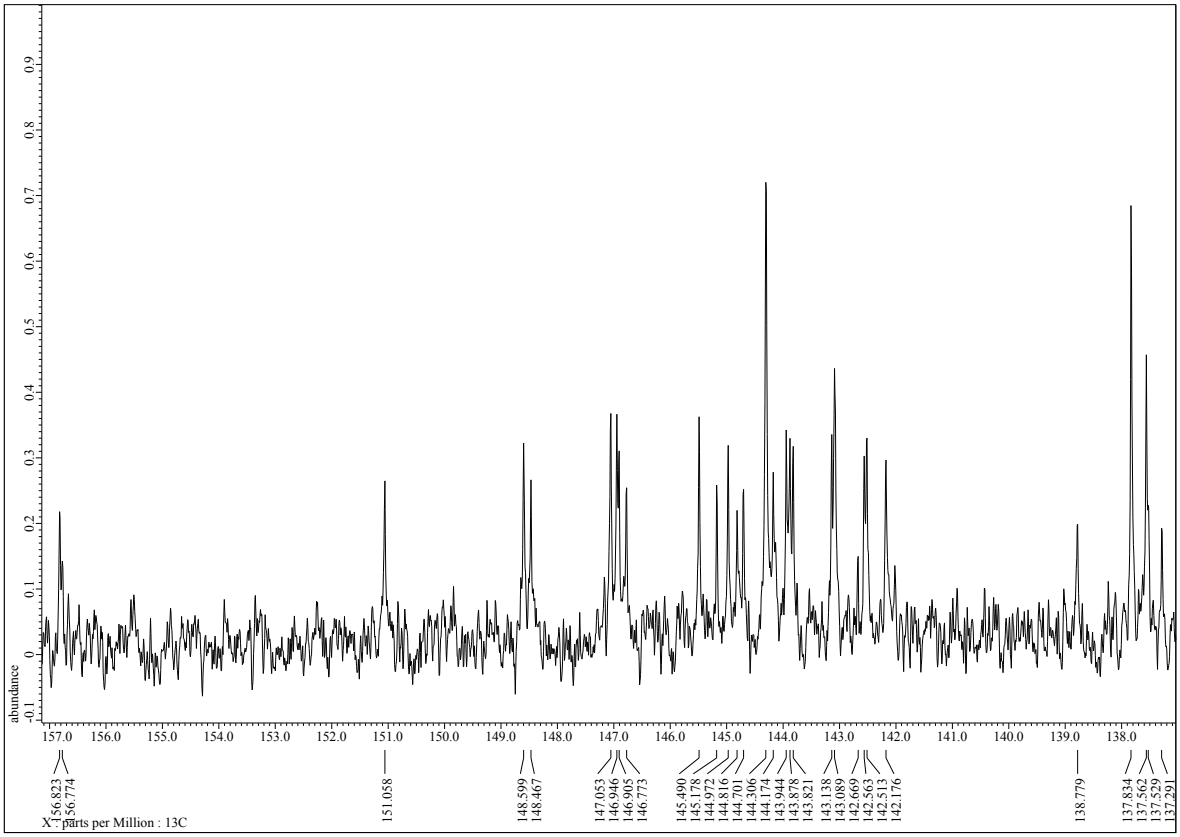


NMR chart of **3** (reported compound)

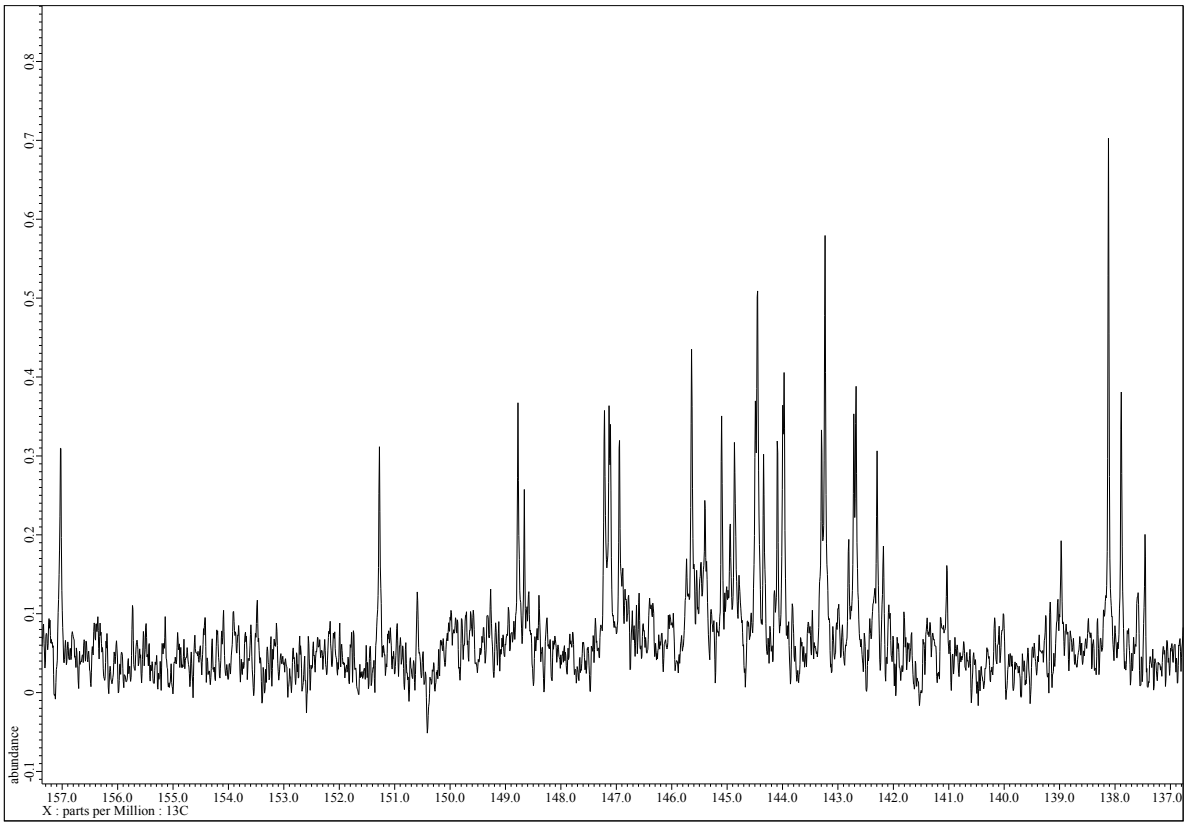




(**x**: remaining toluene and grease)



c.f. 1,4-ditolyl fullerene by acid-catalytic condition (Chem. Asian J., ref.11)



Full citation of Gaussian 09:

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Cartesian coordinates and energies of calculations

Tosyl azafulleroid 1 (5-exo, -3160.43402448 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.185591	0.831090	3.007987
2	6	0	−0.383487	−0.464681	3.325678
3	6	0	0.393413	−1.455812	2.627967
4	6	0	1.498931	−0.819611	1.966565
5	6	0	1.340763	0.646548	2.116054
6	6	0	2.064235	−1.452851	0.864545
7	6	0	−0.212767	−2.575618	2.064146
8	6	0	−1.757062	−0.640987	3.477646
9	6	0	−0.675879	1.919302	2.888948
10	6	0	1.561451	1.599125	1.094856
11	6	0	2.409728	0.030848	−0.726173
12	6	0	1.986759	1.283283	−0.289168
13	6	0	−0.451159	2.891673	1.845035
14	6	0	0.623460	2.725430	0.974183
15	6	0	−2.113424	1.750854	3.048539
16	6	0	−2.646576	0.493876	3.329889
17	6	0	−2.403844	−1.804771	2.889870
18	6	0	−1.648011	−2.750245	2.193110
19	6	0	1.236015	−2.343101	0.068462
20	6	0	0.181331	−2.987757	0.730237
21	6	0	−1.006776	−3.422422	0.041421
22	6	0	−2.141861	−3.290334	0.940044
23	6	0	−1.747572	3.332129	1.349994
24	6	0	−2.773516	2.618451	2.089153
25	6	0	−3.846207	0.038561	2.648813
26	6	0	−3.692978	−1.380933	2.372512
27	6	0	1.217524	2.098942	−1.187571
28	6	0	0.425397	3.032338	−0.429356
29	6	0	1.625087	−0.654074	−1.741655
30	6	0	1.075982	−1.970440	−1.353510
31	6	0	0.746843	1.569555	−2.387078
32	6	0	0.907593	0.149869	−2.637625
33	6	0	−0.810543	3.451173	−0.916650
34	6	0	−1.928163	3.600929	−0.006157
35	6	0	−3.931415	2.186214	1.437564
36	6	0	−4.473951	0.867138	1.718479
37	6	0	−4.172365	−1.913295	1.172780
38	6	0	−3.377724	−2.885383	0.441586
39	6	0	−0.100072	−2.400333	−2.006776
40	6	0	−1.139464	−3.144475	−1.311728
41	6	0	−2.437328	−2.751189	−1.837341
42	6	0	−3.530385	−2.617005	−0.978833
43	6	0	−4.824841	−1.049417	0.203940
44	6	0	−4.975563	0.311928	0.472593
45	6	0	−4.107688	2.449595	0.018945
46	6	0	−3.127350	3.145552	−0.688578
47	6	0	−1.314117	2.905019	−2.168287
48	6	0	−0.553496	1.979556	−2.886280
49	6	0	−0.287549	−0.312153	−3.296898
50	6	0	−0.776530	−1.575298	−2.997270
51	6	0	−4.432482	−1.488001	−1.126256
52	6	0	−4.748873	1.290079	−0.578055
53	6	0	−2.745855	2.710809	−2.022898
54	6	0	−1.192258	0.812899	−3.466293
55	6	0	−2.212087	−1.777294	−2.883174
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57	6	0	−2.565768	0.624648	−3.328979
58	6	0	−4.380934	0.869258	−1.856945
59	6	0	−4.215376	−0.548896	−2.134760
60	6	0	−3.087553	−0.700379	−3.037862
61	7	0	3.122359	−0.765557	0.209188
62	16	0	4.514477	−1.660256	−0.281808
63	8	0	4.436440	−2.017633	−1.705122
64	8	0	4.642511	−2.709029	0.736873
65	6	0	5.802278	−0.444808	−0.079265
66	6	0	7.852297	1.425149	0.249003
67	6	0	6.183564	−0.064859	1.212819
68	6	0	6.426252	0.088978	−1.205839
69	6	0	7.448456	1.023013	−1.030108
70	6	0	7.204137	0.865837	1.364947
71	1	0	5.692558	−0.493318	2.080232
72	1	0	6.122153	−0.224286	−2.198236
73	1	0	7.939581	1.441865	−1.903971
74	1	0	7.506719	1.164125	2.365272
75	6	0	8.959509	2.432750	0.437606
76	1	0	9.792163	1.999522	1.004661
77	1	0	8.606407	3.303880	1.002168
78	1	0	9.349246	2.784400	−0.521677

C60 (−2286.1749514 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.176233	0.382181	3.327756
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3	6	0	−0.726952	−1.000563	3.327756
4	6	0	0.000000	1.236764	3.327756
5	6	0	−1.176233	0.382181	3.327756
6	6	0	2.304731	0.748852	2.594413
7	6	0	2.304731	1.985617	1.830051
8	6	0	3.031683	1.749416	0.593286
9	6	0	3.031683	−0.251711	1.830051
10	6	0	3.480964	0.366671	0.593286
11	6	0	1.424402	−1.960521	2.594413
12	6	0	2.600635	−1.578340	1.830051
13	6	0	2.600635	−2.342702	0.593286
14	6	0	0.697450	−2.961084	1.830051
15	6	0	1.424402	−3.197285	0.593286
16	6	0	−1.424402	−1.960521	2.594413
17	6	0	−0.697450	−2.961084	1.830051
18	6	0	−1.424402	−3.197285	0.593286
19	6	0	−2.600635	−1.578340	1.830051
20	6	0	−2.600635	−2.342702	0.593286
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22	6	0	−1.176233	2.805519	1.830051
23	6	0	−0.726952	3.423901	0.593286
24	6	0	1.176233	2.805519	1.830051
25	6	0	0.726952	3.423901	0.593286
26	6	0	−2.304731	0.748852	2.594413
27	6	0	−3.031683	−0.251711	1.830051
28	6	0	−3.480964	0.366671	0.593286
29	6	0	−2.304731	1.985617	1.830051
30	6	0	−3.031683	1.749416	0.593286
31	6	0	−1.176233	−0.382181	−3.327756
32	6	0	0.000000	−1.236764	−3.327756
33	6	0	1.176233	−0.382181	−3.327756
34	6	0	−0.726952	1.000563	−3.327756
35	6	0	0.726952	1.000563	−3.327756
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40	6	0	−3.031683	−1.749416	−0.593286
41	6	0	−0.000000	−2.423337	−2.594413
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45	6	0	0.726952	−3.423901	−0.593286
46	6	0	2.304731	−0.748852	−2.594413
47	6	0	2.304731	−1.985617	−1.830051
48	6	0	3.031683	−1.749416	−0.593286
49	6	0	3.031683	0.251711	−1.830051
50	6	0	3.480964	−0.366671	−0.593286
51	6	0	−1.424402	1.960521	−2.594413
52	6	0	−0.697450	2.961084	−1.830051
53	6	0	−1.424402	3.197285	−0.593286
54	6	0	−2.600635	1.578340	−1.830051
55	6	0	−2.600635	2.342702	−0.593286
56	6	0	1.424402	1.960521	−2.594413
57	6	0	2.600635	1.578340	−1.830051
58	6	0	2.600635	2.342702	−0.593286
59	6	0	0.697450	2.961084	−1.830051
60	6	0	1.424402	3.197285	−0.593286

PhMgBr (−3003.553841 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.037201	2.230321	0.007399
2	6	0	1.372557	2.129384	−0.008614

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5	6	0	0.264618	4.676557	−0.000019
6	6	0	−0.556752	3.543218	0.011240
7	1	0	1.846465	1.146812	−0.012458
8	1	0	3.290056	3.125572	−0.032230
9	1	0	2.297684	5.409824	−0.024529
10	1	0	−0.177838	5.671030	0.003455
11	1	0	−1.635945	3.699481	0.023380
12	12	0	−1.211755	0.478858	0.023822
13	35	0	−2.363001	−1.653495	0.040723

EtMgBr (−2851.1235234 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.659450	−0.580509	−0.000011
2	1	0	3.513835	−1.220893	−0.880412
3	1	0	3.514014	−1.220759	0.880521
4	1	0	4.721093	−0.282115	−0.000147
5	6	0	2.696190	0.621588	−0.000032
6	1	0	2.909847	1.257596	0.873518
7	1	0	2.909798	1.257590	−0.873602
8	12	0	0.620745	0.179208	0.000062
9	35	0	−1.804325	−0.062525	−0.000010

TS of C60+PhMgBr (284.2i, -5289.69990182 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−1.435980	2.115058	0.157284
2	6	0	−0.901717	2.355438	−1.165232
3	6	0	−1.207332	1.205219	−1.996808
4	6	0	−1.929526	0.243943	−1.194734
5	6	0	−2.196263	0.836677	0.141439
6	6	0	−1.675743	−1.110987	−1.353463
7	6	0	−0.294092	0.781512	−2.965407
8	6	0	0.304971	3.037958	−1.334947
9	6	0	−0.711352	2.519177	1.270685
10	6	0	−2.011516	−0.042572	1.293283
11	6	0	−1.578119	−2.003909	−0.195640
12	6	0	−1.683003	−1.450921	1.079798
13	6	0	−0.602149	1.666070	2.455794
14	6	0	−1.186164	0.400627	2.414688
15	6	0	0.547773	3.221988	1.107359
16	6	0	1.046854	3.479116	−0.171912
17	6	0	1.260465	2.590207	−2.336221
18	6	0	0.967022	1.485997	−3.134668
19	6	0	−0.723161	−1.561895	−2.349815
20	6	0	−0.045965	−0.633621	−3.144810
21	6	0	1.367331	−0.812124	−3.424975
22	6	0	1.994898	0.499073	−3.417399
23	6	0	0.732710	1.820671	2.988216
24	6	0	1.442291	2.788387	2.163735
25	6	0	2.462071	3.307445	−0.447240
26	6	0	2.594679	2.755778	−1.785644
27	6	0	−0.785033	−1.888282	2.131522
28	6	0	−0.479425	−0.742471	2.959819
29	6	0	−0.541709	−2.972316	−0.475199
30	6	0	−0.018756	−2.708348	−1.808153
31	6	0	0.199166	−2.846309	1.865513
32	6	0	0.325906	−3.404779	0.535977
33	6	0	0.800926	−0.583854	3.500092
34	6	0	1.423103	0.723517	3.519010
35	6	0	2.803059	2.624139	1.902277
36	6	0	3.321650	2.884777	0.568471
37	6	0	3.583114	1.807727	−2.055201
38	6	0	3.276975	0.656139	−2.887754
39	6	0	1.339018	−2.883282	−2.077770
40	6	0	2.046476	−1.912635	−2.898669
41	6	0	3.380807	−1.750619	−2.351645
42	6	0	3.983390	−0.490969	−2.343499
43	6	0	4.478806	1.371467	−0.997470
44	6	0	4.351901	1.901598	0.288041
45	6	0	3.516641	1.481995	2.448436
46	6	0	2.835943	0.549348	3.233853
47	6	0	1.826479	−1.573719	3.218547
48	6	0	1.532128	−2.679653	2.419256
49	6	0	1.740493	−3.573514	0.254786
50	6	0	2.239063	−3.325698	−1.025961
51	6	0	4.728934	−0.048376	−1.177822
52	6	0	4.467804	1.031618	1.448062
53	6	0	3.088150	−0.871757	3.053286
54	6	0	2.487962	−3.130420	1.421437
55	6	0	3.497336	−2.619949	−1.191140
56	6	0	4.004672	−1.302931	2.093804
57	6	0	3.698128	−2.455222	1.261124
58	6	0	4.709986	−0.332181	1.274802
59	6	0	4.838276	−0.882693	−0.063754
60	6	0	4.215124	−2.195430	−0.071764
61	1	0	−4.885912	−0.167079	−1.366422
62	6	0	−5.025854	0.903260	−1.215865
63	6	0	−5.352940	3.661950	−0.930004
64	6	0	−5.912917	1.588140	−2.050012
65	6	0	−4.303964	1.573041	−0.205101
66	6	0	−4.470171	2.968822	−0.098231
67	6	0	−6.076028	2.969761	−1.906647
68	1	0	−6.467300	1.051230	−2.815918
69	1	0	−3.893200	3.528958	0.637326
70	1	0	−6.754193	3.507675	−2.563737
71	1	0	−5.472181	4.737553	−0.824525
72	12	0	−4.249175	0.470935	1.699351
73	35	0	−5.409671	−0.241912	3.696423

Reaction of PhMgBr

TS(1−Cα) (energy and imaginary frequency are in Table S1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.594208	−2.414879	−1.741432
2	6	0	0.585339	−2.981836	−0.414321
3	6	0	−0.370544	−2.228053	0.362015
4	6	0	−1.042107	−1.281552	−0.479239
5	6	0	−0.361069	−1.293258	−1.781460
6	6	0	−1.737148	−0.200062	0.169776
7	6	0	−0.117721	−1.945475	1.709457
8	6	0	1.749704	−3.469674	0.176350
9	6	0	1.789245	−2.403208	−2.459131
10	6	0	−0.041848	−0.187554	−2.607162
11	6	0	−1.020828	1.609380	−1.101534
12	6	0	−0.274771	1.213561	−2.201682
13	6	0	2.125064	−1.258432	−3.269117
14	6	0	1.236774	−0.181446	−3.318535
15	6	0	3.013393	−2.911878	−1.856943
16	6	0	2.997188	−3.426061	−0.561266
17	6	0	2.030157	−3.170784	1.569465
18	6	0	1.119009	−2.403189	2.306689
19	6	0	−0.988264	0.357835	1.343962
20	6	0	−0.362100	−0.582851	2.168660
21	6	0	0.699127	−0.231237	3.070991
22	6	0	1.614855	−1.351419	3.177811
23	6	0	3.557851	−1.034410	−3.160211
24	6	0	4.105805	−2.055134	−2.282645
25	6	0	4.056200	−3.087389	0.373188
26	6	0	3.454506	−2.919289	1.687825
27	6	0	0.872037	1.994522	−2.567379
28	6	0	1.789650	1.163389	−3.301107
29	6	0	−0.382625	2.356555	−0.047140
30	6	0	−0.426110	1.714349	1.282517
31	6	0	1.332541	2.996424	−1.713120
32	6	0	0.723172	3.141262	−0.406491
33	6	0	3.161520	1.386817	−3.196443
34	6	0	4.072067	0.262065	−3.123591
35	6	0	5.129045	−1.732653	−1.388213
36	6	0	5.099673	−2.254568	−0.031275
37	6	0	3.927099	−1.920906	2.545544
38	6	0	2.982777	−1.118444	3.301725
39	6	0	0.613189	2.050463	2.185502
40	6	0	1.167724	1.075614	3.100040
41	6	0	2.592452	1.321095	3.257282
42	6	0	3.481827	0.247973	3.346037
43	6	0	5.009614	−1.050708	2.119799
44	6	0	5.588822	−1.216631	0.860600
45	6	0	5.646050	−0.375054	−1.334743
46	6	0	5.128415	0.601701	−2.186161
47	6	0	3.655975	2.430967	−2.309560

48	6	0	2.760651	3.218428	−1.580996
49	6	0	1.772322	3.461060	0.529864
50	6	0	1.709105	2.936774	1.811280
51	6	0	4.739721	0.288105	2.622936
52	6	0	5.924561	−0.054545	0.055184
53	6	0	4.871216	1.942261	−1.683026
54	6	0	3.034054	3.520870	−0.187735
55	6	0	2.928822	2.477437	2.455536
56	6	0	5.137971	2.248232	−0.345272
57	6	0	4.198997	3.053557	0.416957
58	6	0	5.675276	1.230430	0.540863
59	6	0	5.064806	1.404043	1.849475
60	6	0	4.145806	2.525715	1.770483
61	7	0	−2.167187	0.859303	−0.719781
62	1	0	−4.282736	1.015211	1.756371
63	6	0	−4.091617	0.022593	2.154893
64	6	0	−3.606270	−2.492679	3.268404
65	6	0	−4.431985	−0.230517	3.480210
66	6	0	−3.495150	−0.966908	1.330559
67	6	0	−3.248132	−2.223394	1.938884
68	6	0	−4.189635	−1.492918	4.042417
69	1	0	−4.891476	0.550011	4.082124
70	1	0	−2.765265	−3.017885	1.372299
71	1	0	−4.452589	−1.686977	5.078762
72	1	0	−3.412844	−3.473685	3.694759
73	12	0	−4.572785	−1.741529	−0.427756
74	35	0	−6.008801	−3.467685	−1.325544
75	16	0	−3.549082	1.003003	−1.644174
76	8	0	−3.196659	1.709169	−2.870948
77	8	0	−4.154756	−0.357063	−1.816032
78	6	0	−4.721081	1.973925	−0.716257
79	6	0	−4.287129	3.119036	−0.039788
80	6	0	−6.071609	1.624122	−0.763778
81	6	0	−5.229018	3.906324	0.613813
82	1	0	−3.236266	3.386743	−0.010219
83	6	0	−6.996783	2.428380	−0.098714
84	1	0	−6.396698	0.744653	−1.309331
85	6	0	−6.594849	3.574376	0.600464
86	1	0	−4.897525	4.793143	1.146758
87	1	0	−8.048455	2.158460	−0.129012
88	6	0	−7.595668	4.429000	1.337092
89	1	0	−8.621996	4.173792	1.059503
90	1	0	−7.497875	4.293244	2.421553
91	1	0	−7.435821	5.492685	1.130162

TS(2-Cα) (energy and imaginary frequency are in Table S1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.845023	−0.570455	−3.055771
2	6	0	0.995687	−1.925403	−2.581898
3	6	0	−0.056722	−2.156877	−1.619582
4	6	0	−0.920424	−1.014476	−1.563410
5	6	0	−0.305972	0.040488	−2.369149
6	6	0	−1.779575	−0.908206	−0.416713
7	6	0	0.187774	−2.935936	−0.483556
8	6	0	2.254191	−2.497918	−2.408112
9	6	0	1.984946	0.158857	−3.386764
10	6	0	−0.244442	1.424109	−2.080311
11	6	0	−1.499919	1.318923	0.133161
12	6	0	−0.732487	1.991986	−0.808372
13	6	0	2.060300	1.559795	−3.050902
14	6	0	0.978804	2.158597	−2.399229
15	6	0	3.306977	−0.425838	−3.212053
16	6	0	3.440525	−1.724693	−2.723003
17	6	0	2.526211	−3.290248	−1.221707
18	6	0	1.513460	−3.481371	−0.272880
19	6	0	−1.118556	−1.299192	0.863642
20	6	0	−0.290523	−2.424168	0.796449
21	6	0	0.715432	−2.697793	1.784080
22	6	0	1.832359	−3.362867	1.140308
23	6	0	3.424697	1.851144	−2.643986
24	6	0	4.194754	0.621761	−2.740170
25	6	0	4.449527	−2.028206	−1.723556
26	6	0	3.878469	−2.987795	−0.789931
27	6	0	0.226782	2.957103	−0.342903
28	6	0	1.258731	3.108254	−1.335284
29	6	0	−0.970916	1.128981	1.462859
30	6	0	−0.835674	−0.279868	1.882625
31	6	0	0.519736	3.052866	1.016987
32	6	0	−0.052977	2.081340	1.926334
33	6	0	2.565454	3.393746	−0.939600
34	6	0	3.678921	2.751787	−1.608650
35	6	0	5.170099	0.331434	−1.783563
36	6	0	5.295195	−1.019603	−1.260995
37	6	0	4.183617	−2.898429	0.571719
38	6	0	3.133035	−3.086044	1.555628
39	6	0	0.153412	−0.566301	2.856094
40	6	0	0.922244	−1.792112	2.816725
41	6	0	2.277426	−1.523386	3.269628
42	6	0	3.359309	−2.148194	2.645794
43	6	0	5.059677	−1.843957	1.052063
44	6	0	5.609249	−0.926794	0.154773
45	6	0	5.415898	1.259077	−0.691639
46	6	0	4.685839	2.445106	−0.607021
47	6	0	2.883657	3.495808	0.477556
48	6	0	1.881946	3.326149	1.436788
49	6	0	0.950174	1.763372	2.913287
50	6	0	1.041459	0.462478	3.382825
51	6	0	4.556767	−1.387034	2.339189
52	6	0	5.680971	0.481217	0.506648
53	6	0	4.194237	2.905075	0.682423
54	6	0	2.146915	2.534650	2.624763
55	6	0	2.351681	−0.121808	3.620681
56	6	0	4.449636	2.155013	1.833908
57	6	0	3.403166	1.965648	2.823872
58	6	0	5.208384	0.919533	1.744882
59	6	0	4.628996	−0.034098	2.677662
60	6	0	3.508028	0.610279	3.339236
61	7	0	−2.487183	0.354283	−0.244511
62	1	0	−2.629421	−3.736826	0.993017
63	6	0	−2.960652	−3.786566	−0.042328
64	6	0	−3.783465	−3.991524	−2.695458
65	6	0	−3.093494	−5.050456	−0.635416
66	6	0	−3.252378	−2.596575	−0.744385
67	6	0	−3.655504	−2.740345	−2.096636
68	6	0	−3.501243	−5.153624	−1.963529
69	1	0	−2.867515	−5.945318	−0.060719
70	1	0	−3.861821	−1.856839	−2.697701
71	1	0	−3.594338	−6.129319	−2.432913
72	1	0	−4.103421	−4.067357	−3.731998
73	12	0	−4.815684	−1.585171	0.409466
74	35	0	−6.357827	−1.775944	2.261173
75	16	0	−3.770699	0.851112	−1.243986
76	8	0	−3.500533	0.745013	−2.678525
77	8	0	−4.952631	0.064785	−0.746686
78	6	0	−4.050882	2.539156	−0.775326
79	6	0	−4.611120	2.827892	0.474107
80	6	0	−3.769067	3.541730	−1.705382
81	6	0	−4.870954	4.156006	0.792948
82	1	0	−4.850194	2.037116	1.176752
83	6	0	−4.045580	4.863182	−1.363347
84	1	0	−3.350893	3.293073	−2.674137
85	6	0	−4.590366	5.192675	−0.113651
86	1	0	−5.307631	4.391694	1.759231
87	1	0	−3.835375	5.649915	−2.081960
88	6	0	−4.857309	6.628852	0.259723
89	1	0	−5.780309	6.724332	0.840441
90	1	0	−4.041404	7.022745	0.879400
91	1	0	−4.936209	7.265218	−0.626205

TS(3-Cα) (energy and imaginary frequency are in Table S1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.218252	−1.240312	2.696053
2	6	0	−0.455680	−2.447620	1.943190
3	6	0	0.375212	−2.380976	0.766418
4	6	0	1.216637	−1.221815	0.826451
5	6	0	0.772308	−0.420174	1.971008
6	6	0	1.834918	−0.800282	−0.404041
7	6	0	−0.079434	−2.890243	−0.453099
8	6	0	−1.717002	−3.036822	1.884229
9	6	0	−1.272945	−0.678651	3.411295
10	6	0	0.643088	0.988783	2.051981
11	6	0	1.420798	1.472440	−0.311378
12	6	0	0.856507	1.872449	0.892637
13	6	0	−1.426129	0.756633	3.450143

14	6	0	−0.501804	1.553681	2.772081
15	6	0	−2.598724	−1.279116	3.358583
16	6	0	−2.819878	−2.430069	2.603060
17	6	0	−2.216123	−3.541110	0.617097
18	6	0	−1.414843	−3.444767	−0.528162
19	6	0	0.925612	−0.919459	−1.588629
20	6	0	0.137597	−2.073898	−1.643361
21	6	0	−1.048748	−2.158433	−2.449411
22	6	0	−2.010811	−3.015753	−1.781692
23	6	0	−2.847227	1.057479	3.398544
24	6	0	−3.571230	−0.201505	3.337753
25	6	0	−4.007874	−2.545247	1.775460
26	6	0	−3.629711	−3.222900	0.543666
27	6	0	−0.189221	2.855497	0.866345
28	6	0	−1.000565	2.710035	2.046193
29	6	0	0.634405	1.565019	−1.520428
30	6	0	0.428617	0.294829	−2.242909
31	6	0	−0.748109	3.248956	−0.348495
32	6	0	−0.360236	2.553950	−1.559175
33	6	0	−2.361926	3.006378	1.990567
34	6	0	−3.312899	2.162165	2.683715
35	6	0	−4.717589	−0.311507	2.547440
36	6	0	−4.936784	−1.505150	1.746043
37	6	0	−4.202578	−2.830084	−0.669881
38	6	0	−3.370818	−2.720308	−1.854586
39	6	0	−0.732086	0.196215	−3.048361
40	6	0	−1.467789	−1.044578	−3.166132
41	6	0	−2.888357	−0.751121	−3.267154
42	6	0	−3.818865	−1.565132	−2.617747
43	6	0	−5.165287	−1.742356	−0.699223
44	6	0	−5.529861	−1.096625	0.483611
45	6	0	−5.185614	0.833226	1.783280
46	6	0	−4.498263	2.045366	1.851120
47	6	0	−2.958282	3.421195	0.727662
48	6	0	−2.168808	3.539711	−0.418974
49	6	0	−1.539255	2.425549	−2.381884
50	6	0	−1.714645	1.270043	−3.126360
51	6	0	−4.934683	−0.965834	−1.908005
52	6	0	−5.680886	0.348144	0.506161
53	6	0	−4.278813	2.824151	0.642058
54	6	0	−2.659693	3.038991	−1.689743
55	6	0	−3.041638	0.687800	−3.243052
56	6	0	−4.753657	2.354895	−0.585944
57	6	0	−3.926902	2.464754	−1.775414
58	6	0	−5.470729	1.093204	−0.655509
59	6	0	−5.084004	0.422071	−1.886194
60	6	0	−4.123569	1.266871	−2.574789
61	7	0	2.471955	0.501002	−0.260494
62	1	0	3.986353	−1.549019	−2.857754
63	6	0	3.746520	−2.465515	−2.324983
64	6	0	3.148343	−4.863682	−1.022320
65	6	0	3.858949	−3.677185	−3.004525
66	6	0	3.334114	−2.408426	−0.968668
67	6	0	3.015793	−3.638929	−0.353308
68	6	0	3.560885	−4.881940	−2.353104
69	1	0	4.184779	−3.688764	−4.042045
70	1	0	2.667943	−3.649862	0.678615
71	1	0	3.647211	−5.825405	−2.885511
72	1	0	2.913122	−5.792113	−0.507982
73	12	0	4.871772	−1.607269	0.390670
74	35	0	6.079150	−2.184777	2.408817
75	16	0	3.882358	0.954906	−1.108718
76	8	0	5.008517	0.212908	−0.440232
77	8	0	3.792010	0.819706	−2.566094
78	6	0	4.078893	2.660927	−0.661490
79	6	0	4.507631	2.991724	0.629512
80	6	0	3.857123	3.635581	−1.635373
81	6	0	4.703624	4.331674	0.939547
82	1	0	4.690394	2.220494	1.369636
83	6	0	4.064269	4.972343	−1.299314
84	1	0	3.537283	3.355612	−2.632671
85	6	0	4.486980	5.341571	−0.015287
86	1	0	5.036168	4.600570	1.938252
87	1	0	3.896028	5.738274	−2.050623
88	6	0	4.720568	6.787828	0.341823
89	1	0	4.144368	7.071264	1.230013
90	1	0	5.777579	6.964976	0.574752
91	1	0	4.438254	7.454361	−0.477462

TS(4-Cα) (energy and imaginary frequency are in Table S1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.329159	1.646017	2.267686
2	6	0	−0.344085	0.352387	2.907707
3	6	0	0.584463	−0.487129	2.186366
4	6	0	1.262538	0.285242	1.185619
5	6	0	0.608870	1.596359	1.131991
6	6	0	1.913811	−0.445212	0.131834
7	6	0	0.288969	−1.838075	1.975831
8	6	0	−1.518095	−0.179675	3.439055
9	6	0	−1.504961	2.393928	2.230271
10	6	0	0.294560	2.367854	−0.012334
11	6	0	1.217396	0.742716	−1.740284
12	6	0	0.502696	1.880445	−1.391767
13	6	0	−1.835502	3.149568	1.046916
14	6	0	−0.961804	3.113018	−0.042982
15	6	0	−2.737361	1.853198	2.785617
16	6	0	−2.747186	0.587312	3.369473
17	6	0	−1.838837	−1.578501	3.218401
18	6	0	−0.957211	−2.378069	2.479332
19	6	0	1.123221	−1.616777	−0.362535
20	6	0	0.490565	−2.370267	0.630869
21	6	0	−0.592935	−3.266050	0.344297
22	6	0	−1.492049	−3.290201	1.481876
23	6	0	−3.272762	3.066771	0.846348
24	6	0	−3.829966	2.261208	1.920424
25	6	0	−3.834360	−0.335237	3.094277
26	6	0	−3.269208	−1.672287	2.990096
27	6	0	−0.645402	2.236454	−2.179310
28	6	0	−1.531856	3.038816	−1.378321
29	6	0	0.537732	−0.328405	−2.425858
30	6	0	0.549770	−1.619693	−1.712612
31	6	0	−1.143229	1.345567	−3.129812
32	6	0	−0.570370	0.017682	−3.211997
33	6	0	−2.909595	2.960886	−1.578508
34	6	0	−3.805860	2.974265	−0.440174
35	6	0	−4.880574	1.378506	1.659536
36	6	0	−4.878823	0.051406	2.253855
37	6	0	−3.778227	−2.569206	2.045631
38	6	0	−2.865528	−3.392865	1.273639
39	6	0	−0.515507	−2.514237	−1.985504
40	6	0	−1.079327	−3.356688	−0.953611
41	6	0	−2.510425	−3.491487	−1.171390
42	6	0	−3.385020	−3.497770	−0.082526
43	6	0	−4.861275	−2.162676	1.167268
44	6	0	−5.405130	−0.881330	1.271839
45	6	0	−5.418077	1.266092	0.313382
46	6	0	−4.891110	2.048765	−0.714708
47	6	0	−3.442094	2.033383	−2.566600
48	6	0	−2.577368	1.240220	−3.325275
49	6	0	−1.648625	−0.906776	−3.467569
50	6	0	−1.613338	−2.160097	−2.876685
51	6	0	−4.624370	−2.745033	−0.145450
52	6	0	−5.736153	−0.131277	0.072198
53	6	0	−4.666093	1.466866	−2.029132
54	6	0	−2.891775	−0.159508	−3.548497
55	6	0	−2.842549	−2.745436	−2.366071
56	6	0	−4.972215	0.122700	−2.258650
57	6	0	−4.065603	−0.706657	−3.033964
58	6	0	−5.518491	−0.692538	−1.187599
59	6	0	−4.945032	−2.024405	−1.297777
60	6	0	−4.041468	−2.030994	−2.434703
61	7	0	2.373074	0.355503	−0.994212
62	1	0	2.955473	−3.579981	0.562888
63	6	0	3.389708	−2.991268	1.368873
64	6	0	4.463616	−1.542258	3.491818
65	6	0	3.766136	−3.653473	2.545476
66	6	0	3.566081	−1.599028	1.205560
67	6	0	4.093082	−0.896589	2.311906
68	6	0	4.302663	−2.928405	3.608899
69	1	0	3.627396	−4.728408	2.630580
70	1	0	4.196205	0.185378	2.263866
71	1	0	4.583741	−3.434152	4.528648
72	1	0	4.871723	−0.969631	4.321159
73	12	0	5.025845	−1.449010	−0.444959
74	35	0	6.770426	−2.681299	−1.576776
75	16	0	3.734886	1.330949	−1.186209
76	8	0	4.856667	0.561270	−0.563209

77	8	0	3.794436	1.615820	−2.617188
78	6	0	3.685832	2.878591	−0.306254
79	6	0	4.178429	2.967556	0.998037
80	6	0	3.162060	3.997044	−0.964177
81	6	0	4.129334	4.196084	1.651255
82	1	0	4.623572	2.107170	1.481917
83	6	0	3.124006	5.213601	−0.290590
84	1	0	2.809920	3.921687	−1.986261
85	6	0	3.595782	5.333074	1.026202
86	1	0	4.521393	4.272743	2.661290
87	1	0	2.727448	6.087177	−0.800211
88	6	0	3.520848	6.652269	1.752634
89	1	0	4.239078	6.697547	2.576359
90	1	0	3.713617	7.491036	1.076246
91	1	0	2.519814	6.800960	2.177811

TS(1−Cβ) (energy and imaginary frequency are in Table S2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.086998	−2.791004	0.750320
2	6	0	0.184143	−2.171417	2.058179
3	6	0	−0.686624	−1.028827	2.064014
4	6	0	−1.523744	−1.021272	0.851109
5	6	0	−0.844700	−2.026050	−0.074894
6	6	0	−1.878585	0.289713	0.384609
7	6	0	−0.270123	0.149700	2.668422
8	6	0	1.394339	−2.155083	2.754160
9	6	0	1.211006	−3.421518	0.219051
10	6	0	−0.575679	−1.897417	−1.448745
11	6	0	−1.406326	0.487227	−1.812609
12	6	0	−0.770094	−0.665262	−2.267391
13	6	0	1.491765	−3.288840	−1.187650
14	6	0	0.630462	−2.540604	−1.987950
15	6	0	2.476873	−3.413586	0.939046
16	6	0	2.569708	−2.780529	2.175684
17	6	0	1.814608	−0.938382	3.421593
18	6	0	1.000393	0.195447	3.368449
19	6	0	−1.105090	1.444799	0.742965
20	6	0	−0.460828	1.428121	1.993038
21	6	0	0.684332	2.237050	2.265561
22	6	0	1.589020	1.498484	3.134962
23	6	0	2.933202	−3.194454	−1.355619
24	6	0	3.540483	−3.259357	−0.037473
25	6	0	3.720128	−1.950084	2.486510
26	6	0	3.250985	−0.806743	3.252279
27	6	0	0.370312	−0.520846	−3.118454
28	6	0	1.203720	−1.693356	−3.012307
29	6	0	−0.629390	1.705942	−1.687958
30	6	0	−0.549920	2.283480	−0.336331
31	6	0	0.935469	0.737054	−3.343129
32	6	0	0.457645	1.858602	−2.566313
33	6	0	2.582065	−1.588534	−3.183021
34	6	0	3.471008	−2.351358	−2.328101
35	6	0	4.650245	−2.463815	0.258992
36	6	0	4.738416	−1.791430	1.545163
37	6	0	3.816361	0.453517	3.036322
38	6	0	2.966402	1.631614	2.978024
39	6	0	0.572515	3.090207	−0.032430
40	6	0	1.185005	3.088484	1.281900
41	6	0	2.621239	3.234643	1.133622
42	6	0	3.497275	2.525684	1.961114
43	6	0	4.874302	0.618682	2.057128
44	6	0	5.328590	−0.481947	1.327606
45	6	0	5.195495	−1.572414	−0.750657
46	6	0	4.621231	−1.521325	−2.021791
47	6	0	3.181868	−0.281881	−3.412824
48	6	0	2.375604	0.856746	−3.483456
49	6	0	1.595512	2.678995	−2.234845
50	6	0	1.644863	3.299567	−0.994759
51	6	0	4.677919	1.900215	1.394082
52	6	0	5.613445	−0.347291	−0.090837
53	6	0	4.437115	−0.239415	−2.685809
54	6	0	2.786246	2.074261	−2.808667
55	6	0	2.909208	3.372335	−0.279132
56	6	0	4.836172	0.938722	−2.048992
57	6	0	3.990969	2.118140	−2.110420
58	6	0	5.431462	0.883128	−0.724939
59	6	0	4.954724	2.029473	0.031960
60	6	0	4.055432	2.787153	−0.820628
61	1	0	−4.002992	−0.256515	2.455850
62	6	0	−3.937907	−1.339953	2.565794
63	6	0	−3.666722	−4.089774	2.939917
64	6	0	−4.448652	−1.933289	3.720895
65	6	0	−3.312652	−2.099519	1.553828
66	6	0	−3.171043	−3.486736	1.781043
67	6	0	−4.307985	−3.312781	3.909933
68	1	0	−4.937002	−1.326853	4.479886
69	1	0	−2.670530	−4.109115	1.040359
70	1	0	−4.685613	−3.778214	4.816467
71	1	0	−3.553177	−5.160796	3.089289
72	12	0	−4.195974	−1.664396	−0.417552
73	35	0	−5.146538	−3.078681	−2.152383
74	16	0	−3.967141	1.184834	−1.177803
75	8	0	−4.923825	0.278571	−0.452187
76	8	0	−4.090197	1.355922	−2.623397
77	6	0	−4.038063	2.752908	−0.354226
78	6	0	−4.485754	2.831382	0.968646
79	6	0	−3.633761	3.890713	−1.062538
80	6	0	−4.519780	4.078189	1.585932
81	1	0	−4.824139	1.945669	1.492781
82	6	0	−3.679076	5.123996	−0.422079
83	1	0	−3.306801	3.813999	−2.093365
84	6	0	−4.112259	5.238393	0.909328
85	1	0	−4.875234	4.150910	2.609664
86	1	0	−3.377808	6.014053	−0.966873
87	6	0	−4.123908	6.577866	1.600738
88	1	0	−4.850904	6.600212	2.417677
89	1	0	−3.137558	6.795164	2.030915
90	1	0	−4.359202	7.386164	0.901587
91	7	0	−2.493967	0.295911	−0.912903

TS(2−Cβ) (energy and imaginary frequency are in Table S2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.561654	2.925624	−0.668693
2	6	0	−0.399233	2.900918	0.771636
3	6	0	0.680234	2.003021	1.074789
4	6	0	1.361680	1.607584	−0.168621
5	6	0	0.415883	2.026582	−1.282503
6	6	0	1.990563	0.297665	−0.127404
7	6	0	0.577114	1.136621	2.153164
8	6	0	−1.500053	3.007726	1.621991
9	6	0	−1.839188	3.110894	−1.193121
10	6	0	0.032379	1.296409	−2.420559
11	6	0	1.279148	−0.881988	−1.974442
12	6	0	0.377952	−0.126614	−2.716208
13	6	0	−2.234329	2.367469	−2.362078
14	6	0	−1.328733	1.480779	−2.941978
15	6	0	−2.995148	3.229203	−0.315917
16	6	0	−2.829902	3.164514	1.065349
17	6	0	−1.593458	2.133651	2.775358
18	6	0	−0.577120	1.208538	3.028262
19	6	0	1.456514	−0.713719	0.778126
20	6	0	0.952063	−0.270985	2.008568
21	6	0	0.024423	−1.041359	2.774681
22	6	0	−0.913600	−0.142025	3.430069
23	6	0	−3.637142	2.012348	−2.220629
24	6	0	−4.103009	2.534864	−0.947701
25	6	0	−3.750703	2.387458	1.876343
26	6	0	−2.983514	1.745202	2.931404
27	6	0	−0.793019	−0.767908	−3.226738
28	6	0	−1.827601	0.213844	−3.436339
29	6	0	0.781415	−2.027365	−1.242666
30	6	0	0.963148	−1.983944	0.221766
31	6	0	−1.113723	−2.069724	−2.832687
32	6	0	−0.340783	−2.685328	−1.777962
33	6	0	−3.166889	−0.143133	−3.304341
34	6	0	−4.094982	0.774196	−2.672684
35	6	0	−4.993038	1.788978	−0.170669
36	6	0	−4.808294	1.709077	1.269232
37	6	0	−3.302911	0.443646	3.329408
38	6	0	−2.244501	−0.519318	3.585836
39	6	0	0.061909	−2.742564	1.011210
40	6	0	−0.396449	−2.283424	2.305570
41	6	0	−1.781522	−2.680895	2.487475
42	6	0	−2.688949	−1.820367	3.111337

43	6	0	−4.403003	−0.261183	2.698826
44	6	0	−5.143012	0.359749	1.690586
45	6	0	−5.452343	0.491289	−0.635876
46	6	0	−5.015540	−0.004098	−1.865370
47	6	0	−3.513040	−1.496848	−2.892282
48	6	0	−2.507512	−2.437317	−2.655490
49	6	0	−1.249799	−3.439980	−0.953545
50	6	0	−1.041126	−3.485475	0.417052
51	6	0	−4.024562	−1.661149	2.567047
52	6	0	−5.542979	−0.392618	0.513871
53	6	0	−4.650062	−1.407042	−1.995934
54	6	0	−2.591370	−3.305485	−1.495925
55	6	0	−2.182384	−3.432217	1.316800
56	6	0	−4.735454	−2.255540	−0.888689
57	6	0	−3.682160	−3.221934	−0.633309
58	6	0	−5.187115	−1.736973	0.391052
59	6	0	−4.411954	−2.384106	1.437502
60	6	0	−3.474022	−3.293876	0.803758
61	1	0	2.382354	4.236470	1.465009
62	6	0	2.633196	4.441124	0.424596
63	6	0	3.243379	5.019689	−2.238391
64	6	0	2.785248	5.770058	0.018224
65	6	0	2.803603	3.375521	−0.480993
66	6	0	3.090122	3.693934	−1.825001
67	6	0	3.088372	6.059247	−1.315634
68	1	0	2.661852	6.577282	0.736245
69	1	0	3.189245	2.901384	−2.565343
70	1	0	3.194395	7.091935	−1.637337
71	1	0	3.474501	5.243384	−3.277117
72	12	0	3.954452	1.694840	0.338684
73	35	0	4.873940	1.222005	2.539644
74	16	0	3.967027	−0.664676	−1.728162
75	8	0	4.754177	0.403474	−1.023461
76	8	0	4.101221	−0.806012	−3.174602
77	6	0	4.388061	−2.205263	−0.942598
78	6	0	4.795712	−2.224618	0.396774
79	6	0	4.249781	−3.384918	−1.681321
80	6	0	5.067517	−3.453503	0.990721
81	1	0	4.909325	−1.308414	0.967101
82	6	0	4.528911	−4.600307	−1.062163
83	1	0	3.942435	−3.351754	−2.720542
84	6	0	4.939634	−4.656460	0.278096
85	1	0	5.387287	−3.476056	2.028812
86	1	0	4.427578	−5.519821	−1.631602
87	6	0	5.263529	−5.975405	0.933808
88	1	0	6.343627	−6.168488	0.900138
89	1	0	4.966218	−5.979725	1.987256
90	1	0	4.764278	−6.807025	0.428047
91	7	0	2.378904	−0.184993	−1.420044

TS(3-Cβ) (energy and imaginary frequency are in Table S2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.360295	−2.571917	1.312024
2	6	0	−0.847384	−3.128759	0.064102
3	6	0	−0.038351	−2.593889	−0.996945
4	6	0	1.110787	−1.861149	−0.438770
5	6	0	0.754922	−1.670380	1.031029
6	6	0	1.546097	−0.752642	−1.235697
7	6	0	−0.639478	−2.200574	−2.186888
8	6	0	−2.208827	−3.375543	−0.124991
9	6	0	−1.266786	−2.337464	2.345093
10	6	0	0.891514	−0.510547	1.812771
11	6	0	1.750754	1.091254	0.023217
12	6	0	1.294940	0.834976	1.315035
13	6	0	−1.127345	−1.148819	3.147271
14	6	0	−0.086138	−0.262596	2.878824
15	6	0	−2.688016	−2.595873	2.159047
16	6	0	−3.150826	−3.091434	0.942882
17	6	0	−2.830527	−3.006408	−1.381965
18	6	0	−2.060060	−2.419914	−2.388617
19	6	0	0.690827	−0.123382	−2.194819
20	6	0	−0.287741	−0.928014	−2.805021
21	6	0	−1.478449	−0.372157	−3.365199
22	6	0	−2.582031	−1.293463	−3.135844
23	6	0	−2.457910	−0.655829	3.465434
24	6	0	−3.422329	−1.545483	2.842015
25	6	0	−4.358379	−2.547970	0.345825
26	6	0	−4.157334	−2.490414	−1.092772
27	6	0	0.453021	1.803338	1.946476
28	6	0	−0.350653	1.158118	2.956101
29	6	0	0.946943	1.941801	−0.837359
30	6	0	0.463023	1.328337	−2.084133
31	6	0	−0.045872	2.890179	1.224972
32	6	0	0.161594	2.922555	−0.205584
33	6	0	−1.619891	1.646030	3.255862
34	6	0	−2.704234	0.716808	3.509237
35	6	0	−4.586201	−1.022791	2.272838
36	6	0	−5.059479	−1.530808	0.995502
37	6	0	−4.660308	−1.408636	−1.821382
38	6	0	−3.855379	−0.798098	−2.866918
39	6	0	−0.716279	1.853711	−2.662182
40	6	0	−1.686618	1.005875	−3.328394
41	6	0	−3.019078	1.515348	−3.062581
42	6	0	−4.083745	0.637533	−2.837602
43	6	0	−5.388797	−0.351191	−1.146060
44	6	0	−5.586894	−0.411673	0.234751
45	6	0	−4.830690	0.409358	2.303743
46	6	0	−3.910177	1.262534	2.914495
47	6	0	−2.152519	2.774525	2.505729
48	6	0	−1.383984	3.378290	1.507179
49	6	0	−1.040053	3.442193	−0.809506
50	6	0	−1.464134	2.928826	−2.027121
51	6	0	−5.033577	0.912907	−1.775285
52	6	0	−5.447807	0.787439	1.043469
53	6	0	−3.565865	2.529969	2.287350
54	6	0	−1.998406	3.738525	0.243075
55	6	0	−2.884018	2.712929	−2.259201
56	6	0	−4.158166	2.891700	1.074508
57	6	0	−3.355571	3.505141	0.030896
58	6	0	−5.113941	2.000656	0.438846
59	6	0	−4.903199	2.065285	−0.998600
60	6	0	−3.808911	2.987241	−1.250065
61	1	0	3.089998	−2.910009	−2.478586
62	6	0	3.063064	−3.693728	−1.719197
63	6	0	2.866086	−5.739612	0.166888
64	6	0	3.328019	−5.010550	−2.098029
65	6	0	2.733148	−3.356629	−0.389510
66	6	0	2.617893	−4.415818	0.538814
67	6	0	3.224412	−6.036832	−1.152111
68	1	0	3.593700	−5.242901	−3.126530
69	1	0	2.337926	−4.203960	1.570299
70	1	0	3.407975	−7.066894	−1.446184
71	1	0	2.778914	−6.538466	0.899483
72	12	0	3.967697	−1.686086	0.367941
73	35	0	4.980100	−1.187240	2.530019
74	16	0	3.940560	0.506606	−1.590678
75	8	0	3.624634	0.595717	−3.014547
76	8	0	4.872791	−0.597664	−1.163414
77	6	0	4.529998	2.055565	−0.969378
78	6	0	4.340983	3.191448	−1.763890
79	6	0	5.163900	2.122290	0.278065
80	6	0	4.805981	4.415960	−1.294536
81	1	0	3.848945	3.114679	−2.726801
82	6	0	5.611707	3.361185	0.723304
83	1	0	5.301141	1.239915	0.895427
84	6	0	5.446715	4.522049	−0.050613
85	1	0	4.667934	5.303253	−1.905341
86	1	0	6.101674	3.426546	1.690529
87	6	0	5.969415	5.848228	0.439017
88	1	0	7.044562	5.935127	0.235526
89	1	0	5.469978	6.684369	−0.058462
90	1	0	5.834719	5.953784	1.520132
91	7	0	2.537110	0.060878	−0.582060

TS(4-Cβ) (energy and imaginary frequency are in Table S2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.012382	−1.245131	2.415607
2	6	0	−0.298261	−2.409164	1.599009
3	6	0	0.474066	−2.297053	0.392819
4	6	0	1.420306	−1.175992	0.509918
5	6	0	0.941186	−0.383963	1.715417
6	6	0	1.767759	−0.541990	−0.746453
7	6	0	−0.094466	−2.639101	−0.826522
8	6	0	−1.571316	−2.980386	1.580723

9	6	0	−1.024341	−0.733811	3.225990
10	6	0	0.800917	1.009387	1.836484
11	6	0	1.475370	1.718736	−0.520030
12	6	0	0.976465	2.013455	0.744786
13	6	0	−1.167178	0.693838	3.357567
14	6	0	−0.289257	1.531408	2.671594
15	6	0	−2.354976	−1.325332	3.220043
16	6	0	−2.626917	−2.418907	2.402171
17	6	0	−2.152209	−3.381294	0.313732
18	6	0	−1.428589	−3.205222	−0.868521
19	6	0	0.834395	−0.602308	−1.862619
20	6	0	0.067014	−1.767866	−1.990997
21	6	0	−1.162085	−1.793202	−2.719210
22	6	0	−2.090224	−2.693197	−2.051659
23	6	0	−2.586040	1.003613	3.431663
24	6	0	−3.319906	−0.246000	3.332961
25	6	0	−3.865060	−2.475501	1.644538
26	6	0	−3.569089	−3.066871	0.349879
27	6	0	−0.075179	2.975102	0.856947
28	6	0	−0.819426	2.736576	2.067929
29	6	0	0.596945	1.875586	−1.661351
30	6	0	0.331366	0.652716	−2.442147
31	6	0	−0.710374	3.464738	−0.287153
32	6	0	−0.403898	2.858723	−1.563127
33	6	0	−2.175712	3.045366	2.126548
34	6	0	−3.085330	2.152898	2.817603
35	6	0	−4.513408	−0.298380	2.608450
36	6	0	−4.788229	−1.433637	1.742651
37	6	0	−4.205183	−2.582629	−0.797062
38	6	0	−3.449499	−2.394526	−2.024532
39	6	0	−0.878333	0.598177	−3.178257
40	6	0	−1.622394	−0.634038	−3.339029
41	6	0	−3.043331	−0.335587	−3.323915
42	6	0	−3.940325	−1.193324	−2.681008
43	6	0	−5.166001	−1.500584	−0.695236
44	6	0	−5.453615	−0.938146	0.550140
45	6	0	−5.019731	0.896176	1.954446
46	6	0	−4.322484	2.100466	2.061706
47	6	0	−2.849603	3.553735	0.939336
48	6	0	−2.133122	3.751943	−0.243654
49	6	0	−1.631961	2.777023	−2.313206
50	6	0	−1.858005	1.674376	−3.123819
51	6	0	−5.003447	−0.643066	−1.861132
52	6	0	−5.598869	0.501309	0.681748
53	6	0	−4.172523	2.960200	0.896524
54	6	0	−2.705851	3.340726	−1.511794
55	6	0	−3.191943	1.098801	−3.195009
56	6	0	−4.727088	2.577641	−0.327995
57	6	0	−3.976171	2.770141	−1.555898
58	6	0	−5.450322	1.322275	−0.437456
59	6	0	−5.146711	0.739725	−1.734525
60	6	0	−4.226800	1.629235	−2.421811
61	7	0	2.466608	0.705668	−0.578852
62	1	0	2.424159	−4.143092	1.466528
63	6	0	2.996760	−3.434818	2.064835
64	6	0	4.433940	−1.651580	3.658716
65	6	0	3.509946	−3.858767	3.294134
66	6	0	3.211929	−2.125559	1.589704
67	6	0	3.916468	−1.237226	2.429267
68	6	0	4.230538	−2.965741	4.092419
69	1	0	3.342617	−4.878740	3.631925
70	1	0	4.051974	−0.198954	2.130932
71	1	0	4.620588	−3.288066	5.054276
72	1	0	4.983670	−0.951343	4.283261
73	12	0	3.667046	−2.057510	−0.576661
74	35	0	3.811827	−3.940222	−2.093641
75	16	0	3.870065	0.928976	−1.516015
76	8	0	4.581184	−0.380899	−1.313310
77	8	0	3.621691	1.344797	−2.898221
78	6	0	4.777706	2.192728	−0.668135
79	6	0	5.605647	1.851692	0.405947
80	6	0	4.639002	3.516342	−1.095820
81	6	0	6.299220	2.864891	1.060273
82	1	0	5.718931	0.817731	0.711417
83	6	0	5.338469	4.512403	−0.419509
84	1	0	4.006384	3.760471	−1.941899
85	6	0	6.177406	4.206203	0.662807
86	1	0	6.949466	2.609123	1.891950
87	1	0	5.233828	5.544163	−0.742639
88	6	0	6.956776	5.290351	1.363680
89	1	0	7.919991	5.455839	0.863792
90	1	0	6.416006	6.241526	1.352723
91	1	0	7.168993	5.021928	2.402829

Reaction of EtMgBr

TS(1−Cα) (energy and imaginary frequency are in Table S3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.252406	2.298523	−1.698946
2	6	0	−0.314939	2.916073	−0.394719
3	6	0	0.619466	2.217889	0.453888
4	6	0	1.377208	1.272321	−0.331946
5	6	0	0.718942	1.199571	−1.660838
6	6	0	1.995257	0.176063	0.394596
7	6	0	0.305267	1.962876	1.791559
8	6	0	−1.518855	3.391302	0.125676
9	6	0	−1.413627	2.236614	−2.471911
10	6	0	0.464742	0.058559	−2.452048
11	6	0	1.423014	−1.680312	−0.855292
12	6	0	0.714543	−1.330719	−1.994153
13	6	0	−1.686335	1.058746	−3.253507
14	6	0	−0.775247	−0.000252	−3.222641
15	6	0	−2.673870	2.736797	−1.943192
16	6	0	−2.728937	3.294208	−0.666657
17	6	0	−1.857567	3.132065	1.512628
18	6	0	−0.966777	2.410668	2.317312
19	6	0	1.223545	−0.344062	1.543197
20	6	0	0.549631	0.615963	2.303879
21	6	0	−0.539889	0.273313	3.175273
22	6	0	−1.480745	1.376745	3.200146
23	6	0	−3.118071	0.806613	−3.205470
24	6	0	−3.728034	1.843334	−2.390256
25	6	0	−3.823809	2.963596	0.228740
26	6	0	−3.281340	2.853241	1.574274
27	6	0	−0.398785	−2.145468	−2.386761
28	6	0	−1.298627	−1.356306	−3.186649
29	6	0	0.748395	−2.404455	0.196321
30	6	0	0.706953	−1.718125	1.504948
31	6	0	−0.879683	−3.130184	−1.522551
32	6	0	−0.328518	−3.218964	−0.185727
33	6	0	−2.668648	−1.606024	−3.139480
34	6	0	−3.604748	−0.499200	−3.147030
35	6	0	−4.784558	1.527624	−1.533158
36	6	0	−4.829680	2.094959	−0.194863
37	6	0	−3.771494	1.872469	2.441437
38	6	0	−2.847281	1.116808	3.268240
39	6	0	−0.366669	−2.039805	2.368816
40	6	0	−0.981978	−1.042670	3.221582
41	6	0	−2.405466	−1.315020	3.324364
42	6	0	−3.318808	−0.258329	3.334823
43	6	0	−4.814485	0.965050	1.997258
44	6	0	−5.337537	1.076161	0.707928
45	6	0	−5.275136	0.161656	−1.457271
46	6	0	−4.696346	−0.831060	−2.249255
47	6	0	−3.183341	−2.631000	−2.242159
48	6	0	−2.307736	−3.375916	−1.447890
49	6	0	−1.414545	−3.527184	0.712477
50	6	0	−1.424425	−2.961799	1.978179
51	6	0	−4.540942	−0.350026	2.557932
52	6	0	−5.611214	−0.119195	−0.071720
53	6	0	−4.435051	−2.148055	−1.688952
54	6	0	−2.640305	−3.637512	−0.059490
55	6	0	−2.681067	−2.505411	2.549317
56	6	0	−4.759278	−2.415892	−0.356057
57	6	0	−3.840873	−3.174892	0.475148
58	6	0	−5.358523	−1.381439	0.468651
59	6	0	−4.806869	−1.498056	1.809221
60	6	0	−3.862852	−2.601729	1.810972
61	7	0	2.521968	−0.880629	−0.428978
62	12	0	3.615050	2.063222	0.024751
63	35	0	4.498151	4.300613	−0.309888
64	16	0	3.892645	−0.723780	−1.400773
65	8	0	3.632690	−1.367455	−2.684016
66	8	0	4.245873	0.731922	−1.413734
67	6	0	5.199630	−1.578547	−0.543739
68	6	0	4.952568	−2.845235	−0.005163
69	6	0	6.470903	−1.002679	−0.505530
70	6	0	6.004094	−3.533055	0.591038

71	1	0	3.960946	−3.284199	−0.037058
72	6	0	7.508055	−1.713543	0.096588
73	1	0	6.649101	−0.022090	−0.932290
74	6	0	7.294564	−2.981276	0.655056
75	1	0	5.818965	−4.515447	1.016401
76	1	0	8.499459	−1.271000	0.130970
77	6	0	8.415115	−3.729913	1.332074
78	1	0	9.393752	−3.371805	1.000029
79	1	0	8.365697	−3.597759	2.420626
80	1	0	8.352428	−4.804528	1.132958
81	6	0	3.997206	0.629382	1.758704
82	1	0	3.879640	−0.449383	1.852945
83	1	0	5.028573	0.786631	1.391228
84	6	0	3.788762	1.344095	3.087419
85	1	0	3.961506	2.424338	3.012610
86	1	0	2.776226	1.194006	3.476539
87	1	0	4.481568	0.960458	3.853468

TS(2-Cα) (energy and imaginary frequency are in Table S3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.777206	0.494767	−3.199043
2	6	0	1.188451	−0.886073	−3.245884
3	6	0	0.186451	−1.648074	−2.534410
4	6	0	−0.897158	−0.787284	−2.154857
5	6	0	−0.482817	0.581553	−2.440110
6	6	0	−1.768232	−1.270430	−1.111119
7	6	0	0.568286	−2.736752	−1.741750
8	6	0	2.534571	−1.243268	−3.176609
9	6	0	1.749525	1.490599	−3.139050
10	6	0	−0.708893	1.747274	−1.667123
11	6	0	−1.960360	0.604567	0.243995
12	6	0	−1.316873	1.697120	−0.322741
13	6	0	1.534990	2.653216	−2.312790
14	6	0	0.344712	2.754712	−1.585821
15	6	0	3.159544	1.134082	−3.073600
16	6	0	3.544456	−0.206071	−3.080616
17	6	0	2.943035	−2.359334	−2.343796
18	6	0	1.971355	−3.067298	−1.621825
19	6	0	−1.046996	−1.969704	−0.003518
20	6	0	−0.023592	−2.832921	−0.407092
21	6	0	1.000835	−3.268282	0.499994
22	6	0	2.238066	−3.430446	−0.239034
23	6	0	2.805235	3.012438	−1.706989
24	6	0	3.809716	2.071361	−2.175726
25	6	0	4.577936	−0.673099	−2.173811
26	6	0	4.198209	−1.999833	−1.710111
27	6	0	−0.581190	2.576708	0.545690
28	6	0	0.412303	3.271956	−0.228888
29	6	0	−1.421845	0.028616	1.453609
30	6	0	−0.998211	−1.380689	1.337876
31	6	0	−0.336130	2.212488	1.869432
32	6	0	−0.716931	0.886683	2.309690
33	6	0	1.628865	3.622022	0.357221
34	6	0	2.858842	3.492315	−0.397247
35	6	0	4.809265	1.626436	−1.307771
36	6	0	5.195883	0.224389	−1.303174
37	6	0	4.458550	−2.372179	−0.387315
38	6	0	3.450048	−3.098087	0.362757
39	6	0	0.009964	−1.831990	2.224365
40	6	0	1.007366	−2.791511	1.805972
41	6	0	2.272981	−2.474166	2.445733
42	6	0	3.466948	−2.612151	1.735007
43	6	0	5.095744	−1.433109	0.519906
44	6	0	5.464008	−0.163419	0.071376
45	6	0	4.846883	2.106265	0.063875
46	6	0	3.891608	3.020650	0.509124
47	6	0	1.899044	3.242470	1.736834
48	6	0	0.937523	2.550863	2.478131
49	6	0	0.317584	0.407767	3.195669
50	6	0	0.662925	−0.934300	3.167860
51	6	0	4.491650	−1.589555	1.834543
52	6	0	5.245114	0.998338	0.915814
53	6	0	3.298470	2.867520	1.829092
54	6	0	1.339105	1.433915	3.314223
55	6	0	2.059688	−1.317653	3.289492
56	6	0	3.683096	1.801302	2.646781
57	6	0	2.681289	1.069480	3.403480
58	6	0	4.676620	0.848638	2.182578
59	6	0	4.285148	−0.472325	2.646664
60	6	0	3.048786	−0.337002	3.396157
61	7	0	−2.734690	−0.311759	−0.553877
62	6	0	−2.935544	−3.025701	−2.054124
63	12	0	−4.124906	−2.178695	−0.300063
64	35	0	−4.983160	−3.012604	1.790990
65	16	0	−4.002066	0.365337	−1.583607
66	8	0	−3.569928	0.737281	−2.925248
67	8	0	−5.020463	−0.735602	−1.469432
68	6	0	−4.602183	1.767363	−0.688251
69	6	0	−5.345136	1.574953	0.482758
70	6	0	−4.370028	3.039830	−1.217507
71	6	0	−5.848191	2.694109	1.135849
72	1	0	−5.536685	0.580299	0.871473
73	6	0	−4.892557	4.141490	−0.546540
74	1	0	−3.802477	3.162054	−2.132930
75	6	0	−5.629595	3.990217	0.637804
76	1	0	−6.428549	2.558623	2.043786
77	1	0	−4.725400	5.134910	−0.951989
78	6	0	−6.164166	5.192160	1.373414
79	1	0	−5.492090	5.466948	2.196663
80	1	0	−6.250502	6.059987	0.713629
81	1	0	−7.146082	4.986871	1.811139
82	1	0	−2.133792	−2.903776	−2.774949
83	1	0	−3.865458	−2.789004	−2.598179
84	6	0	−2.911075	−4.450884	−1.487095
85	1	0	−2.040479	−4.606871	−0.840020
86	1	0	−3.799760	−4.720053	−0.899038
87	1	0	−2.844215	−5.188832	−2.300390

TS(3-Cα) (energy and imaginary frequency are in Table S3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.499921	−0.933418	−2.388736
2	6	0	−0.114300	−2.222488	−1.863586
3	6	0	−0.729609	−2.356250	−0.566187
4	6	0	−1.614669	−1.239462	−0.330656
5	6	0	−1.350171	−0.252818	−1.404038
6	6	0	−1.938596	−0.948338	1.052507
7	6	0	−0.039517	−2.966803	0.483674
8	6	0	1.154479	−2.751937	−2.099373
9	6	0	0.400288	−0.238265	−3.197940
10	6	0	−1.256808	1.153571	−1.301733
11	6	0	−1.630516	1.342419	1.215186
12	6	0	−1.280748	1.887523	−0.012567
13	6	0	0.516948	1.191553	−3.069059
14	6	0	−0.280623	1.855174	−2.133150
15	6	0	1.724098	−0.784128	−3.458744
16	6	0	2.098638	−2.010654	−2.911795
17	6	0	1.882166	−3.388297	−1.016963
18	6	0	1.298164	−3.468878	0.253746
19	6	0	−0.847808	−1.177510	2.024800
20	6	0	−0.048500	−2.299491	1.784781
21	6	0	1.260532	−2.442790	2.359010
22	6	0	2.100845	−3.171785	1.428258
23	6	0	1.917514	1.546079	−3.232936
24	6	0	2.664532	0.322460	−3.469186
25	6	0	3.418133	−2.178771	−2.328661
26	6	0	3.280809	−3.021819	−1.150827
27	6	0	−0.274366	2.908857	−0.052155
28	6	0	0.315169	2.936260	−1.365128
29	6	0	−0.639515	1.313002	2.267033
30	6	0	−0.277554	−0.035689	2.753809
31	6	0	0.489165	3.174351	1.085349
32	6	0	0.338379	2.319556	2.245573
33	6	0	1.656890	3.281306	−1.516091
34	6	0	2.482241	2.569578	−2.471859
35	6	0	3.935764	0.162104	−2.913741
36	6	0	4.317313	−1.112629	−2.326664
37	6	0	4.053474	−2.758537	−0.015999
38	6	0	3.445625	−2.832457	1.300786
39	6	0	1.013258	−0.193586	3.312820
40	6	0	1.779015	−1.410034	3.129536
41	6	0	3.188908	−1.076249	3.022294
42	6	0	4.001010	−1.763725	2.117397
43	6	0	4.985223	−1.644694	−0.013197
44	6	0	5.120145	−0.841242	−1.146541

45	6	0	4.512255	1.219993	−2.100804
46	6	0	3.799721	2.400410	−1.885612
47	6	0	2.464378	3.562117	−0.337170
48	6	0	1.893848	3.507078	0.937468
49	6	0	1.649349	2.130640	2.817024
50	6	0	1.975876	0.898614	3.361451
51	6	0	4.961343	−1.036137	1.308818
52	6	0	5.238600	0.600036	−1.005863
53	6	0	3.788219	3.012870	−0.565796
54	6	0	2.615909	2.870043	2.023537
55	6	0	3.311504	0.358837	3.163298
56	6	0	4.486584	2.413665	0.486224
57	6	0	3.886187	2.340220	1.807060
58	6	0	5.226589	1.184355	0.262113
59	6	0	5.079032	0.348409	1.443083
60	6	0	4.244388	1.060005	2.395255
61	7	0	−2.601691	0.307612	1.263084
62	12	0	−3.764954	−2.333741	−0.025707
63	35	0	−4.735122	−3.951431	−1.554291
64	16	0	−4.261940	0.536626	1.065135
65	8	0	−4.674571	−0.499273	0.056766
66	8	0	−4.941406	0.508026	2.359646
67	6	0	−4.499541	2.129073	0.325337
68	6	0	−4.556164	2.248646	−1.066780
69	6	0	−4.692227	3.229120	1.166549
70	6	0	−4.800592	3.503370	−1.615682
71	1	0	−4.428189	1.381302	−1.703517
72	6	0	−4.926989	4.474483	0.591276
73	1	0	−4.673339	3.111705	2.244235
74	6	0	−4.981485	4.633723	−0.801959
75	1	0	−4.858301	3.604863	−2.695626
76	1	0	−5.080834	5.334396	1.236630
77	6	0	−5.216462	5.990910	−1.415318
78	1	0	−5.724998	6.662838	−0.717996
79	1	0	−4.262090	6.459214	−1.688977
80	1	0	−5.815661	5.917406	−2.328223
81	6	0	−3.530433	−2.439378	2.243104
82	1	0	−3.315222	−1.673656	2.986605
83	1	0	−4.632765	−2.446397	2.137247
84	6	0	−3.006009	−3.806573	2.661325
85	1	0	−1.917407	−3.803190	2.781759
86	1	0	−3.428162	−4.107833	3.633690
87	1	0	−3.259943	−4.598446	1.945910

TS(4-Cα) (energy and imaginary frequency are in Table S3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.424652	1.626287	−2.710946
2	6	0	0.420457	0.247821	−3.131982
3	6	0	−0.571194	−0.434658	−2.332937
4	6	0	−1.268448	0.507709	−1.517147
5	6	0	−0.576962	1.793037	−1.641519
6	6	0	−2.045036	−0.020107	−0.424781
7	6	0	−0.370153	−1.764229	−1.935146
8	6	0	1.590678	−0.404731	−3.507357
9	6	0	1.627460	2.327778	−2.722350
10	6	0	−0.303062	2.732931	−0.621108
11	6	0	−1.385065	1.415662	1.259713
12	6	0	−0.609018	2.469220	0.798855
13	6	0	1.925764	3.248204	−1.651294
14	6	0	0.990950	3.420946	−0.627978
15	6	0	2.861543	1.660350	−3.110660
16	6	0	2.846538	0.318016	−3.490305
17	6	0	1.835607	−1.767835	−3.063068
18	6	0	0.880128	−2.416538	−2.271703
19	6	0	−1.353491	−1.170231	0.282850
20	6	0	−0.675609	−2.084067	−0.552341
21	6	0	0.355080	−2.963038	−0.058709
22	6	0	1.317103	−3.186524	−1.119307
23	6	0	3.344630	3.142586	−1.352455
24	6	0	3.921938	2.158413	−2.253764
25	6	0	3.874121	−0.589836	−3.013133
26	6	0	3.244830	−1.874469	−2.739826
27	6	0	0.517205	2.884773	1.588611
28	6	0	1.482350	3.527050	0.735209
29	6	0	−0.783874	0.436547	2.136113
30	6	0	−0.814592	−0.950242	1.644249
31	6	0	0.920814	2.134388	2.691974
32	6	0	0.286010	0.857369	2.938744
33	6	0	2.841958	3.427637	1.030892
34	6	0	3.800271	3.231402	−0.036856
35	6	0	4.914023	1.288315	−1.796524
36	6	0	4.886269	−0.114285	−2.179792
37	6	0	3.662636	−2.633767	−1.642119
38	6	0	2.673397	−3.294633	−0.812548
39	6	0	0.185467	−1.827839	2.117286
40	6	0	0.768494	−2.843899	1.260946
41	6	0	2.175906	−2.994823	1.590454
42	6	0	3.108987	−3.200175	0.572498
43	6	0	4.712154	−2.131585	−0.770840
44	6	0	5.316097	−0.901981	−1.036517
45	6	0	5.370660	1.367152	−0.418660
46	6	0	4.825603	2.319242	0.443096
47	6	0	3.275781	2.644616	2.179768
48	6	0	2.335139	2.010568	2.994452
49	6	0	1.303767	−0.052931	3.403999
50	6	0	1.245211	−1.380398	3.010698
51	6	0	4.376850	−2.492953	0.597621
52	6	0	5.612667	0.014076	0.051892
53	6	0	4.501797	1.958012	1.814083
54	6	0	2.572459	0.652471	3.449418
55	6	0	2.472439	−2.082689	2.674259
56	6	0	4.732280	0.654594	2.264231
57	6	0	3.746674	−0.010793	3.098247
58	6	0	5.300755	−0.336013	1.367161
59	6	0	4.662228	−1.612926	1.642866
60	6	0	3.696075	−1.410276	2.708897
61	12	0	−3.582682	−2.067303	0.106504
62	35	0	−4.441450	−4.331388	0.244204
63	16	0	−3.929196	0.757672	1.434111
64	8	0	−3.709942	1.425651	2.714499
65	8	0	−4.237793	−0.714544	1.496232
66	6	0	−5.243750	1.551943	0.539392
67	6	0	−5.020222	2.807838	−0.034233
68	6	0	−6.503336	0.949044	0.516732
69	6	0	−6.083518	3.454057	−0.655716
70	1	0	−4.035565	3.261689	−0.013259
71	6	0	−7.552320	1.619751	−0.109361
72	1	0	−6.663306	−0.021084	0.973825
73	6	0	−7.361675	2.873266	−0.707865
74	1	0	−5.917245	4.426176	−1.111289
75	1	0	−8.534473	1.156487	−0.133162
76	6	0	−8.493503	3.574682	−1.415768
77	1	0	−8.448257	4.657605	−1.262671
78	1	0	−8.440442	3.396997	−2.497686
79	1	0	−9.466690	3.214987	−1.069706
80	7	0	−2.518944	0.999887	0.488932
81	6	0	−3.980971	−0.555258	−1.603044
82	1	0	−4.981228	−0.852587	−1.227591
83	1	0	−4.020347	0.530610	−1.665263
84	6	0	−3.735751	−1.171832	−2.974631
85	1	0	−2.783429	−0.843592	−3.400085
86	1	0	−3.738647	−2.268145	−2.957688
87	1	0	−4.519932	−0.856878	−3.680250

TS(1-Cβ) (energy and imaginary frequency are in Table S4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.408210	−2.691755	1.528994
2	6	0	0.497426	−1.765918	2.642514
3	6	0	−0.522540	−0.769602	2.468348
4	6	0	−1.437651	−1.161102	1.377451
5	6	0	−0.665190	−2.262071	0.633220
6	6	0	−1.982916	−0.042465	0.644413
7	6	0	−0.235246	0.561605	2.733606
8	6	0	1.733303	−1.437395	3.204295
9	6	0	1.576894	−3.289305	1.057905
10	6	0	−0.489500	−2.433092	−0.753007
11	6	0	−1.664757	−0.334321	−1.588197
12	6	0	−0.901981	−1.475256	−1.823191
13	6	0	1.755854	−3.468109	−0.360161
14	6	0	0.756059	−3.043182	−1.232916
15	6	0	2.870017	−2.957900	1.640827
16	6	0	2.947100	−2.038486	2.683103

17	6	0	2.019592	−0.054713	3.529891
18	6	0	1.055381	0.926822	3.286552
19	6	0	−1.350394	1.241913	0.640959
20	6	0	−0.640801	1.609768	1.799673
21	6	0	0.395491	2.587482	1.772114
22	6	0	1.443723	2.194564	2.704276
23	6	0	3.158166	−3.246656	−0.673453
24	6	0	3.843750	−2.917879	0.563977
25	6	0	3.988669	−1.025693	2.688776
26	6	0	3.411546	0.203669	3.206860
27	6	0	0.154118	−1.407548	−2.780606
28	6	0	1.146742	−2.408523	−2.474183
29	6	0	−1.061332	0.963997	−1.815411
30	6	0	−0.983359	1.856164	−0.647896
31	6	0	0.526336	−0.179812	−3.336377
32	6	0	−0.056845	1.028503	−2.799890
33	6	0	2.484612	−2.183435	−2.785441
34	6	0	3.517847	−2.605408	−1.859622
35	6	0	4.849050	−1.947419	0.567025
36	6	0	4.917915	−0.978132	1.648780
37	6	0	3.783576	1.432685	2.653827
38	6	0	2.777341	2.450790	2.398867
39	6	0	0.034685	2.841599	−0.640567
40	6	0	0.716004	3.232608	0.576701
41	6	0	2.107616	3.507840	0.271992
42	6	0	3.120417	3.130944	1.159953
43	6	0	4.750100	1.482560	1.573471
44	6	0	5.308543	0.300895	1.081570
45	6	0	5.206510	−1.267459	−0.666350
46	6	0	4.558485	−1.594641	−1.858606
47	6	0	2.884289	−0.908615	−3.365424
48	6	0	1.925922	0.074001	−3.627131
49	6	0	0.974830	2.035669	−2.769894
50	6	0	1.010364	2.938727	−1.717466
51	6	0	4.340181	2.532949	0.651188
52	6	0	5.489923	0.121928	−0.348843
53	6	0	4.161200	−0.542190	−2.782726
54	6	0	2.202875	1.458136	−3.291489
55	6	0	2.292165	3.333340	−1.153919
56	6	0	4.430434	0.793963	−2.474497
57	6	0	3.428399	1.813008	−2.732224
58	6	0	5.103423	1.132012	−1.231851
59	6	0	4.518574	2.362001	−0.722969
60	6	0	3.475120	2.777085	−1.644354
61	12	0	−3.612134	−2.379268	0.494648
62	35	0	−4.408948	−4.562886	−0.195358
63	16	0	−4.294780	0.080441	−0.857622
64	8	0	−4.965347	−0.821050	0.145983
65	8	0	−4.557127	−0.097185	−2.283547
66	6	0	−4.598976	1.747822	−0.353758
67	6	0	−4.875442	2.031068	0.988268
68	6	0	−4.527071	2.757096	−1.321607
69	6	0	−5.086840	3.355918	1.356171
70	1	0	−4.934477	1.236582	1.721631
71	6	0	−4.744320	4.072228	−0.925825
72	1	0	−4.318675	2.515965	−2.357969
73	6	0	−5.024905	4.393620	0.412822
74	1	0	−5.305113	3.587332	2.394636
75	1	0	−4.696321	4.863016	−1.668835
76	6	0	−5.281897	5.821108	0.822798
77	1	0	−4.690774	6.520604	0.224029
78	1	0	−6.339183	6.077766	0.676414
79	1	0	−5.048304	5.981109	1.879392
80	7	0	−2.643923	−0.457348	−0.562055
81	6	0	−2.959110	−2.184051	2.686575
82	1	0	−2.111443	−2.563133	3.253560
83	6	0	−3.692856	−1.046359	3.375173
84	1	0	−3.841210	−1.244014	4.445878
85	1	0	−3.131123	−0.105501	3.299563
86	1	0	−4.684357	−0.871672	2.941477
87	1	0	−3.616318	−3.069581	2.555797

TS(2–Cβ) (energy and imaginary frequency are in Table S4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.867587	−2.791342	1.477483
2	6	0	−0.715801	−3.179516	0.087573
3	6	0	0.479057	−2.556882	−0.409819
4	6	0	1.225577	−1.946458	0.706739
5	6	0	0.235075	−1.908294	1.857629
6	6	0	2.040320	−0.791265	0.329823
7	6	0	0.487044	−1.997352	−1.680087
8	6	0	−1.830970	−3.348913	−0.735133
9	6	0	−2.152991	−2.651262	1.997294
10	6	0	−0.028823	−0.856538	2.752565
11	6	0	1.515170	0.925208	1.786254
12	6	0	0.522126	0.531146	2.676484
13	6	0	−2.424530	−1.575447	2.915044
14	6	0	−1.395476	−0.703546	3.266955
15	6	0	−3.322985	−2.834123	1.149845
16	6	0	−3.164541	−3.162624	−0.194016
17	6	0	−1.810358	−2.807494	−2.078999
18	6	0	−0.673583	−2.133635	−2.536380
19	6	0	1.633251	0.013904	−0.819539
20	6	0	1.060394	−0.664457	−1.901979
21	6	0	0.245460	−0.003361	−2.868937
22	6	0	−0.817761	−0.903467	−3.289135
23	6	0	−3.763786	−1.077232	2.646713
24	6	0	−4.312908	−1.847979	1.545025
25	6	0	−3.972802	−2.505999	−1.206691
26	6	0	−3.131252	−2.281125	−2.371081
27	6	0	−0.539327	1.442059	2.966436
28	6	0	−1.702430	0.706080	3.396680
29	6	0	1.180019	1.894862	0.764716
30	6	0	1.336036	1.440654	−0.631731
31	6	0	−0.674632	2.623728	2.232441
32	6	0	0.168436	2.822286	1.075316
33	6	0	−2.977699	1.199871	3.137172
34	6	0	−4.034156	0.287968	2.743108
35	6	0	−5.095083	−1.216973	0.574199
36	6	0	−4.915893	−1.548607	−0.830148
37	6	0	−3.264902	−1.099732	−3.106710
38	6	0	−2.081833	−0.397655	−3.577527
39	6	0	0.544498	2.082853	−1.618969
40	6	0	0.012499	1.366250	−2.757390
41	6	0	−1.302904	1.891442	−3.077208
42	6	0	−2.330332	1.032043	−3.476136
43	6	0	−4.245362	−0.105354	−2.715681
44	6	0	−5.057494	−0.325823	−1.601434
45	6	0	−5.357924	0.209028	0.667542
46	6	0	−4.842372	0.946395	1.734599
47	6	0	−3.130622	2.430816	2.373430
48	6	0	−2.002778	3.122895	1.924825
49	6	0	−0.631688	3.453058	0.055396
50	6	0	−0.433563	3.104867	−1.272716
51	6	0	−3.668595	1.211699	−2.946501
52	6	0	−5.333300	0.760101	−0.676794
53	6	0	−4.277993	2.267972	1.500995
54	6	0	−1.973588	3.656093	0.575901
55	6	0	−1.580326	2.975678	−2.158348
56	6	0	−4.252093	2.795454	0.207132
57	6	0	−3.073946	3.501056	−0.264298
58	6	0	−4.786533	2.024848	−0.902659
59	6	0	−3.938048	2.256423	−2.060573
60	6	0	−2.872919	3.160358	−1.663251
61	12	0	3.625728	−2.501603	0.234601
62	35	0	4.728674	−2.828872	−1.893459
63	16	0	4.129392	0.180226	1.763295
64	8	0	4.695885	−1.145370	1.341147
65	8	0	4.268788	0.605710	3.152582
66	6	0	4.857602	1.407091	0.700387
67	6	0	5.294669	1.058829	−0.582598
68	6	0	4.928824	2.725232	1.164680
69	6	0	5.815247	2.058202	−1.400852
70	1	0	5.245265	0.034180	−0.936930
71	6	0	5.453297	3.703849	0.326179
72	1	0	4.593081	2.975031	2.164994
73	6	0	5.905175	3.389076	−0.964960
74	1	0	6.161690	1.795586	−2.396407
75	1	0	5.515930	4.728337	0.682257
76	6	0	6.501784	4.453721	−1.851081
77	1	0	6.412778	4.189892	−2.908960
78	1	0	6.018091	5.422610	−1.691824
79	1	0	7.569806	4.582916	−1.632468
80	7	0	2.491263	−0.044637	1.464417
81	6	0	2.398161	−3.809514	1.625607
82	1	0	1.420670	−4.278310	1.536018
83	1	0	3.100123	−4.520161	1.138862

84	6	0	2.800166	−3.547611	3.070812
85	1	0	2.724901	−4.462084	3.678926
86	1	0	3.831576	−3.187381	3.162456
87	1	0	2.148625	−2.799801	3.537372

TS(3-Cβ) (energy and imaginary frequency are in Table S4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.461609	−2.830705	1.104773
2	6	0	−1.017030	−3.253295	−0.167801
3	6	0	−0.180171	−2.724966	−1.209707
4	6	0	1.060465	−2.159326	−0.633221
5	6	0	0.725449	−2.014164	0.861682
6	6	0	1.562470	−1.018428	−1.365749
7	6	0	−0.763855	−2.192980	−2.351379
8	6	0	−2.398509	−3.367671	−0.342333
9	6	0	−1.329025	−2.587064	2.169553
10	6	0	0.971402	−0.921189	1.712182
11	6	0	1.942934	0.723507	0.020921
12	6	0	1.487865	0.419526	1.302759
13	6	0	−1.072981	−1.473399	3.046110
14	6	0	0.037027	−0.663358	2.813090
15	6	0	−2.770634	−2.708730	1.998706
16	6	0	−3.294123	−3.076387	0.762502
17	6	0	−3.004720	−2.860817	−1.556904
18	6	0	−2.200822	−2.274840	−2.537749
19	6	0	0.744596	−0.247121	−2.246184
20	6	0	−0.309502	−0.916576	−2.895165
21	6	0	−1.453826	−0.223315	−3.385915
22	6	0	−2.631758	−1.058540	−3.195035
23	6	0	−2.349595	−0.890070	3.425810
24	6	0	−3.398486	−1.647521	2.765949
25	6	0	−4.458740	−2.391349	0.229314
26	6	0	−4.276292	−2.253114	−1.206218
27	6	0	0.744190	1.408700	2.014943
28	6	0	−0.099932	0.766094	2.992825
29	6	0	1.202530	1.693843	−0.764908
30	6	0	0.647087	1.208744	−2.036480
31	6	0	0.330508	2.582501	1.377704
32	6	0	0.517159	2.694727	−0.050952
33	6	0	−1.316134	1.340025	3.351700
34	6	0	−2.473613	0.492831	3.565475
35	6	0	−4.520801	−0.987745	2.258316
36	6	0	−5.057523	−1.364262	0.960534
37	6	0	−4.692234	−1.083399	−1.849495
38	6	0	−3.852377	−0.474494	−2.868360
39	6	0	−0.490166	1.873592	−2.554687
40	6	0	−1.540574	1.163735	−3.257136
41	6	0	−2.818606	1.765285	−2.927653
42	6	0	−3.954270	0.970353	−2.739661
43	6	0	−5.314448	−0.015941	−1.089924
44	6	0	−5.496434	−0.153843	0.287831
45	6	0	−4.637083	0.454704	2.389512
46	6	0	−3.635898	1.180908	3.036834
47	6	0	−1.758772	2.561042	2.693164
48	6	0	−0.955469	3.162666	1.720561
49	6	0	−0.643913	3.355719	−0.593558
50	6	0	−1.130052	2.964579	−1.832916
51	6	0	−4.858347	1.253071	−1.640798
52	6	0	−5.239081	0.970388	1.171763
53	6	0	−3.191318	2.454576	2.489510
54	6	0	−1.556035	3.660560	0.496907
55	6	0	−2.566610	2.888636	−2.048416
56	6	0	−3.768017	2.947593	1.316053
57	6	0	−2.931328	3.560124	0.299107
58	6	0	−4.807790	2.188211	0.642559
59	6	0	−4.615170	2.333870	−0.791171
60	6	0	−3.448229	3.172081	−1.003850
61	12	0	3.660803	−2.303083	0.057789
62	35	0	5.063778	−2.332515	2.050991
63	16	0	4.059566	0.005294	−1.658825
64	8	0	3.751155	0.344634	−3.045939
65	8	0	4.765696	−1.303976	−1.408919
66	6	0	4.919828	1.330570	−0.861701
67	6	0	4.913334	2.582344	−1.486415
68	6	0	5.579062	1.114579	0.355242
69	6	0	5.587297	3.634306	−0.873077
70	1	0	4.404018	2.723828	−2.432822
71	6	0	6.239090	2.185682	0.946220
72	1	0	5.580737	0.140611	0.834328
73	6	0	6.254414	3.457319	0.348355
74	1	0	5.596371	4.607893	−1.353983
75	1	0	6.757518	2.028793	1.887888
76	6	0	6.962921	4.606215	1.019216
77	1	0	6.387798	4.959812	1.884320
78	1	0	7.947316	4.301354	1.389878
79	1	0	7.094591	5.450616	0.337266
80	7	0	2.616699	−0.333821	−0.661391
81	6	0	2.345275	−3.955059	−0.847144
82	1	0	1.475046	−4.537503	−0.550340
83	1	0	3.168476	−4.409156	−0.249986
84	6	0	2.643897	−4.034151	−2.336912
85	1	0	1.820616	−3.612791	−2.924998
86	1	0	3.552579	−3.484294	−2.613878
87	1	0	2.783911	−5.072809	−2.667180

TS(4-Cβ) (energy and imaginary frequency are in Table S4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−1.597121	−1.546872	3.027483
2	6	0	−1.042090	−0.381079	3.690388
3	6	0	−1.550346	0.782384	3.019054
4	6	0	−2.596197	0.387868	2.062658
5	6	0	−2.458966	−1.114442	1.925993
6	6	0	−2.740323	1.268158	0.917909
7	6	0	−0.712509	1.860548	2.769139
8	6	0	0.255405	−0.397084	4.205145
9	6	0	−0.829325	−2.708336	2.965332
10	6	0	−2.476332	−1.884444	0.748050
11	6	0	−2.705550	−0.023631	−0.981850
12	6	0	−2.513583	−1.361516	−0.651706
13	6	0	−0.849413	−3.499448	1.762138
14	6	0	−1.639255	−3.089830	0.689064
15	6	0	0.522119	−2.738897	3.507211
16	6	0	1.059120	−1.601036	4.103492
17	6	0	1.122039	0.743385	3.984016
18	6	0	0.647301	1.846936	3.268667
19	6	0	−1.586994	2.041650	0.465070
20	6	0	−0.705614	2.503426	1.450434
21	6	0	0.645010	2.861528	1.155622
22	6	0	1.491561	2.482552	2.276739
23	6	0	0.487333	−4.029390	1.544162
24	6	0	1.338098	−3.546348	2.617613
25	6	0	2.427710	−1.204837	3.820867
26	6	0	2.463980	0.246406	3.741559
27	6	0	−1.601865	−2.133840	−1.434842
28	6	0	−1.108482	−3.238216	−0.650639
29	6	0	−1.629075	0.689628	−1.635564
30	6	0	−1.093831	1.856594	−0.907043
31	6	0	−0.788702	−1.513759	−2.386995
32	6	0	−0.764379	−0.069722	−2.444558
33	6	0	0.171113	−3.736878	−0.876122
34	6	0	0.995034	−4.134469	0.248947
35	6	0	2.656491	−3.170790	2.346878
36	6	0	3.209489	−1.972077	2.956467
37	6	0	3.278705	0.870075	2.792015
38	6	0	2.781744	2.014497	2.045331
39	6	0	0.243880	2.239287	−1.181169
40	6	0	1.115399	2.765667	−0.152350
41	6	0	2.468029	2.293141	−0.387523
42	6	0	3.285738	1.923595	0.683925
43	6	0	4.091694	0.072598	1.894057
44	6	0	4.060230	−1.321157	1.975480
45	6	0	3.175323	−3.264142	0.992796
46	6	0	2.362101	−3.742475	−0.035575
47	6	0	1.028603	−3.098259	−1.865321
48	6	0	0.560464	−2.005578	−2.599368
49	6	0	0.595560	0.333841	−2.701211
50	6	0	1.086875	1.480570	−2.094854
51	6	0	4.098228	0.725218	0.592201
52	6	0	4.041788	−2.120324	0.762759
53	6	0	2.380262	−3.094728	−1.339349
54	6	0	1.421273	−0.857469	−2.812704
55	6	0	2.453722	1.497980	−1.597257

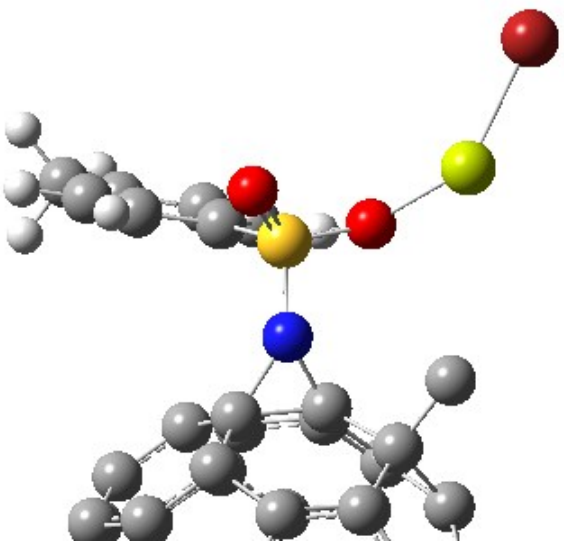
56	6	0	3.212135	−1.993194	−1.558545
57	6	0	2.719983	−0.851031	−2.308296
58	6	0	4.055109	−1.494546	−0.485294
59	6	0	4.084148	−0.043562	−0.572934
60	6	0	3.250234	0.355100	−1.693393
61	12	0	−4.414252	2.144513	2.351876
62	35	0	−4.614589	4.238548	3.562179
63	16	0	−4.803816	1.689918	−0.709213
64	8	0	−4.387377	2.771188	−1.606708
65	8	0	−5.461371	2.114942	0.579465
66	6	0	−5.864616	0.568504	−1.576725
67	6	0	−6.108569	0.800819	−2.931812
68	6	0	−6.448892	−0.508823	−0.900009
69	6	0	−6.954881	−0.068906	−3.617084
70	1	0	−5.645891	1.641542	−3.435868
71	6	0	−7.289261	−1.361146	−1.605412
72	1	0	−6.249726	−0.679063	0.151429
73	6	0	−7.558044	−1.156206	−2.970354
74	1	0	−7.147407	0.102918	−4.672072
75	1	0	−7.745587	−2.201275	−1.089498
76	6	0	−8.491251	−2.080715	−3.710577
77	1	0	−8.390540	−1.969618	−4.793720
78	1	0	−8.302036	−3.127245	−3.449378
79	1	0	−9.535059	−1.865859	−3.448264
80	7	0	−3.561469	0.705599	−0.120436
81	6	0	−4.531409	0.206804	3.540301
82	1	0	−3.793383	−0.315749	4.145613
83	1	0	−4.985874	0.959149	4.215346
84	6	0	−5.584654	−0.725956	2.960682
85	1	0	−6.068264	−1.336763	3.739140
86	1	0	−6.385850	−0.178956	2.447049
87	1	0	−5.142428	−1.425847	2.240864

Ring-opening process of 1+PhMgBr

INT1(Cβ1-adduct) (-6164.0431319 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.729621	2.749524	−1.492727
2	6	0	−0.608256	3.187175	−0.114506
3	6	0	0.502983	2.494860	0.471803
4	6	0	1.368152	1.859972	−0.621888
5	6	0	0.284866	1.746518	−1.770555
6	6	0	2.068569	0.547182	−0.053814
7	6	0	0.369896	1.974855	1.743477
8	6	0	−1.751725	3.498915	0.628975
9	6	0	−1.989894	2.729243	−2.092637
10	6	0	−0.020439	0.717132	−2.659743
11	6	0	1.285203	−1.160173	−1.535668
12	6	0	0.391080	−0.713227	−2.499350
13	6	0	−2.316053	1.658098	−2.993961
14	6	0	−1.359715	0.676369	−3.252107
15	6	0	−3.181048	3.062634	−1.326111
16	6	0	−3.064405	3.423096	0.013267
17	6	0	−1.862442	3.014433	1.985472
18	6	0	−0.824512	2.243246	2.518673
19	6	0	1.346814	−0.184423	1.016057
20	6	0	0.784687	0.584589	2.038257
21	6	0	−0.147023	0.048063	2.970226
22	6	0	−1.134678	1.063045	3.298434
23	6	0	−3.710236	1.303735	−2.791623
24	6	0	−4.242063	2.166041	−1.749848
25	6	0	−3.990966	2.888806	0.995474
26	6	0	−3.243090	2.628753	2.215170
27	6	0	−0.735694	−1.527843	−2.827589
28	6	0	−1.794450	−0.700540	−3.352463
29	6	0	0.790067	−2.061339	−0.520868
30	6	0	0.908104	−1.570840	0.864361
31	6	0	−1.033349	−2.666066	−2.071101
32	6	0	−0.283378	−2.903842	−0.861959
33	6	0	−3.126776	−1.057105	−3.159290
34	6	0	−4.109261	−0.032125	−2.861412
35	6	0	−5.136190	1.650449	−0.807943
36	6	0	−5.003750	2.015889	0.593812
37	6	0	−3.535754	1.493185	2.977459
38	6	0	−2.456388	0.696086	3.535656
39	6	0	0.006932	−2.104379	1.824173
40	6	0	−0.510398	−1.298340	2.900477
41	6	0	−1.886469	−1.677954	3.160689
42	6	0	−2.842132	−0.705649	3.468512
43	6	0	−4.586272	0.585987	2.560071
44	6	0	−5.309834	0.842829	1.393171
45	6	0	−5.533383	0.254622	−0.871844
46	6	0	−5.033476	−0.569327	−1.882174
47	6	0	−3.445359	−2.237107	−2.366900
48	6	0	−2.420207	−3.021605	−1.831039
49	6	0	−1.200303	−3.415704	0.128250
50	6	0	−1.045059	−3.042161	1.454163
51	6	0	−4.159583	−0.772636	2.867969
52	6	0	−5.638535	−0.245476	0.488755
53	6	0	−4.618346	−1.930721	−1.572355
54	6	0	−2.522844	−3.504138	−0.466073
55	6	0	−2.220572	−2.765932	2.264277
56	6	0	−4.720501	−2.409620	−0.263232
57	6	0	−3.649447	−3.211430	0.300799
58	6	0	−5.236268	−1.548588	0.787423
59	6	0	−4.482570	−1.818800	2.000822
60	6	0	−3.495607	−2.840043	1.698406
61	1	0	2.550641	3.992971	0.697953
62	6	0	2.995467	3.819758	−0.278537
63	6	0	4.101530	3.462257	−2.810177
64	6	0	4.056705	4.630571	−0.701164
65	6	0	2.478860	2.813023	−1.115543
66	6	0	3.043526	2.653777	−2.392908
67	6	0	4.613986	4.452358	−1.966987
68	1	0	4.432775	5.404577	−0.038571
69	1	0	2.653587	1.894831	−3.062236
70	1	0	5.434380	5.082343	−2.297612
71	1	0	4.523990	3.318958	−3.800641
72	12	0	4.056191	1.299623	0.658194
73	35	0	5.541660	1.976455	2.450912
74	16	0	3.928854	−0.931729	−1.464474
75	8	0	4.829829	0.025282	−0.735410
76	8	0	4.099831	−1.074274	−2.908847
77	6	0	4.166016	−2.533641	−0.714871
78	6	0	4.571154	−2.639345	0.620928
79	6	0	3.901717	−3.671139	−1.482789
80	6	0	4.709668	−3.904724	1.181914
81	1	0	4.794864	−1.757605	1.211512
82	6	0	4.045726	−4.927495	−0.898209
83	1	0	3.600723	−3.576313	−2.519965
84	6	0	4.448952	−5.066706	0.437271
85	1	0	5.030676	−3.990918	2.216336
86	1	0	3.842626	−5.813455	−1.493100
87	6	0	4.626211	−6.429746	1.058207
88	1	0	5.688960	−6.700882	1.099708
89	1	0	4.247381	−6.450247	2.085368
90	1	0	4.108961	−7.202636	0.482708
91	7	0	2.378253	−0.325189	−1.180200

INT2(5,6-close) (-6164.01394925 au)



(phenyl group except for ipso carbon is omitted for clarity)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.857598	−3.181361	−0.830873
2	6	0	0.680504	−3.187444	0.612424
3	6	0	−0.376286	−2.275069	0.938261
4	6	0	−1.139650	−1.868238	−0.335402
5	6	0	−0.097316	−2.283411	−1.412446
6	6	0	−1.401622	−0.326076	−0.388744
7	6	0	−0.272640	−1.484296	2.062105
8	6	0	1.783952	−3.342459	1.460641
9	6	0	2.142529	−3.363180	−1.368912
10	6	0	0.306588	−1.459852	−2.459076
11	6	0	−0.916358	0.526680	−1.581393
12	6	0	−0.101055	−0.073991	−2.629830
13	6	0	2.539995	−2.553110	−2.491524
14	6	0	1.642535	−1.621221	−3.021260
15	6	0	3.286318	−3.496163	−0.482327
16	6	0	3.117670	−3.500481	0.902149
17	6	0	1.882569	−2.531516	2.650729
18	6	0	0.869166	−1.607899	2.938010
19	6	0	−1.095487	0.512111	0.825310
20	6	0	−0.634260	−0.048026	2.000367
21	6	0	0.284735	0.671887	2.849748
22	6	0	1.217487	−0.284710	3.420851
23	6	0	3.934783	−2.190104	−2.323571
24	6	0	4.400028	−2.774337	−1.076641
25	6	0	4.037562	−2.763194	1.748391
26	6	0	3.274277	−2.169736	2.836613
27	6	0	1.028984	0.634899	−3.120053
28	6	0	2.098528	−0.317332	−3.425057
29	6	0	−0.438398	1.826879	−1.013758
30	6	0	−0.588384	1.799836	0.414969
31	6	0	1.382197	1.940121	−2.700140
32	6	0	0.637820	2.498767	−1.581024
33	6	0	3.439778	0.038162	−3.274694
34	6	0	4.374404	−0.919484	−2.703703
35	6	0	5.286803	−2.067216	−0.262711
36	6	0	5.103078	−2.060780	1.179917
37	6	0	3.605464	−0.893025	3.300919
38	6	0	2.554353	0.064969	3.608615
39	6	0	0.274370	2.534098	1.246929
40	6	0	0.731393	1.947167	2.481894
41	6	0	2.125112	2.309823	2.669204
42	6	0	3.018477	1.386905	3.217253
43	6	0	4.714344	−0.166101	2.716805
44	6	0	5.443686	−0.736476	1.667844
45	6	0	5.745789	−0.747704	−0.662347
46	6	0	5.296536	−0.186830	−1.859392
47	6	0	3.798232	1.363662	−2.808679
48	6	0	2.767702	2.269406	−2.497071
49	6	0	1.557808	3.235793	−0.730609
50	6	0	1.378631	3.257703	0.653629
51	6	0	4.348899	1.240876	2.658255
52	6	0	5.847692	0.072963	0.533101
53	6	0	4.928519	1.223898	−1.916574
54	6	0	2.883123	3.091076	−1.295881
55	6	0	2.527276	3.123540	1.533693
56	6	0	5.041661	2.015533	−0.768922
57	6	0	3.989146	2.965434	−0.454394
58	6	0	5.493885	1.424112	0.476899
59	6	0	4.734111	2.020250	1.563990
60	6	0	3.804014	2.974757	0.989336
61	12	0	−5.801440	−1.309977	0.289193
62	35	0	−8.055480	−1.215605	1.140754
63	16	0	−3.844580	0.852796	−1.129053
64	8	0	−4.446750	0.096669	0.039458
65	8	0	−4.582153	0.829209	−2.393831
66	6	0	−3.734047	2.543827	−0.579948
67	6	0	−3.812466	2.855506	0.778785
68	6	0	−3.574327	3.538877	−1.551021
69	6	0	−3.735355	4.193064	1.162517
70	1	0	−3.940770	2.074340	1.518622
71	6	0	−3.492437	4.865189	−1.142026
72	1	0	−3.532718	3.282826	−2.604055
73	6	0	−3.569029	5.214451	0.216771
74	1	0	−3.807743	4.444996	2.216575
75	1	0	−3.374346	5.643772	−1.890540
76	6	0	−3.465167	6.658157	0.640513
77	1	0	−2.442129	7.029556	0.501921
78	1	0	−4.122888	7.295283	0.039089
79	1	0	−3.728614	6.787505	1.693888
80	7	0	−2.393903	0.095399	−1.393309
81	6	0	−2.478747	−2.617039	−0.450779
82	6	0	−5.005469	−3.862425	−0.689837
83	6	0	−2.975874	−3.010268	−1.701291
84	6	0	−3.257514	−2.864361	0.686465
85	6	0	−4.515208	−3.480271	0.574030
86	6	0	−4.227176	−3.618998	−1.825266
87	1	0	−2.377841	−2.832690	−2.588638
88	1	0	−2.887065	−2.590703	1.669150
89	1	0	−5.067150	−3.745977	1.474129
90	1	0	−4.588420	−3.913950	−2.805594
91	1	0	−5.964415	−4.365761	−0.772797

TS(α1scission) (238.9i, -6163.99064668 au)

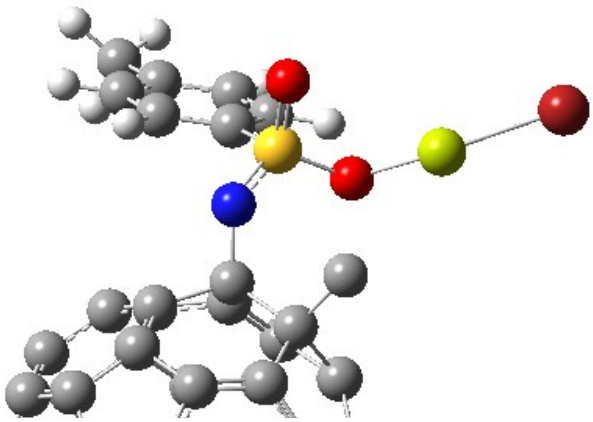
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.808477	−3.250217	0.222332
2	6	0	−0.713617	−3.028860	−1.210574
3	6	0	0.379260	−2.132690	−1.459211
4	6	0	1.237329	−1.975833	−0.173982
5	6	0	0.223211	−2.507164	0.877944
6	6	0	1.490564	−0.472198	0.092594
7	6	0	0.253593	−1.161870	−2.428150
8	6	0	−1.877361	−2.976860	−1.989006
9	6	0	−2.060892	−3.463753	0.817052
10	6	0	−0.044789	−1.874838	2.084475
11	6	0	1.310610	0.133223	1.462558
12	6	0	0.474497	−0.576795	2.458324
13	6	0	−2.333524	−2.842507	2.088351
14	6	0	−1.348080	−2.068333	2.707646
15	6	0	−3.263887	−3.382364	0.005905
16	6	0	−3.181625	−3.157408	−1.367872
17	6	0	−2.000126	−1.970839	−3.017840
18	6	0	−0.948403	−1.070124	−3.224439
19	6	0	1.261567	0.540984	−0.909105
20	6	0	0.701735	0.218840	−2.145765
21	6	0	−0.206697	1.123876	−2.784865
22	6	0	−1.238476	0.334784	−3.444300
23	6	0	−3.707207	−2.382272	2.084784
24	6	0	−4.287880	−2.716679	0.794391
25	6	0	−4.103202	−2.236089	−2.007018
26	6	0	−3.373910	−1.506463	−3.033356
27	6	0	−0.572495	0.097372	3.139159
28	6	0	−1.686438	−0.832257	3.358073
29	6	0	0.830236	1.548883	1.167723
30	6	0	0.870755	1.765227	−0.245217
31	6	0	−0.867561	1.474482	2.976620
32	6	0	−0.162302	2.170837	1.917082
33	6	0	−3.007740	−0.383848	3.364585
34	6	0	−4.036743	−1.174675	2.707230
35	6	0	−5.175163	−1.832324	0.179754
36	6	0	−5.081172	−1.585572	−1.250489
37	6	0	−3.647364	−0.152106	−3.247138
38	6	0	−2.555708	0.784491	−3.464374
39	6	0	0.021581	2.683225	−0.881394
40	6	0	−0.550240	2.334336	−2.156076
41	6	0	−1.921504	2.806460	−2.183808
42	6	0	−2.904738	2.041365	−2.814626
43	6	0	−4.665705	0.522208	−2.468699
44	6	0	−5.363150	−0.180499	−1.480426
45	6	0	−5.519371	−0.579198	0.830190
46	6	0	−4.959524	−0.259060	2.068991
47	6	0	−3.306937	1.020406	3.157615
48	6	0	−2.240431	1.908328	2.932039
49	6	0	−1.083365	3.096413	1.271391
50	6	0	−0.991454	3.353080	−0.096487
51	6	0	−4.204824	1.875394	−2.197690
52	6	0	−5.640026	0.440348	−0.197857
53	6	0	−4.497295	1.098522	2.339005
54	6	0	−2.377285	2.931067	1.899463
55	6	0	−2.198117	3.434504	−0.902400
56	6	0	−4.630301	2.082252	1.354056
57	6	0	−3.539354	3.013953	1.130742
58	6	0	−5.195782	1.739884	0.061409

59	6	0	−4.467042	2.471879	−0.960149
60	6	0	−3.444525	3.263374	−0.300496
61	12	0	4.632296	−1.380517	1.032087
62	35	0	5.936263	−1.313567	−1.034277
63	16	0	3.824224	1.182285	1.829731
64	8	0	5.150474	0.450151	1.822583
65	8	0	3.371733	1.741796	3.106508
66	6	0	3.973867	2.506427	0.642490
67	6	0	4.622378	2.284119	−0.576411
68	6	0	3.446293	3.757486	0.972342
69	6	0	4.725951	3.340551	−1.476807
70	1	0	5.057170	1.317779	−0.812342
71	6	0	3.568505	4.798979	0.056276
72	1	0	2.955403	3.910318	1.926262
73	6	0	4.199644	4.608359	−1.182035
74	1	0	5.233692	3.177290	−2.423478
75	1	0	3.167262	5.776218	0.309810
76	6	0	4.296227	5.732598	−2.182839
77	1	0	5.224574	5.674494	−2.759768
78	1	0	3.464876	5.684657	−2.898274
79	1	0	4.251816	6.709857	−1.693120
80	7	0	2.830692	−0.104032	1.368545
81	6	0	2.478664	−2.892142	−0.212351
82	6	0	4.578929	−4.780914	−0.219935
83	6	0	3.042946	−3.349761	0.999876
84	6	0	2.995632	−3.382820	−1.414756
85	6	0	4.028339	−4.325269	−1.415882
86	6	0	4.089615	−4.285641	0.991924
87	1	0	2.593450	−3.059913	1.946507
88	1	0	2.583100	−3.042543	−2.358069
89	1	0	4.404334	−4.698445	−2.363505
90	1	0	4.489382	−4.646265	1.935471
91	1	0	5.377404	−5.515949	−0.226502

TS(α2scission) (103.1i, -6164.01392188 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.845755	−3.186374	−0.808472
2	6	0	0.658208	−3.174008	0.633192
3	6	0	−0.394534	−2.250370	0.940197
4	6	0	−1.147073	−1.854163	−0.342966
5	6	0	−0.099532	−2.288733	−1.406728
6	6	0	−1.403507	−0.308026	−0.420937
7	6	0	−0.295621	−1.449200	2.056745
8	6	0	1.754150	−3.326379	1.491373
9	6	0	2.133518	−3.379766	−1.334907
10	6	0	0.318024	−1.479802	−2.457986
11	6	0	−0.883258	0.521094	−1.601251
12	6	0	−0.078921	−0.090775	−2.640691
13	6	0	2.544061	−2.584579	−2.463425
14	6	0	1.655635	−1.653140	−3.009459
15	6	0	3.270188	−3.510227	−0.438512
16	6	0	3.090898	−3.498072	0.944494
17	6	0	1.848671	−2.503126	2.673250
18	6	0	0.839044	−1.570110	2.942259
19	6	0	−1.099670	0.538387	0.793280
20	6	0	−0.649186	−0.011910	1.976879
21	6	0	0.268770	0.711732	2.825246
22	6	0	1.191490	−0.243974	3.413780
23	6	0	3.939578	−2.227730	−2.288793
24	6	0	4.392273	−2.801261	−1.032201
25	6	0	4.009131	−2.757517	1.789842
26	6	0	3.241220	−2.147511	2.865509
27	6	0	1.057697	0.607020	−3.137303
28	6	0	2.122105	−0.355453	−3.424142
29	6	0	−0.414567	1.825919	−1.053648
30	6	0	−0.578582	1.817581	0.374030
31	6	0	1.415703	1.913387	−2.728162
32	6	0	0.666767	2.489666	−1.622253
33	6	0	3.464705	−0.006823	−3.267544
34	6	0	4.389326	−0.963832	−2.679167
35	6	0	5.277269	−2.090693	−0.219371
36	6	0	5.082800	−2.067584	1.221583
37	6	0	3.576576	−0.868023	3.318638
38	6	0	2.529107	0.099562	3.608041
39	6	0	0.282099	2.556237	1.203068
40	6	0	0.726217	1.980224	2.447754
41	6	0	2.120697	2.336514	2.641266
42	6	0	3.004324	1.414244	3.205831
43	6	0	4.694054	−0.154142	2.734569
44	6	0	5.428000	−0.740233	1.697905
45	6	0	5.747223	−0.778360	−0.629824
46	6	0	5.309916	−0.227768	−1.836096
47	6	0	3.827806	1.321238	−2.812472
48	6	0	2.802354	2.237729	−2.519392
49	6	0	1.584510	3.230679	−0.772954
50	6	0	1.395259	3.266772	0.609658
51	6	0	4.337969	1.254515	2.658549
52	6	0	5.845100	0.054610	0.557285
53	6	0	4.951602	1.184324	−1.911124
54	6	0	2.913442	3.071830	−1.326549
55	6	0	2.536272	3.135176	1.499841
56	6	0	5.060422	1.987465	−0.771392
57	6	0	4.012054	2.947795	−0.475124
58	6	0	5.500358	1.407130	0.484191
59	6	0	4.736128	2.019584	1.558900
60	6	0	3.816247	2.973468	0.966936
61	12	0	−5.807202	−1.299674	0.292617
62	35	0	−8.061263	−1.207308	1.144724
63	16	0	−3.850807	0.850102	−1.132675
64	8	0	−4.451111	0.102520	0.045444
65	8	0	−4.610784	0.833075	−2.385342
66	6	0	−3.728224	2.541373	−0.581937
67	6	0	−3.811942	2.854564	0.775934
68	6	0	−3.553024	3.535475	−1.551212
69	6	0	−3.724219	4.191364	1.160788
70	1	0	−3.952092	2.074497	1.514713
71	6	0	−3.461069	4.861122	−1.141734
72	1	0	−3.507229	3.279503	−2.604165
73	6	0	−3.542748	5.211274	0.216566
74	1	0	−3.800302	4.443618	2.214573
75	1	0	−3.331030	5.638614	−1.889465
76	6	0	−3.428572	6.654038	0.641362
77	1	0	−2.403273	7.019022	0.502526
78	1	0	−4.082583	7.296209	0.041173
79	1	0	−3.690653	6.784218	1.695010
80	7	0	−2.411249	0.097122	−1.421957
81	6	0	−2.487039	−2.601844	−0.455996
82	6	0	−5.011552	−3.852864	−0.690415
83	6	0	−2.985764	−2.996167	−1.705611
84	6	0	−3.263166	−2.851207	0.682477
85	6	0	−4.519889	−3.469746	0.572380
86	6	0	−4.235720	−3.607899	−1.827270
87	1	0	−2.390047	−2.817327	−2.594228
88	1	0	−2.892046	−2.576796	1.664589
89	1	0	−5.069670	−3.736407	1.473504
90	1	0	−4.598061	−3.903576	−2.806973
91	1	0	−5.969609	−4.358134	−0.771801

INT3 (-6164.05621247 au)



(phenyl group except for ipso carbon is omitted for clarity)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.498593	−3.049241	−0.709944
2	6	0	0.060212	−2.794255	0.648410
3	6	0	−0.861508	−1.689874	0.623819
4	6	0	−1.301028	−1.391039	−0.825096
5	6	0	−0.146901	−2.099640	−1.574338

6	6	0	−1.416444	0.226371	−1.161441
7	6	0	−0.824299	−0.766291	1.643718
8	6	0	0.944682	−2.984564	1.715960
9	6	0	1.807698	−3.481498	−0.952634
10	6	0	0.556879	−1.560880	−2.625887
11	6	0	−0.325516	0.703460	−2.148574
12	6	0	0.463268	−0.113621	−2.922563
13	6	0	2.538360	−2.929761	−2.066704
14	6	0	1.920346	−1.972010	−2.878550
15	6	0	2.731839	−3.658650	0.155821
16	6	0	2.309685	−3.415824	1.461737
17	6	0	0.966986	−2.025263	2.792158
18	6	0	0.102978	−0.926574	2.742685
19	6	0	−1.045317	1.116045	0.049704
20	6	0	−0.918684	0.680747	1.347699
21	6	0	−0.045736	1.371628	2.271637
22	6	0	0.582091	0.386685	3.132810
23	6	0	3.919738	−2.753910	−1.658313
24	6	0	4.041447	−3.207154	−0.281602
25	6	0	3.177419	−2.709800	2.388369
26	6	0	2.344642	−1.848561	3.212345
27	6	0	1.773002	0.326726	−3.352666
28	6	0	2.670713	−0.813290	−3.326917
29	6	0	0.176203	1.987967	−1.747312
30	6	0	−0.263428	2.240940	−0.388311
31	6	0	2.248459	1.593826	−2.998921
32	6	0	1.427530	2.445756	−2.173615
33	6	0	4.004052	−0.650053	−2.949236
34	6	0	4.638706	−1.636815	−2.089437
35	6	0	4.875536	−2.525174	0.606720
36	6	0	4.434902	−2.271634	1.969244
37	6	0	2.804167	−0.583204	3.583755
38	6	0	1.901822	0.557191	3.551886
39	6	0	0.563999	2.943150	0.494230
40	6	0	0.676816	2.496848	1.861715
41	6	0	2.054972	2.668607	2.281190
42	6	0	2.657055	1.718394	3.109501
43	6	0	4.110919	−0.129462	3.150226
44	6	0	4.910693	−0.955851	2.357433
45	6	0	5.623186	−1.365018	0.155009
46	6	0	5.506203	−0.931131	−1.167287
47	6	0	4.491250	0.664821	−2.564384
48	6	0	3.629693	1.764123	−2.589917
49	6	0	2.295231	3.158792	−1.250045
50	6	0	1.872811	3.400892	0.055943
51	6	0	4.019930	1.293777	2.856911
52	6	0	5.645918	−0.395451	1.236743
53	6	0	5.415625	0.491935	−1.461235
54	6	0	3.660451	2.734476	−1.506705
55	6	0	2.796877	3.229744	1.163254
56	6	0	5.445097	1.422654	−0.420216
57	6	0	4.549793	2.565956	−0.443509
58	6	0	5.558899	0.969125	0.955423
59	6	0	4.732508	1.831682	1.782643
60	6	0	4.108774	2.818550	0.919009
61	12	0	−5.435577	−1.227743	0.476776
62	35	0	−7.219736	−2.136771	1.819666
63	16	0	−3.966653	0.992730	−1.025364
64	8	0	−4.173460	0.243885	0.319262
65	8	0	−5.162753	0.849362	−1.891691
66	6	0	−3.905495	2.716802	−0.501437
67	6	0	−4.410137	3.119103	0.735932
68	6	0	−3.396451	3.658606	−1.401152
69	6	0	−4.398097	4.473698	1.070356
70	1	0	−4.800762	2.383606	1.429917
71	6	0	−3.397236	5.006923	−1.053579
72	1	0	−2.994766	3.337526	−2.356892
73	6	0	−3.893183	5.437483	0.187061
74	1	0	−4.788335	4.784962	2.036073
75	1	0	−3.001920	5.737208	−1.755192
76	6	0	−3.855601	6.897921	0.568062
77	1	0	−2.867430	7.175299	0.958012
78	1	0	−4.054062	7.541378	−0.295497
79	1	0	−4.590999	7.127933	1.345076
80	7	0	−2.685948	0.576497	−1.805731
81	6	0	−2.599919	−2.140015	−1.177482
82	6	0	−4.967688	−3.531989	−1.866044
83	6	0	−3.039795	−2.209943	−2.506367
84	6	0	−3.348220	−2.814466	−0.199050
85	6	0	−4.524520	−3.506787	−0.536432
86	6	0	−4.212476	−2.887823	−2.846537
87	1	0	−2.469237	−1.716833	−3.284920
88	1	0	−3.003946	−2.830593	0.831325
89	1	0	−5.052676	−4.072768	0.226459
90	1	0	−4.532868	−2.912447	−3.883776
91	1	0	−5.873359	−4.069845	−2.128888

INT2'(5,6-close, rotated)(-6164.03264452 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.369375	−0.378454	−2.884671
2	6	0	0.619749	−1.771201	−2.559721
3	6	0	−0.206965	−2.123994	−1.442871
4	6	0	−1.276127	−1.037064	−1.206037
5	6	0	−0.624572	0.139981	−1.984646
6	6	0	−1.384794	−0.681265	0.307179
7	6	0	0.293299	−2.949674	−0.460443
8	6	0	1.902993	−2.310657	−2.707119
9	6	0	1.411603	0.414420	−3.381211
10	6	0	−0.491298	1.433826	−1.509984
11	6	0	−1.189331	0.766812	0.783729
12	6	0	−0.902083	1.905144	−0.152580
13	6	0	1.533743	1.767423	−2.909977
14	6	0	0.608423	2.252060	−1.979801
15	6	0	2.748889	−0.141564	−3.510998
16	6	0	2.992870	−1.475686	−3.187674
17	6	0	2.421893	−3.191494	−1.688524
18	6	0	1.628527	−3.491129	−0.574610
19	6	0	−0.675404	−1.524573	1.337101
20	6	0	0.064407	−2.629934	0.967538
21	6	0	1.258369	−2.994693	1.696163
22	6	0	2.225002	−3.521345	0.747879
23	6	0	2.943991	2.070838	−2.748646
24	6	0	3.698789	0.886190	−3.121757
25	6	0	4.186687	−1.837030	−2.448387
26	6	0	3.833595	−2.902267	−1.519926
27	6	0	0.212625	2.781518	0.256448
28	6	0	1.046112	3.085966	−0.885891
29	6	0	−0.448665	0.691048	2.085910
30	6	0	−0.188690	−0.685010	2.403559
31	6	0	0.791508	2.773244	1.525298
32	6	0	0.456419	1.670766	2.440725
33	6	0	2.404692	3.393880	−0.733301
34	6	0	3.371458	2.864096	−1.682061
35	6	0	4.849318	0.539381	−2.409866
36	6	0	5.098491	−0.850082	−2.065785
37	6	0	4.403788	−2.929539	−0.245653
38	6	0	3.584120	−3.253730	0.911057
39	6	0	0.947600	−1.039451	3.147243
40	6	0	1.692990	−2.217202	2.775178
41	6	0	3.106944	−1.929168	2.940751
42	6	0	4.032004	−2.433604	2.025694
43	6	0	5.351925	−1.905586	0.151828
44	6	0	5.689720	−0.883265	−0.739636
45	6	0	5.291506	1.364588	−1.298809
46	6	0	4.567126	2.505098	−0.944555
47	6	0	3.000859	3.377283	0.581394
48	6	0	2.199160	3.042816	1.683231
49	6	0	1.646369	1.318927	3.187686
50	6	0	1.888658	−0.012467	3.535949
51	6	0	5.119257	−1.596898	1.552819
52	6	0	5.811938	0.484043	−0.267360
53	6	0	4.332946	2.815239	0.459657
54	6	0	2.728302	2.160011	2.713853
55	6	0	3.228175	−0.559685	3.414847
56	6	0	4.837898	1.969659	1.449089
57	6	0	4.016824	1.638161	2.602014
58	6	0	5.585021	0.781247	1.079102
59	6	0	5.234686	−0.280354	2.007548
60	6	0	4.268236	0.248283	2.951973
61	1	0	−2.663092	−3.329778	−0.645813
62	6	0	−3.186021	−2.712772	−1.371791
63	6	0	−4.536717	−1.163143	−3.252819
64	6	0	−4.401596	−3.152501	−1.895278
65	6	0	−2.630289	−1.492866	−1.782885
66	6	0	−3.317585	−0.723788	−2.728499
67	6	0	−5.081422	−2.379160	−2.840104
68	1	0	−4.814452	−4.102757	−1.568357

69	1	0	−2.895127	0.217030	−3.067782
70	1	0	−6.025544	−2.724191	−3.252188
71	1	0	−5.054415	−0.552833	−3.987754
72	12	0	−3.059389	2.571397	0.086090
73	35	0	−4.836691	3.935230	−0.848096
74	16	0	−3.661999	0.247779	1.945043
75	8	0	−3.927101	1.729950	1.831480
76	8	0	−3.198331	−0.265748	3.233603
77	6	0	−5.115527	−0.630938	1.436642
78	6	0	−6.041668	−0.022076	0.581950
79	6	0	−5.311867	−1.922754	1.933299
80	6	0	−7.178084	−0.737604	0.219943
81	1	0	−5.893393	0.990863	0.222176
82	6	0	−6.457628	−2.616579	1.553806
83	1	0	−4.590632	−2.370401	2.607887
84	6	0	−7.405557	−2.039677	0.695719
85	1	0	−7.904888	−0.273121	−0.440408
86	1	0	−6.618439	−3.620966	1.934826
87	6	0	−8.658145	−2.786367	0.311825
88	1	0	−9.504197	−2.464775	0.932748
89	1	0	−8.931062	−2.595172	−0.730953
90	1	0	−8.539425	−3.865039	0.448255
91	7	0	−2.563725	0.154473	0.652259

TS'(α2scission) (274.3i, -6164.03070335 au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.344691	0.192354	2.893391
2	6	0	−0.523179	−1.246043	2.811841
3	6	0	0.319642	−1.741042	1.762391
4	6	0	1.332437	−0.661302	1.335162
5	6	0	0.623094	0.594395	1.910640
6	6	0	1.443709	−0.551154	−0.227461
7	6	0	−0.129506	−2.753038	0.945006
8	6	0	−1.776840	−1.816763	3.058591
9	6	0	−1.429145	1.006408	3.244204
10	6	0	0.416667	1.771212	1.213941
11	6	0	1.079660	0.734949	−0.921784
12	6	0	0.772921	1.977233	−0.216104
13	6	0	−1.618691	2.248863	2.543727
14	6	0	−0.717213	2.610435	1.536484
15	6	0	−2.736310	0.413726	3.476294
16	6	0	−2.909590	−0.967382	3.393097
17	6	0	−2.246340	−2.886560	2.210780
18	6	0	−1.435300	−3.334007	1.161123
19	6	0	0.777713	−1.619248	−1.083484
20	6	0	0.089328	−2.674510	−0.517953
21	6	0	−1.084403	−3.223355	−1.162983
22	6	0	−2.025362	−3.624031	−0.131483
23	6	0	−3.041964	2.445382	2.338355
24	6	0	−3.736350	1.307420	2.918122
25	6	0	−4.080726	−1.513727	2.734657
26	6	0	−3.670195	−2.704319	2.003591
27	6	0	−0.342398	2.757169	−0.768519
28	6	0	−1.191103	3.215889	0.313257
29	6	0	0.413087	0.415344	−2.198415
30	6	0	0.236323	−1.008142	−2.272832
31	6	0	−0.922167	2.500073	−2.014466
32	6	0	−0.534298	1.277402	−2.722268
33	6	0	−2.563925	3.416985	0.117179
34	6	0	−3.505291	3.014671	1.150517
35	6	0	−4.865127	0.782216	2.286020
36	6	0	−5.041337	−0.657398	2.191518
37	6	0	−4.235719	−2.984259	0.757980
38	6	0	−3.396798	−3.462517	−0.329774
39	6	0	−0.875741	−1.542928	−2.936718
40	6	0	−1.558887	−2.673219	−2.358825
41	6	0	−2.985582	−2.491377	−2.563275
42	6	0	−3.884567	−2.874177	−1.567143
43	6	0	−5.235154	−2.096499	0.194471
44	6	0	−5.626902	−0.952388	0.895494
45	6	0	−5.345815	1.376109	1.050204
46	6	0	−4.679646	2.471472	0.496156
47	6	0	−3.158488	3.142257	−1.170817
48	6	0	−2.342217	2.666798	−2.206350
49	6	0	−1.699521	0.737396	−3.392600
50	6	0	−1.868809	−0.646346	−3.491357
51	6	0	−5.015237	−2.025609	−1.240702
52	6	0	−5.818071	0.303462	0.192222
53	6	0	−4.460443	2.543213	−0.942013
54	6	0	−2.824694	1.591551	−3.064853
55	6	0	−3.177180	−1.233454	−3.267716
56	6	0	−4.920119	1.513480	−1.764815
57	6	0	−4.082590	1.029069	−2.849207
58	6	0	−5.605591	0.371470	−1.186951
59	6	0	−5.199111	−0.816894	−1.917648
60	6	0	−4.259239	−0.412149	−2.946771
61	12	0	3.085421	2.386343	−0.541423
62	35	0	4.526425	4.078100	0.404319
63	16	0	3.718828	−0.049568	−1.976749
64	8	0	4.108995	1.402650	−2.140865
65	8	0	3.156700	−0.749490	−3.132825
66	6	0	5.142887	−0.933809	−1.389775
67	6	0	6.142175	−0.257751	−0.679695
68	6	0	5.237634	−2.299848	−1.666429
69	6	0	7.250414	−0.975494	−0.245154
70	1	0	6.066760	0.807370	−0.489317
71	6	0	6.357908	−2.996543	−1.218113
72	1	0	4.461238	−2.802634	−2.232364
73	6	0	7.376685	−2.351555	−0.502846
74	1	0	8.035523	−0.457472	0.298666
75	1	0	6.442816	−4.057561	−1.434497
76	6	0	8.589276	−3.107755	−0.020770
77	1	0	8.548324	−4.160509	−0.313010
78	1	0	9.509525	−2.674961	−0.430351
79	1	0	8.671099	−3.059894	1.071656
80	7	0	2.670399	0.185187	−0.677101
81	6	0	2.698167	−0.959059	1.984889
82	6	0	5.156307	−1.565800	3.210503
83	6	0	3.342649	−0.016587	2.793677
84	6	0	3.300849	−2.211120	1.796050
85	6	0	4.519431	−2.512384	2.403628
86	6	0	4.565652	−0.316413	3.400608
87	1	0	2.883805	0.952741	2.963870
88	1	0	2.812160	−2.961837	1.180842
89	1	0	4.968539	−3.489428	2.249223
90	1	0	5.049013	0.428184	4.027041
91	1	0	6.102514	−1.802798	3.688776