Supporting Information

Density Functional Theory Study of the Mechanism and Origins of Stereoselectivity in the Asymmetric Simmons–Smith Cyclopropanation with Charette Chiral Dioxaborolane Ligand

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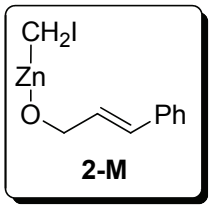
Content

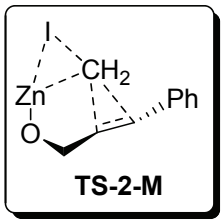
1. Coordinates of All Stationary Points



2-M

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-0.736185	1.004271	-0.164624
2	8	0	-0.312503	2.713624	0.213053
3	6	0	1.058678	3.061241	0.162481
4	6	0	1.940647	1.893993	0.523436
5	6	0	2.743870	1.259594	-0.351735
6	6	0	-1.415304	-0.776680	-0.538529
7	53	0	-3.554887	-0.879569	0.066012
8	6	0	3.587139	0.077406	-0.118719
9	6	0	4.269620	-0.492517	-1.208297
10	6	0	5.074196	-1.619837	-1.047726
11	6	0	5.216432	-2.202473	0.212234
12	6	0	4.550063	-1.644757	1.308292
13	6	0	3.747629	-0.519113	1.146651
14	1	0	1.339517	3.435781	-0.837019
15	1	0	1.226519	3.888173	0.870660
16	1	0	1.851410	1.545582	1.553471
17	1	0	2.791395	1.658122	-1.367146
18	1	0	-1.420791	-1.048691	-1.593887
19	1	0	-0.935045	-1.572253	0.030912
20	1	0	4.162538	-0.043007	-2.193030
21	1	0	5.589670	-2.041819	-1.906283
22	1	0	5.843168	-3.080332	0.342595
23	1	0	4.660773	-2.088073	2.294363
24	1	0	3.247615	-0.094593	2.012470



Imaginary frequency: -277.6 cm^{-1}

Standard orientation:

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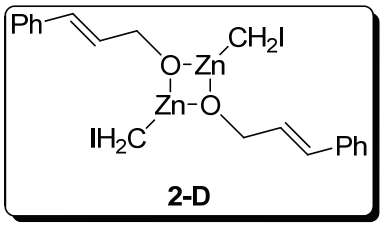
1	30	0	-1.467498	1.078383	0.115809
2	8	0	-0.943282	2.834309	0.259111
3	6	0	0.370965	2.912354	-0.251605
4	6	0	1.303903	1.795143	0.185723
5	6	0	2.161005	1.124514	-0.627531
6	6	0	-0.161513	-0.340045	-0.289373
7	53	0	-2.864797	-1.215278	-0.010936
8	6	0	3.222753	0.183847	-0.243827
9	6	0	3.938123	-0.478848	-1.258021
10	6	0	4.952276	-1.384511	-0.951503
11	6	0	5.276242	-1.646249	0.380629
12	6	0	4.580739	-0.989693	1.401193
13	6	0	3.569782	-0.083611	1.094866
14	1	0	0.391467	2.979616	-1.355282
15	1	0	0.819813	3.851820	0.118992
16	1	0	1.332215	1.629672	1.263274
17	1	0	2.096784	1.332089	-1.696924
18	1	0	0.044147	-0.697833	-1.303241
19	1	0	0.304191	-1.000735	0.446809
20	1	0	3.689282	-0.280009	-2.298054
21	1	0	5.489033	-1.884831	-1.752872
22	1	0	6.066750	-2.350580	0.623916
23	1	0	4.833222	-1.180655	2.440722
24	1	0	3.052882	0.427798	1.901772



2-D

Standard orientation:

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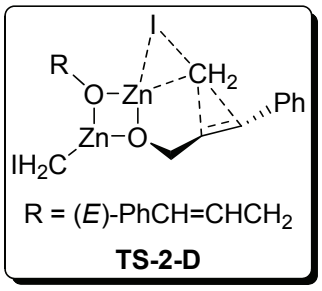
1	30	0	-1.242843	0.589794	-0.578248
2	8	0	-0.707871	-0.863223	0.602855
3	6	0	-1.499391	-1.948929	1.079155
4	6	0	-2.958549	-1.607490	1.012081
5	6	0	-3.847015	-2.280747	0.262526
6	6	0	-2.805234	1.535929	-1.301929
7	53	0	-3.429889	3.055115	0.224591
8	6	0	-5.284184	-2.010247	0.107848
9	6	0	-6.079477	-2.945436	-0.577958
10	6	0	-7.447120	-2.738793	-0.753618
11	6	0	-8.048835	-1.584152	-0.251244
12	6	0	-7.270562	-0.639632	0.425665
13	6	0	-5.905802	-0.848160	0.604094
14	1	0	-1.297958	-2.855808	0.489489
15	1	0	-1.207097	-2.163319	2.118772
16	1	0	-3.266697	-0.751327	1.611742
17	1	0	-3.483458	-3.143430	-0.298731
18	1	0	-2.639623	2.133998	-2.198007
19	1	0	-3.701362	0.930036	-1.433710
20	1	0	-5.615141	-3.846309	-0.973043
21	1	0	-8.041006	-3.477971	-1.284598
22	1	0	-9.113536	-1.416928	-0.389325
23	1	0	-7.728455	0.267184	0.811453
24	1	0	-5.317857	-0.094987	1.120399
25	30	0	1.242842	-0.591023	0.578408
26	8	0	0.707881	0.862035	-0.602774
27	6	0	1.499273	1.948499	-1.077544
28	6	0	2.958518	1.607511	-1.010134
29	6	0	3.846481	2.280543	-0.259788
30	6	0	2.805815	-1.537147	1.300836
31	53	0	3.430241	-3.054364	-0.227898
32	6	0	5.283700	2.010425	-0.104865
33	6	0	6.078566	2.945608	0.581442

34	6	0	7.446232	2.739304	0.757328
35	6	0	8.048393	1.585005	0.254700
36	6	0	7.270542	0.640488	-0.422696
37	6	0	5.905759	0.848682	-0.601361
38	1	0	1.297245	2.854733	-0.487081
39	1	0	1.207428	2.163842	-2.117093
40	1	0	3.267186	0.751902	-1.610315
41	1	0	3.482441	3.142691	0.301980
42	1	0	2.640995	-2.136406	2.196260
43	1	0	3.701804	-0.931076	1.432736
44	1	0	5.613881	3.846210	0.976735
45	1	0	8.039788	3.478480	1.288683
46	1	0	9.113110	1.418040	0.392966
47	1	0	7.728778	-0.266070	-0.808681
48	1	0	5.318144	0.095513	-1.118052



Imaginary frequency: -316.1 cm^{-1}

Standard orientation:

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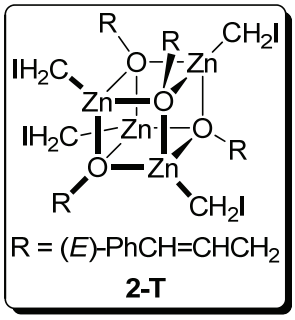
1	30	0	-1.274377	1.368788	-0.421987
2	8	0	-0.744066	0.019170	-1.843454
3	6	0	-1.756236	-0.937285	-2.083724
4	6	0	-2.580641	-1.273294	-0.854138
5	6	0	-3.915271	-1.541655	-0.882892
6	6	0	-3.183348	0.927254	-0.158355
7	53	0	-2.828823	3.647418	0.200436
8	6	0	-4.739739	-2.127894	0.175929
9	6	0	-6.128845	-2.231528	-0.028449
10	6	0	-6.961059	-2.782399	0.943784
11	6	0	-6.421348	-3.243208	2.145855
12	6	0	-5.042542	-3.152211	2.363749
13	6	0	-4.210655	-2.605379	1.391893

14	1	0	-2.423342	-0.582483	-2.884211
15	1	0	-1.300723	-1.874227	-2.443171
16	1	0	-1.996475	-1.536738	0.027420
17	1	0	-4.449821	-1.309068	-1.804998
18	1	0	-3.895148	1.105973	-0.963186
19	1	0	-3.692673	0.726594	0.784832
20	1	0	-6.554797	-1.871426	-0.962098
21	1	0	-8.030228	-2.850691	0.763060
22	1	0	-7.066807	-3.673557	2.906332
23	1	0	-4.614336	-3.515187	3.294090
24	1	0	-3.141232	-2.557482	1.575194
25	30	0	1.093040	-0.215153	-1.206074
26	8	0	0.601529	1.243367	0.015482
27	6	0	1.445931	2.104831	0.782650
28	6	0	2.768969	1.446574	1.034773
29	6	0	3.938797	1.938813	0.594660
30	6	0	2.572130	-1.467322	-1.532569
31	53	0	2.279896	-3.214211	-0.154268
32	6	0	5.281291	1.364800	0.768799
33	6	0	6.397987	2.123024	0.374635
34	6	0	7.693458	1.627462	0.516379
35	6	0	7.899508	0.355198	1.051520
36	6	0	6.799384	-0.415405	1.441538
37	6	0	5.506371	0.081344	1.303076
38	1	0	1.590938	3.059109	0.256294
39	1	0	0.940267	2.328308	1.733153
40	1	0	2.729709	0.516651	1.601393
41	1	0	3.915334	2.884240	0.049934
42	1	0	2.607031	-1.930478	-2.518345
43	1	0	3.564864	-1.103747	-1.269381
44	1	0	6.243039	3.114829	-0.044282
45	1	0	8.540420	2.234180	0.207294
46	1	0	8.907100	-0.036483	1.160702
47	1	0	6.950080	-1.410312	1.851766
48	1	0	4.665490	-0.537631	1.602193

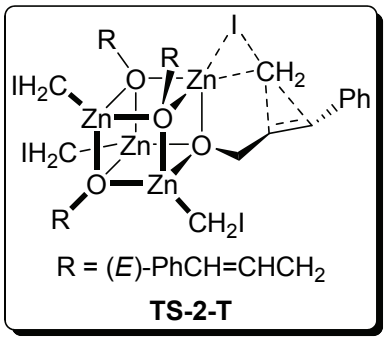


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.112494	-1.091856	-1.091362
2	8	0	0.981597	-0.995262	-0.968601
3	6	0	1.793092	-1.853737	-1.810075
4	6	0	3.251630	-1.725791	-1.495520
5	6	0	3.985470	-2.744713	-1.016012
6	6	0	-2.169804	-2.162389	-2.378224
7	53	0	-1.618314	-4.328994	-2.237743
8	6	0	5.421160	-2.754894	-0.700642
9	6	0	5.956865	-3.877232	-0.042860
10	6	0	7.311550	-3.944324	0.279772
11	6	0	8.162567	-2.890291	-0.056193
12	6	0	7.646385	-1.769330	-0.714663
13	6	0	6.292775	-1.700760	-1.033134
14	1	0	1.461004	-2.889370	-1.678585
15	1	0	1.598928	-1.572743	-2.854786
16	1	0	3.701696	-0.752007	-1.689772
17	1	0	3.473280	-3.688443	-0.826284
18	1	0	-3.244326	-2.174996	-2.191840
19	1	0	-2.004472	-1.937974	-3.433050
20	1	0	5.296896	-4.700186	0.220777
21	1	0	7.701721	-4.820623	0.790238
22	1	0	9.220423	-2.942190	0.186829
23	1	0	8.301698	-0.946740	-0.987312
24	1	0	5.914561	-0.826565	-1.554650
25	30	0	1.112678	1.091961	-1.091032
26	8	0	-0.981575	0.995225	-0.968604
27	6	0	-1.793025	1.853669	-1.810206
28	6	0	-3.251548	1.725870	-1.495599
29	6	0	-3.985280	2.744863	-1.016070
30	6	0	2.169953	2.162524	-2.377890
31	53	0	1.618232	4.329081	-2.237788

32	6	0	-5.420920	2.755122	-0.700509
33	6	0	-5.956390	3.877330	-0.042309
34	6	0	-7.311003	3.944447	0.280616
35	6	0	-8.162169	2.890572	-0.055466
36	6	0	-7.646222	1.769753	-0.714364
37	6	0	-6.292689	1.701164	-1.033147
38	1	0	-1.598852	1.572482	-2.854863
39	1	0	-1.460826	2.889284	-1.678875
40	1	0	-3.701728	0.752128	-1.689798
41	1	0	-3.473007	3.688562	-0.826420
42	1	0	2.004691	1.937836	-3.432672
43	1	0	3.244453	2.175335	-2.191431
44	1	0	-5.296285	4.700140	0.221438
45	1	0	-7.701004	4.820637	0.791399
46	1	0	-9.219972	2.942482	0.187787
47	1	0	-8.301672	0.947292	-0.987076
48	1	0	-5.914644	0.827102	-1.555007
49	30	0	-1.112768	1.091826	1.091311
50	8	0	0.981410	0.995113	0.968893
51	6	0	1.792863	1.853559	1.810464
52	6	0	3.251372	1.725941	1.495625
53	6	0	3.984903	2.745035	1.016011
54	6	0	-2.170304	2.162249	2.378067
55	53	0	-1.618548	4.328811	2.238095
56	6	0	5.420502	2.755479	0.700247
57	6	0	5.955735	3.877715	0.041905
58	6	0	7.310309	3.945023	-0.281145
59	6	0	8.161687	2.891330	0.054973
60	6	0	7.645981	1.770489	0.714021
61	6	0	6.292476	1.701694	1.032898
62	1	0	1.460540	2.889158	1.679318
63	1	0	1.598927	1.572213	2.855119
64	1	0	3.701661	0.752225	1.689706
65	1	0	3.472495	3.688685	0.826477
66	1	0	-3.244761	2.175000	2.191323
67	1	0	-2.005338	1.937603	3.432901
68	1	0	5.295481	4.700405	-0.221849
69	1	0	7.700116	4.821230	-0.792048
70	1	0	9.219463	2.943407	-0.188359
71	1	0	8.301586	0.948178	0.986812
72	1	0	5.914629	0.827622	1.554887
73	30	0	1.112265	-1.092100	1.091495
74	8	0	-0.981660	-0.995451	0.968792
75	6	0	-1.793053	-1.854223	1.810117

76	6	0	-3.251573	-1.726422	1.495502
77	6	0	-3.985240	-2.745240	1.015512
78	6	0	2.170320	-2.162384	2.377936
79	53	0	1.618937	-4.329048	2.238284
80	6	0	-5.420882	-2.755414	0.699935
81	6	0	-5.956279	-3.877298	0.041124
82	6	0	-7.310889	-3.944325	-0.281835
83	6	0	-8.162127	-2.890696	0.054833
84	6	0	-7.646253	-1.770209	0.714353
85	6	0	-6.292721	-1.701701	1.033162
86	1	0	-1.598981	-1.573275	2.854857
87	1	0	-1.460746	-2.889774	1.678548
88	1	0	-3.701808	-0.752782	1.690096
89	1	0	-3.472932	-3.688837	0.825456
90	1	0	2.005514	-1.937616	3.432776
91	1	0	3.244737	-2.175003	2.190982
92	1	0	-5.296123	-4.699923	-0.223069
93	1	0	-7.700831	-4.820262	-0.793099
94	1	0	-9.219929	-2.942544	-0.188437
95	1	0	-8.301768	-0.947959	0.987546
96	1	0	-5.914735	-0.827913	1.555523



Imaginary frequency: -349.7 cm^{-1}

Standard orientation:

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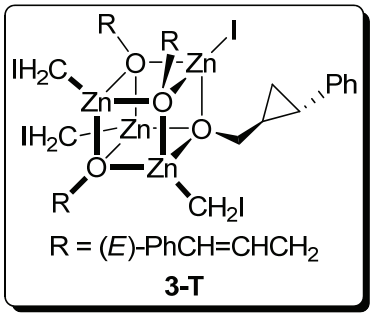
1	30	0	-1.188743	0.988933	0.893806
2	8	0	0.872419	1.129332	0.826585
3	6	0	1.590908	1.992860	1.748766
4	6	0	3.070903	1.923229	1.532678
5	6	0	3.803171	2.983884	1.151240
6	6	0	-2.802010	2.147984	1.025596

7	53	0	-1.990840	1.683872	3.637485
8	6	0	5.257039	3.055163	0.946853
9	6	0	5.802851	4.235613	0.410136
10	6	0	7.174350	4.362597	0.194160
11	6	0	8.032271	3.310145	0.517107
12	6	0	7.506045	2.131157	1.055267
13	6	0	6.136060	2.003564	1.267650
14	1	0	1.235404	3.021024	1.615022
15	1	0	1.325373	1.681281	2.766313
16	1	0	3.539496	0.958187	1.725963
17	1	0	3.273625	3.918422	0.963155
18	1	0	-2.713177	3.230600	1.122804
19	1	0	-3.801871	1.816643	1.294335
20	1	0	5.137893	5.058402	0.158316
21	1	0	7.571882	5.283943	-0.222875
22	1	0	9.102619	3.407499	0.356734
23	1	0	8.165380	1.307427	1.314138
24	1	0	5.749752	1.082816	1.694601
25	30	0	1.194556	-0.954477	0.838961
26	8	0	-0.895160	-1.027192	0.627307
27	6	0	-1.646408	-2.035178	1.361656
28	6	0	-3.121553	-1.790773	1.289139
29	6	0	-3.971217	-2.596659	0.629712
30	6	0	2.305849	-2.001853	2.097741
31	53	0	1.880310	-4.191133	1.901493
32	6	0	-5.433707	-2.464743	0.540692
33	6	0	-6.130111	-3.246163	-0.399231
34	6	0	-7.515762	-3.157030	-0.525791
35	6	0	-8.238716	-2.289839	0.295348
36	6	0	-7.562864	-1.514955	1.244055
37	6	0	-6.177661	-1.600173	1.366651
38	1	0	-1.310706	-2.004027	2.405398
39	1	0	-1.390723	-3.018254	0.953212
40	1	0	-3.483723	-0.920305	1.835384
41	1	0	-3.553254	-3.450431	0.094229
42	1	0	2.123059	-1.811514	3.156137
43	1	0	3.379537	-1.948348	1.913868
44	1	0	-5.572533	-3.929191	-1.035974
45	1	0	-8.030740	-3.770012	-1.260508
46	1	0	-9.320040	-2.227413	0.208249
47	1	0	-8.118844	-0.853285	1.903138
48	1	0	-5.674067	-1.011528	2.128056
49	30	0	-0.929950	-0.997268	-1.454295
50	8	0	1.140332	-0.737799	-1.224008

51	6	0	2.043954	-1.496952	-2.067691
52	6	0	3.473834	-1.317763	-1.660917
53	6	0	4.226034	-2.327260	-1.190026
54	6	0	-1.901410	-2.108707	-2.772781
55	53	0	-1.298037	-4.256929	-2.599760
56	6	0	5.639060	-2.288758	-0.787021
57	6	0	6.168349	-3.386382	-0.083573
58	6	0	7.500880	-3.403242	0.325797
59	6	0	8.336342	-2.324725	0.030075
60	6	0	7.827223	-1.229895	-0.675970
61	6	0	6.494802	-1.210518	-1.079906
62	1	0	1.763199	-2.555126	-2.018342
63	1	0	1.893301	-1.160761	-3.103433
64	1	0	3.886292	-0.314896	-1.773768
65	1	0	3.747677	-3.300308	-1.074637
66	1	0	-2.982786	-2.146161	-2.634477
67	1	0	-1.698243	-1.880908	-3.820176
68	1	0	5.520081	-4.227762	0.149063
69	1	0	7.886473	-4.259762	0.872010
70	1	0	9.377824	-2.338459	0.339839
71	1	0	8.472138	-0.390057	-0.919284
72	1	0	6.121597	-0.358415	-1.640248
73	30	0	1.102867	1.354503	-1.226509
74	8	0	-0.944293	1.055527	-1.269737
75	6	0	-1.881021	1.953014	-1.862329
76	6	0	-3.240234	1.917066	-1.202178
77	6	0	-4.042677	3.019560	-1.129357
78	6	0	2.119215	2.668973	-2.304269
79	53	0	1.326417	4.734210	-1.911173
80	6	0	-5.471207	3.077854	-0.829791
81	6	0	-6.094364	4.339819	-0.768697
82	6	0	-7.456037	4.457140	-0.500667
83	6	0	-8.225899	3.312507	-0.284390
84	6	0	-7.623021	2.051311	-0.340280
85	6	0	-6.264066	1.932268	-0.611994
86	1	0	-2.011569	1.680875	-2.921376
87	1	0	-1.480464	2.974242	-1.838435
88	1	0	-3.673975	0.924225	-1.091956
89	1	0	-3.574473	3.985205	-1.324571
90	1	0	2.029377	2.582009	-3.388111
91	1	0	3.174430	2.768491	-2.048887
92	1	0	-5.497518	5.233545	-0.934900
93	1	0	-7.915383	5.440798	-0.459216
94	1	0	-9.288385	3.400539	-0.075328

95	1	0	-8.211823	1.153753	-0.175036
96	1	0	-5.821597	0.941466	-0.655599

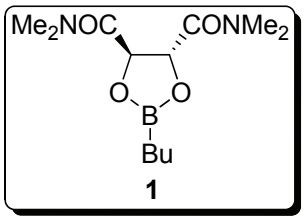


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-1.006386	0.311734	2.004746
2	8	0	0.998222	0.387147	1.583859
3	6	0	1.958207	0.817132	2.585080
4	6	0	3.348265	0.866396	2.031703
5	6	0	4.057510	2.004846	1.944955
6	6	0	-3.253276	2.155228	-2.386467
7	53	0	-2.094998	0.973131	4.183735
8	6	0	5.434643	2.177723	1.461280
9	6	0	5.937751	3.483829	1.319350
10	6	0	7.237517	3.709895	0.868416
11	6	0	8.065565	2.630989	0.555143
12	6	0	7.581484	1.326040	0.694273
13	6	0	6.282517	1.100540	1.141183
14	1	0	1.659644	1.802857	2.958868
15	1	0	1.899675	0.110820	3.424381
16	1	0	3.772283	-0.085966	1.713553
17	1	0	3.569852	2.926366	2.264649
18	1	0	-3.881978	1.332003	-2.056135
19	1	0	-2.953624	2.095284	-3.429278
20	1	0	5.296258	4.327160	1.563502
21	1	0	7.603380	4.727852	0.765535
22	1	0	9.081567	2.802992	0.210327
23	1	0	8.219667	0.478915	0.458931
24	1	0	5.930485	0.079182	1.251514
25	30	0	1.080766	-1.547864	0.740257
26	8	0	-1.007041	-1.474141	1.008387
27	6	0	-1.756159	-2.630382	1.484757

28	6	0	-3.212919	-2.312735	1.613118
29	6	0	-4.160123	-2.877374	0.844156
30	6	0	2.301311	-3.007648	1.281362
31	53	0	1.641074	-4.961782	0.417881
32	6	0	-5.609521	-2.635460	0.886887
33	6	0	-6.422905	-3.243722	-0.086057
34	6	0	-7.802078	-3.038240	-0.102824
35	6	0	-8.397833	-2.221193	0.858830
36	6	0	-7.603478	-1.613861	1.837202
37	6	0	-6.226992	-1.818266	1.853504
38	1	0	-1.332839	-2.919756	2.455331
39	1	0	-1.592337	-3.455515	0.784321
40	1	0	-3.474563	-1.587744	2.383013
41	1	0	-3.838764	-3.596912	0.089978
42	1	0	2.340419	-3.212915	2.352220
43	1	0	3.321895	-2.908727	0.910117
44	1	0	-5.962781	-3.882237	-0.836622
45	1	0	-8.409828	-3.517708	-0.865428
46	1	0	-9.472440	-2.060531	0.851108
47	1	0	-8.060945	-0.981316	2.593254
48	1	0	-5.629249	-1.345092	2.627115
49	30	0	-1.460268	-0.666745	-0.865118
50	8	0	0.635862	-0.521658	-1.003270
51	6	0	1.291022	-0.890393	-2.246154
52	6	0	2.781072	-0.917271	-2.102196
53	6	0	3.499280	-2.048715	-2.207851
54	6	0	-2.661876	-1.318958	-2.295766
55	53	0	-2.105705	-3.399337	-2.910561
56	6	0	4.958229	-2.200835	-2.112548
57	6	0	5.494012	-3.494859	-1.978593
58	6	0	6.869999	-3.696306	-1.879624
59	6	0	7.740810	-2.606290	-1.924459
60	6	0	7.223994	-1.314441	-2.067286
61	6	0	5.849372	-1.112381	-2.159704
62	1	0	0.919095	-1.872568	-2.557456
63	1	0	0.988117	-0.160671	-3.010010
64	1	0	3.267223	0.039069	-1.908066
65	1	0	2.954326	-2.978626	-2.374014
66	1	0	-3.707956	-1.421811	-2.005098
67	1	0	-2.616253	-0.767624	-3.235118
68	1	0	4.818572	-4.346177	-1.943240
69	1	0	7.261013	-4.704337	-1.772116
70	1	0	8.814310	-2.760634	-1.857349
71	1	0	7.894576	-0.460895	-2.115130

72	1	0	5.467264	-0.103761	-2.286831
73	30	0	0.795695	1.402372	-0.223256
74	8	0	-1.270652	1.159305	0.147059
75	6	0	-2.200903	2.261494	0.015960
76	6	0	-2.298023	2.770975	-1.398163
77	6	0	-3.550023	3.528140	-1.817974
78	6	0	1.712611	3.014067	-0.912673
79	53	0	1.234334	4.767584	0.398126
80	6	0	-3.482007	4.771238	-2.641525
81	6	0	-4.360382	5.828117	-2.361699
82	6	0	-4.329570	7.007714	-3.106438
83	6	0	-3.415347	7.154383	-4.150268
84	6	0	-2.534930	6.109759	-4.440633
85	6	0	-2.568636	4.931807	-3.695292
86	1	0	-1.867976	3.065835	0.682344
87	1	0	-3.187209	1.926600	0.363039
88	1	0	-1.365869	3.169566	-1.795891
89	1	0	-4.340418	3.550488	-1.069817
90	1	0	1.416457	3.361553	-1.903400
91	1	0	2.801586	2.969337	-0.870799
92	1	0	-5.076004	5.723550	-1.549296
93	1	0	-5.020805	7.811933	-2.868352
94	1	0	-3.387973	8.071772	-4.731716
95	1	0	-1.818009	6.211349	-5.251259
96	1	0	-1.873697	4.132410	-3.942176

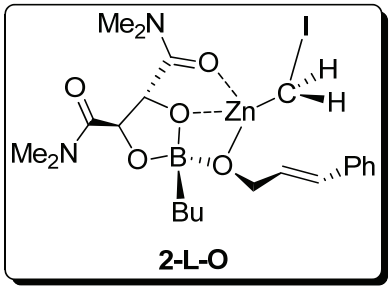


1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570694	0.413392	0.514722
2	6	0	-1.011552	-0.397671	-0.735845
3	8	0	0.175166	-1.141580	-1.078715
4	5	0	1.252285	-0.487949	-0.511882
5	8	0	0.858447	0.516868	0.349530
6	6	0	-1.356329	1.715323	0.748358

7	8	0	-2.232933	1.659665	1.608001
8	7	0	-1.113001	2.841408	0.011523
9	6	0	-0.190453	2.962334	-1.107525
10	6	0	-1.966594	4.003145	0.234903
11	6	0	-2.319700	-1.189350	-0.565353
12	8	0	-3.318507	-0.683432	-1.072167
13	7	0	-2.360447	-2.359065	0.142090
14	6	0	-1.261708	-2.963495	0.880690
15	6	0	-3.657669	-2.997765	0.334590
16	6	0	6.255022	-0.147151	0.820435
17	6	0	5.229963	-0.651297	-0.200783
18	6	0	3.780857	-0.332012	0.188887
19	6	0	2.747569	-0.838308	-0.833624
20	1	0	-0.757759	-0.156196	1.429286
21	1	0	-1.235684	0.273476	-1.569909
22	1	0	0.533296	2.153089	-1.103207
23	1	0	0.359968	3.907104	-1.020481
24	1	0	-0.729636	2.972619	-2.065824
25	1	0	-2.583488	3.818990	1.112666
26	1	0	-1.347136	4.894724	0.391112
27	1	0	-2.616039	4.177259	-0.633662
28	1	0	-0.306420	-2.565423	0.552091
29	1	0	-1.377089	-2.804144	1.962610
30	1	0	-1.256579	-4.045018	0.698044
31	1	0	-3.965640	-2.935686	1.387122
32	1	0	-4.392705	-2.486888	-0.284816
33	1	0	-3.597229	-4.055558	0.050939
34	1	0	7.278945	-0.389389	0.513482
35	1	0	6.087194	-0.598339	1.806282
36	1	0	6.191834	0.941438	0.941188
37	1	0	5.443879	-0.210112	-1.185123
38	1	0	5.340190	-1.738174	-0.326191
39	1	0	3.567474	-0.768787	1.174842
40	1	0	3.668071	0.753256	0.316121
41	1	0	2.981069	-0.423125	-1.828281
42	1	0	2.836537	-1.926816	-0.964091

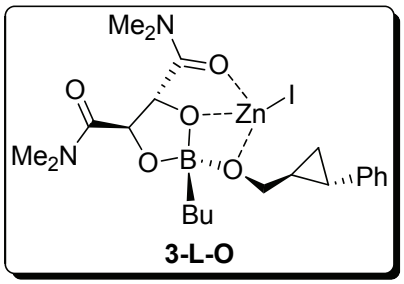


2-L-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.275891	1.056824	-0.148653
2	6	0	-2.821984	-0.213437	-0.897180
3	8	0	-2.596959	-1.285931	-0.019336
4	5	0	-1.500838	-0.982540	0.884441
5	8	0	-1.454405	0.548856	0.889637
6	8	0	-0.135219	-1.234728	0.213209
7	30	0	0.624857	0.631778	0.422662
8	6	0	0.515947	-2.504840	0.234730
9	6	0	2.252034	1.326627	1.301124
10	53	0	2.138001	3.555993	1.491999
11	6	0	1.714534	-2.471942	-0.664731
12	6	0	2.968344	-2.691508	-0.237603
13	6	0	-4.327909	-0.115717	-1.223007
14	8	0	-4.976539	0.893295	-0.926138
15	7	0	-4.895694	-1.178349	-1.859252
16	6	0	-4.207289	-2.404856	-2.242642
17	6	0	-6.312687	-1.127342	-2.196967
18	6	0	-2.976811	-5.012799	3.883969
19	6	0	-2.443289	-3.576721	3.834740
20	6	0	-2.186294	-3.068982	2.408778
21	6	0	-1.663708	-1.620966	2.351460
22	6	0	-1.403462	1.921428	-1.074638
23	8	0	-0.184357	1.624315	-1.181643
24	7	0	-1.914850	2.945606	-1.773705
25	6	0	-3.294729	3.429796	-1.687515
26	6	0	-1.032202	3.757692	-2.614605
27	1	0	-3.102621	1.621336	0.284487
28	1	0	-2.263854	-0.349254	-1.839882
29	1	0	0.809472	-2.770470	1.259568
30	1	0	-0.202205	-3.260685	-0.113822
31	1	0	2.399469	1.002020	2.331823

32	1	0	3.182536	1.174091	0.753402
33	1	0	1.507665	-2.249023	-1.710870
34	1	0	-4.136999	-2.481806	-3.336593
35	1	0	-4.777065	-3.268308	-1.877516
36	1	0	-3.217170	-2.451670	-1.796787
37	1	0	-6.713006	-0.164075	-1.885387
38	1	0	-6.854370	-1.933217	-1.685603
39	1	0	-6.448394	-1.252308	-3.279162
40	1	0	-3.154267	-5.343156	4.914396
41	1	0	-2.268129	-5.715577	3.427226
42	1	0	-3.924745	-5.101065	3.338168
43	1	0	-3.156527	-2.903250	4.331320
44	1	0	-1.512067	-3.511160	4.416162
45	1	0	-1.479665	-3.754432	1.916665
46	1	0	-3.117271	-3.134928	1.829046
47	1	0	-2.372411	-0.982063	2.899956
48	1	0	-0.719086	-1.552199	2.915608
49	1	0	-3.963761	2.678292	-1.270780
50	1	0	-3.640156	3.667808	-2.699313
51	1	0	-3.331801	4.347718	-1.087444
52	1	0	-0.011702	3.391730	-2.531058
53	1	0	-1.076786	4.801640	-2.284429
54	1	0	-1.364164	3.704866	-3.657833
55	6	0	4.204833	-2.696276	-1.033645
56	6	0	5.437858	-2.809910	-0.367480
57	6	0	4.219161	-2.591729	-2.437451
58	6	0	6.641914	-2.808201	-1.070549
59	1	0	5.447056	-2.895225	0.716793
60	6	0	5.420254	-2.589752	-3.140648
61	1	0	3.283175	-2.518629	-2.983636
62	6	0	6.638238	-2.696537	-2.461449
63	1	0	7.581614	-2.894248	-0.531586
64	1	0	5.408070	-2.508572	-4.224415
65	1	0	7.573938	-2.696160	-3.013749
66	1	0	3.112128	-2.888663	0.825865

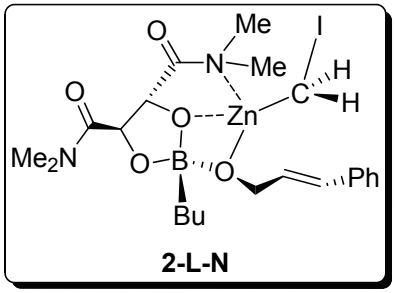


3-L-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.036238	-0.062922	1.027121
2	30	0	0.346118	1.674721	0.033061
3	8	0	0.541938	0.882947	-1.833734
4	6	0	-0.529250	0.552560	-2.409663
5	7	0	-0.539878	0.293878	-3.726073
6	6	0	0.691872	0.418518	-4.507100
7	8	0	-1.653123	1.061539	-0.333363
8	5	0	-1.607629	0.012603	0.787521
9	6	0	-2.700246	0.297319	1.926330
10	6	0	-2.646990	-0.649278	3.138506
11	6	0	-3.745031	-0.391294	4.180155
12	6	0	-3.677541	-1.335156	5.385947
13	8	0	-1.721706	-1.256339	0.063125
14	6	0	-2.153550	-1.067164	-1.250199
15	6	0	-3.659399	-1.340476	-1.540902
16	7	0	-4.317095	-2.329618	-0.878434
17	6	0	-5.728908	-2.544766	-1.182183
18	6	0	-1.821210	0.432952	-1.586774
19	8	0	-0.175621	0.205848	1.295005
20	6	0	0.654688	-0.871532	1.743822
21	6	0	1.873820	-1.013138	0.865471
22	6	0	3.181867	-1.513128	1.451092
23	1	0	3.170905	-1.677436	2.527028
24	53	0	1.457809	3.893438	0.510621
25	6	0	4.056594	-2.471398	0.713027
26	8	0	-4.208893	-0.667149	-2.422510
27	6	0	-3.726243	-3.335008	-0.000166
28	6	0	-1.729422	-0.061176	-4.503383
29	1	0	-2.655897	0.894341	-2.116153
30	1	0	-1.597006	-1.745931	-1.916092
31	1	0	0.954120	-0.664789	2.779664
32	1	0	0.066230	-1.793712	1.730420

33	1	0	2.987136	0.687452	1.812368
34	1	0	3.573730	0.258792	0.139452
35	1	0	1.654857	-1.345227	-0.147704
36	1	0	-3.856557	-4.331470	-0.444361
37	1	0	-4.236912	-3.325748	0.970747
38	1	0	-2.672881	-3.134990	0.167191
39	1	0	-6.099559	-1.705873	-1.768185
40	1	0	-6.294005	-2.628161	-0.246658
41	1	0	-5.865370	-3.472872	-1.753786
42	1	0	-4.476576	-1.126866	6.107326
43	1	0	-2.720197	-1.236534	5.913188
44	1	0	-3.774771	-2.383510	5.075381
45	1	0	-4.728316	-0.483430	3.696297
46	1	0	-3.675291	0.650229	4.524779
47	1	0	-1.667508	-0.560710	3.632067
48	1	0	-2.720520	-1.694166	2.798609
49	1	0	-3.704118	0.241805	1.474992
50	1	0	-2.593636	1.334211	2.280631
51	1	0	-2.606052	-0.219087	-3.874884
52	1	0	-1.527960	-0.982438	-5.062442
53	1	0	-1.946044	0.736377	-5.224421
54	1	0	1.503402	0.735272	-3.855932
55	1	0	0.547309	1.158660	-5.302287
56	1	0	0.938069	-0.545612	-4.966657
57	6	0	4.736015	-3.472099	1.423102
58	6	0	5.563362	-4.386400	0.769435
59	6	0	5.728641	-4.318436	-0.614371
60	6	0	5.058452	-3.326805	-1.334716
61	6	0	4.232581	-2.414507	-0.679040
62	1	0	4.615548	-3.532308	2.502465
63	1	0	6.079155	-5.151154	1.344391
64	1	0	6.373411	-5.027343	-1.126527
65	1	0	5.181284	-3.260876	-2.412896
66	1	0	3.724782	-1.648315	-1.260057

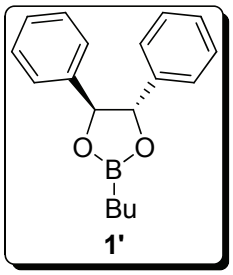


2-L-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.803234	-0.047282	-1.753954
2	6	0	2.838346	0.950205	-1.191822
3	8	0	2.898971	0.703432	0.199904
4	5	0	2.083608	-0.430340	0.560954
5	8	0	1.680312	-1.077014	-0.763231
6	8	0	0.651556	0.030835	1.001476
7	30	0	-0.351929	-1.311832	-0.080470
8	6	0	0.374882	1.098422	1.914312
9	6	0	-1.399718	-2.923042	0.399092
10	53	0	-3.527023	-2.858659	-0.282663
11	6	0	-0.625318	2.038913	1.312403
12	6	0	-1.847666	2.260337	1.822319
13	6	0	4.207628	0.747112	-1.893326
14	8	0	4.286887	0.030602	-2.893701
15	7	0	5.286026	1.414043	-1.388013
16	6	0	5.261682	2.368519	-0.288142
17	6	0	6.578450	1.254603	-2.041238
18	6	0	4.397835	-1.249575	5.163961
19	6	0	3.934129	-1.863343	3.838439
20	6	0	3.212333	-0.864850	2.922118
21	6	0	2.743156	-1.470871	1.587161
22	6	0	0.448784	0.620335	-2.023428
23	8	0	0.291650	1.815378	-2.160496
24	7	0	-0.674949	-0.279523	-2.038008
25	6	0	-0.537177	-1.420799	-2.989129
26	6	0	-1.968471	0.420681	-2.213555
27	1	0	2.195248	-0.478958	-2.681170
28	1	0	2.503485	1.976917	-1.387209
29	1	0	0.007175	0.689192	2.864634
30	1	0	1.322556	1.616131	2.103642
31	1	0	-1.028740	-3.850219	-0.039868

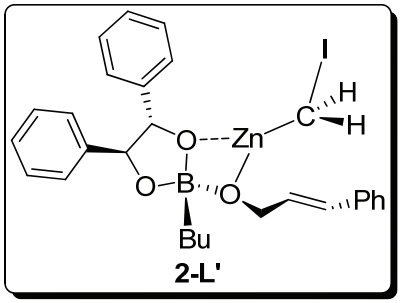
32	1	0	-1.493265	-3.070859	1.475411
33	1	0	-0.298696	2.534568	0.400135
34	1	0	5.489492	3.379500	-0.654973
35	1	0	6.026325	2.096714	0.450890
36	1	0	4.298614	2.363513	0.214349
37	1	0	6.479534	0.517224	-2.836184
38	1	0	7.328950	0.919911	-1.313876
39	1	0	6.914143	2.209307	-2.468669
40	1	0	4.913888	-1.985966	5.791364
41	1	0	3.548655	-0.859604	5.739557
42	1	0	5.089518	-0.414924	4.992924
43	1	0	4.800217	-2.278739	3.303453
44	1	0	3.267899	-2.714539	4.040878
45	1	0	2.352358	-0.447801	3.468343
46	1	0	3.882332	-0.016409	2.720397
47	1	0	3.607929	-1.932278	1.086193
48	1	0	2.047799	-2.300008	1.798545
49	1	0	0.392516	-1.960264	-2.805325
50	1	0	-0.552383	-1.060909	-4.025458
51	1	0	-1.378007	-2.100252	-2.834136
52	1	0	-2.081583	1.181106	-1.440808
53	1	0	-2.768357	-0.314900	-2.118511
54	1	0	-2.017689	0.907225	-3.194286
55	6	0	-2.890678	3.151581	1.290618
56	6	0	-4.096147	3.284114	2.001721
57	6	0	-2.744563	3.878991	0.092949
58	6	0	-5.119345	4.112142	1.541361
59	1	0	-4.228065	2.727879	2.927028
60	6	0	-3.766844	4.703834	-0.368140
61	1	0	-1.827718	3.797172	-0.483919
62	6	0	-4.958819	4.826261	0.353378
63	1	0	-6.041283	4.197855	2.110253
64	1	0	-3.633567	5.255893	-1.294806
65	1	0	-5.753698	5.472060	-0.009520
66	1	0	-2.120337	1.734797	2.739145



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.220946	0.412505	0.396145
2	6	0	-0.655355	-0.581393	-0.741822
3	8	0	0.555879	-1.291954	-1.051977
4	5	0	1.616094	-0.605299	-0.503479
5	8	0	1.212775	0.445979	0.288185
6	6	0	6.593501	-0.174082	0.900073
7	6	0	5.589124	-0.739688	-0.109605
8	6	0	4.131641	-0.404836	0.233270
9	6	0	3.118842	-0.973414	-0.776278
10	1	0	-0.473355	-0.022395	1.371481
11	1	0	-0.944952	-0.006480	-1.630595
12	1	0	7.623997	-0.431422	0.628862
13	1	0	6.406150	-0.566560	1.907384
14	1	0	6.526418	0.919601	0.955272
15	1	0	5.820869	-0.354488	-1.113280
16	1	0	5.705192	-1.831532	-0.170742
17	1	0	3.901559	-0.784945	1.238897
18	1	0	4.012790	0.685446	0.295510
19	1	0	3.371459	-0.617292	-1.788878
20	1	0	3.210684	-2.067641	-0.837867
21	6	0	-0.834678	1.788259	0.284097
22	6	0	-0.234443	2.787329	-0.491985
23	6	0	-2.048238	2.062743	0.927397
24	6	0	-0.840254	4.037158	-0.624693
25	1	0	0.718277	2.586852	-0.971970
26	6	0	-2.658589	3.310514	0.787968
27	1	0	-2.515993	1.297006	1.541618
28	6	0	-2.055711	4.301466	0.011117
29	1	0	-0.359949	4.807457	-1.222433
30	1	0	-3.599285	3.510422	1.294220
31	1	0	-2.525598	5.275915	-0.091921
32	6	0	-1.780458	-1.512087	-0.355796

33	6	0	-3.105403	-1.159782	-0.641523
34	6	0	-1.526728	-2.707606	0.328275
35	6	0	-4.160910	-1.980174	-0.238672
36	1	0	-3.311393	-0.239807	-1.183487
37	6	0	-2.580698	-3.531495	0.723848
38	1	0	-0.500216	-2.998689	0.528592
39	6	0	-3.900885	-3.168616	0.445745
40	1	0	-5.184067	-1.694731	-0.468461
41	1	0	-2.370565	-4.461046	1.246464
42	1	0	-4.720590	-3.812192	0.753707



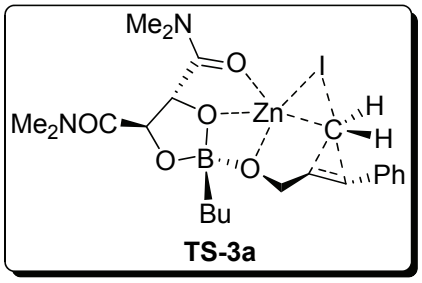
2-L'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.490386	-0.822056	-0.180076
2	6	0	-2.806237	0.354228	0.792053
3	8	0	-2.460235	1.501873	0.036657
4	5	0	-1.353583	1.214159	-0.827522
5	8	0	-1.357429	-0.332528	-0.937102
6	8	0	0.017840	1.294520	-0.080563
7	30	0	0.523131	-0.600423	-0.242878
8	6	0	0.742060	2.511385	0.133662
9	6	0	2.006913	-1.861894	-0.054083
10	53	0	2.710694	-2.433119	-2.094697
11	6	0	1.855240	2.270839	1.106634
12	6	0	3.154266	2.397953	0.790179
13	6	0	-2.296906	5.595319	-3.518146
14	6	0	-1.902854	4.115219	-3.574662
15	6	0	-1.763886	3.466680	-2.190096
16	6	0	-1.368727	1.978585	-2.239727
17	1	0	-3.324622	-0.914832	-0.888761
18	1	0	-2.154005	0.264420	1.677779
19	1	0	1.133850	2.887635	-0.820339

20	1	0	0.033244	3.251342	0.527418
21	1	0	2.897351	-1.457703	0.426437
22	1	0	1.739423	-2.812292	0.405815
23	1	0	1.547491	1.971665	2.107971
24	1	0	-2.393136	6.026210	-4.521894
25	1	0	-1.548081	6.184873	-2.973909
26	1	0	-3.256940	5.729664	-3.004199
27	1	0	-2.651113	3.558809	-4.157611
28	1	0	-0.954744	4.008403	-4.121897
29	1	0	-1.026119	4.039936	-1.608392
30	1	0	-2.712184	3.565094	-1.644710
31	1	0	-2.094426	1.454810	-2.881855
32	1	0	-0.400909	1.872881	-2.756861
33	6	0	4.319436	2.190826	1.662886
34	6	0	5.605071	2.233025	1.094995
35	6	0	4.214278	1.949296	3.045862
36	6	0	6.744746	2.030454	1.872227
37	1	0	5.706468	2.421841	0.028741
38	6	0	5.351160	1.746908	3.822818
39	1	0	3.236852	1.928600	3.519184
40	6	0	6.622242	1.784915	3.240367
41	1	0	7.726974	2.065037	1.408784
42	1	0	5.247435	1.563464	4.889003
43	1	0	7.507601	1.628387	3.850383
44	1	0	3.398733	2.684397	-0.233934
45	6	0	-2.171925	-2.186676	0.399798
46	6	0	-1.481799	-3.115699	-0.398668
47	6	0	-2.565400	-2.574334	1.687907
48	6	0	-1.174072	-4.387184	0.086328
49	1	0	-1.191517	-2.841054	-1.408851
50	6	0	-2.261067	-3.849024	2.171356
51	1	0	-3.125262	-1.889225	2.314262
52	6	0	-1.560729	-4.757040	1.376496
53	1	0	-0.637713	-5.088328	-0.547178
54	1	0	-2.573676	-4.129972	3.173562
55	1	0	-1.323414	-5.747129	1.756107
56	6	0	-4.248710	0.445947	1.248623
57	6	0	-4.586209	0.337738	2.602222
58	6	0	-5.270706	0.670053	0.315628
59	6	0	-5.917347	0.422651	3.017713
60	1	0	-3.799240	0.199306	3.341091
61	6	0	-6.600023	0.756567	0.726168
62	1	0	-5.015029	0.802338	-0.731719
63	6	0	-6.928489	0.627412	2.078815

64	1	0	-6.160695	0.337820	4.073567
65	1	0	-7.381433	0.931296	-0.008813
66	1	0	-7.965001	0.696040	2.398109



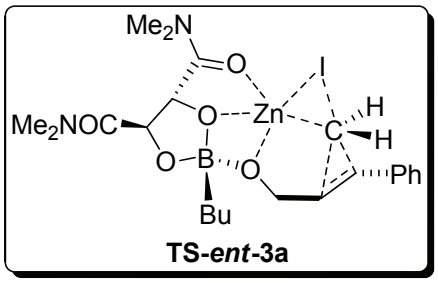
TS-3a

Imaginary frequency: -361.7 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.426072	-0.256063	-0.451510
2	30	0	0.544842	-0.776244	-0.036675
3	8	0	-0.449938	-2.060036	1.159969
4	6	0	-1.673240	-2.197932	0.892214
5	7	0	-2.357704	-3.245058	1.376425
6	6	0	-1.677468	-4.247758	2.197280
7	8	0	-1.407812	-0.349207	-0.628232
8	5	0	-1.422008	1.101922	-0.072877
9	6	0	-1.667709	2.169830	-1.252706
10	6	0	-1.934549	3.620474	-0.811196
11	6	0	-2.266381	4.571732	-1.970365
12	6	0	-2.541532	6.010898	-1.520726
13	8	0	-2.481863	1.031261	0.939563
14	6	0	-3.223683	-0.145305	0.880968
15	6	0	-4.655589	-0.008916	0.284713
16	7	0	-5.415589	1.069380	0.622529
17	6	0	-6.759076	1.176840	0.064344
18	6	0	-2.374898	-1.147801	0.014946
19	8	0	-0.087451	1.161175	0.624338
20	6	0	0.918256	2.131881	0.415532
21	6	0	2.269240	1.579057	0.813759
22	6	0	3.441862	2.028316	0.273905
23	1	0	3.375140	2.605237	-0.649217
24	53	0	1.978275	-2.651940	-1.793704
25	6	0	4.798576	1.818308	0.771999
26	8	0	-5.090481	-0.912775	-0.439994

27	6	0	-5.086732	2.081644	1.620820
28	6	0	-3.773952	-3.512552	1.122012
29	1	0	-3.009074	-1.631781	-0.729652
30	1	0	-3.361298	-0.542632	1.901050
31	1	0	0.945143	2.478813	-0.626067
32	1	0	0.708948	3.008352	1.048076
33	1	0	2.660290	0.217500	-1.403468
34	1	0	3.319281	-0.664214	0.016329
35	1	0	2.278794	1.065267	1.773408
36	1	0	-5.799314	2.023326	2.455577
37	1	0	-5.168294	3.080817	1.174616
38	1	0	-4.071178	1.956808	1.984257
39	1	0	-6.887128	0.413087	-0.700604
40	1	0	-6.897988	2.172677	-0.373337
41	1	0	-7.515723	1.035252	0.848217
42	1	0	-2.774976	6.662597	-2.371067
43	1	0	-1.672929	6.438033	-1.003334
44	1	0	-3.390096	6.053805	-0.826014
45	1	0	-3.139337	4.183168	-2.514311
46	1	0	-1.436190	4.565512	-2.691573
47	1	0	-1.067839	4.024533	-0.266218
48	1	0	-2.764653	3.629632	-0.090471
49	1	0	-2.542352	1.818449	-1.822009
50	1	0	-0.839971	2.157142	-1.980948
51	1	0	-4.249424	-2.721117	0.542949
52	1	0	-4.299282	-3.612217	2.079547
53	1	0	-3.872940	-4.458966	0.576947
54	1	0	-0.613547	-4.024613	2.232894
55	1	0	-1.831621	-5.239584	1.758270
56	1	0	-2.091835	-4.244767	3.212479
57	6	0	5.882457	2.266309	-0.008740
58	6	0	7.197213	2.092686	0.416574
59	6	0	7.460389	1.464716	1.635518
60	6	0	6.396449	1.017107	2.425976
61	6	0	5.082767	1.193536	2.004055
62	1	0	5.682808	2.751197	-0.961424
63	1	0	8.016139	2.445004	-0.204459
64	1	0	8.484667	1.326547	1.970073
65	1	0	6.593737	0.532146	3.378135
66	1	0	4.270816	0.849898	2.638221



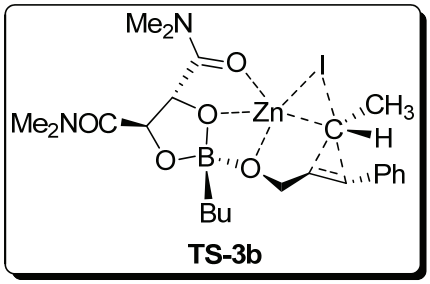
TS-*ent*-3a

Imaginary frequency: -302.9 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.528119	-0.052491	-0.866165
2	30	0	0.751103	-0.782799	-0.383999
3	8	0	0.110940	-1.879061	1.205475
4	6	0	-1.116736	-2.151713	1.169588
5	7	0	-1.617046	-3.153411	1.910031
6	6	0	-0.727346	-3.961989	2.743873
7	8	0	-1.265402	-0.553252	-0.623544
8	5	0	-1.400678	0.985926	-0.323392
9	6	0	-2.148795	1.716321	-1.551976
10	6	0	-2.544484	3.186092	-1.319801
11	6	0	-3.324310	3.813772	-2.483982
12	6	0	-3.723275	5.272890	-2.236752
13	8	0	-2.139459	0.960479	0.946377
14	6	0	-2.814878	-0.239812	1.142889
15	6	0	-4.328169	-0.258500	0.774184
16	7	0	-5.103103	0.814252	1.097460
17	6	0	-6.524161	0.767998	0.771056
18	6	0	-2.041308	-1.306657	0.282733
19	8	0	-0.006614	1.404951	-0.022336
20	6	0	0.771339	2.171504	-0.906195
21	6	0	2.244983	2.091531	-0.560944
22	6	0	2.728524	1.960201	0.711806
23	1	0	2.011652	1.635746	1.464439
24	53	0	2.122274	-2.755871	-1.952588
25	6	0	4.092076	2.171819	1.180963
26	8	0	-4.802512	-1.272440	0.247723
27	6	0	-4.700474	1.944600	1.927971
28	6	0	-3.020367	-3.568006	1.918785
29	1	0	-2.744466	-1.936102	-0.264516
30	1	0	-2.769829	-0.503842	2.212556
31	1	0	0.641732	1.857573	-1.951666

32	1	0	0.479437	3.233012	-0.860512
33	1	0	2.849360	0.202015	-1.878057
34	1	0	3.402960	-0.329673	-0.273654
35	1	0	2.899040	2.485465	-1.337779
36	1	0	-5.213794	1.899261	2.899307
37	1	0	-4.990264	2.880988	1.435846
38	1	0	-3.623604	1.955412	2.070012
39	1	0	-6.707438	-0.071836	0.103127
40	1	0	-6.819502	1.705328	0.285160
41	1	0	-7.128862	0.644266	1.680262
42	1	0	-4.281362	5.688809	-3.084034
43	1	0	-2.839922	5.904725	-2.078471
44	1	0	-4.355775	5.365347	-1.344460
45	1	0	-4.225821	3.214253	-2.676614
46	1	0	-2.719985	3.749401	-3.400482
47	1	0	-1.650971	3.799443	-1.126853
48	1	0	-3.149293	3.256663	-0.404578
49	1	0	-3.065483	1.144295	-1.766025
50	1	0	-1.557764	1.642820	-2.479221
51	1	0	-3.653742	-2.902053	1.333193
52	1	0	-3.385146	-3.579778	2.952860
53	1	0	-3.104716	-4.584032	1.514338
54	1	0	0.296586	-3.617022	2.618883
55	1	0	-0.799882	-5.013346	2.443237
56	1	0	-1.023487	-3.876102	3.795977
57	6	0	4.391724	1.876450	2.526087
58	6	0	5.673102	2.070043	3.036553
59	6	0	6.685433	2.563436	2.211470
60	6	0	6.405401	2.864511	0.873447
61	6	0	5.126333	2.674634	0.363542
62	1	0	3.604846	1.490701	3.169596
63	1	0	5.881740	1.834765	4.076405
64	1	0	7.686305	2.715351	2.605615
65	1	0	7.189301	3.251784	0.228567
66	1	0	4.926964	2.920760	-0.675165



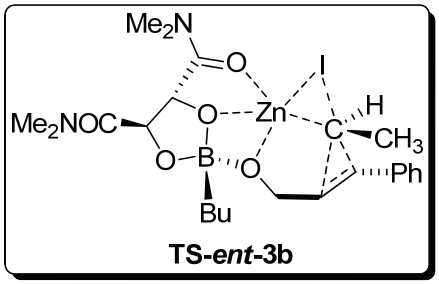
TS-3b

Imaginary frequency: -251.1 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.399325	-0.721531	0.095180
2	30	0	-0.370049	-0.906555	0.237902
3	8	0	0.788573	-1.878246	-1.139920
4	6	0	2.016182	-1.932935	-0.856457
5	7	0	2.769638	-2.944926	-1.308941
6	6	0	2.142188	-4.029590	-2.066735
7	8	0	1.605140	-0.356421	0.892114
8	5	0	1.392728	1.157561	0.742424
9	6	0	1.353017	1.944595	2.142546
10	6	0	1.503712	3.474531	2.050675
11	6	0	1.570553	4.175369	3.414898
12	6	0	1.731501	5.696252	3.313292
13	8	0	2.498224	1.558155	-0.119292
14	6	0	2.940165	0.465226	-0.880281
15	6	0	4.443143	0.613072	-1.189688
16	7	0	4.819845	1.690816	-1.934900
17	6	0	6.226996	1.863758	-2.270926
18	6	0	2.607106	-0.796637	-0.005537
19	8	0	0.077649	1.122123	-0.037907
20	6	0	-0.992807	2.025144	0.097736
21	6	0	-2.197059	1.543825	-0.676924
22	6	0	-3.470722	1.801125	-0.265619
23	1	0	-3.598446	2.139588	0.763410
24	53	0	-1.289447	-2.893729	1.957063
25	6	0	-4.708622	1.684203	-1.028841
26	8	0	5.260267	-0.222370	-0.788310
27	6	0	3.923046	2.721001	-2.443981
28	6	0	4.190025	-3.146349	-1.008580
29	1	0	3.490001	-1.113534	0.551218
30	1	0	2.387723	0.396487	-1.834453
31	1	0	-1.260763	2.184633	1.152292

32	1	0	-0.700199	3.005268	-0.312637
33	1	0	-2.936996	-0.429306	0.999365
34	1	0	-1.996161	1.246366	-1.704837
35	1	0	3.838667	2.656090	-3.538004
36	1	0	4.330009	3.708585	-2.193678
37	1	0	2.941837	2.641617	-1.982542
38	1	0	6.791687	1.031463	-1.854015
39	1	0	6.603603	2.807704	-1.856592
40	1	0	6.356646	1.889315	-3.360985
41	1	0	1.775047	6.165545	4.303460
42	1	0	0.892907	6.148652	2.768139
43	1	0	2.652069	5.962270	2.778410
44	1	0	2.406565	3.755458	3.992219
45	1	0	0.661472	3.940611	3.987890
46	1	0	0.672072	3.910864	1.475449
47	1	0	2.412881	3.708353	1.479433
48	1	0	2.181086	1.553547	2.752175
49	1	0	0.441199	1.698987	2.711388
50	1	0	4.677037	-2.214277	-0.726356
51	1	0	4.680129	-3.522944	-1.912468
52	1	0	4.303140	-3.897023	-0.216486
53	1	0	1.067403	-3.869595	-2.106757
54	1	0	2.354882	-4.984101	-1.572744
55	1	0	2.552986	-4.060643	-3.082621
56	6	0	-5.938475	1.815898	-0.351660
57	6	0	-7.149082	1.716911	-1.031830
58	6	0	-7.160651	1.485743	-2.409693
59	6	0	-5.951553	1.356948	-3.099869
60	6	0	-4.740105	1.456289	-2.421134
61	1	0	-5.934140	1.995764	0.720738
62	1	0	-8.083840	1.820293	-0.487929
63	1	0	-8.103974	1.411063	-2.943274
64	1	0	-5.953586	1.185516	-4.172792
65	1	0	-3.810020	1.375527	-2.975836
66	6	0	-3.273851	-1.461864	-0.871956
67	1	0	-4.121262	-0.842506	-1.198474
68	1	0	-2.733148	-1.810275	-1.757297
69	1	0	-3.717491	-2.331966	-0.372607



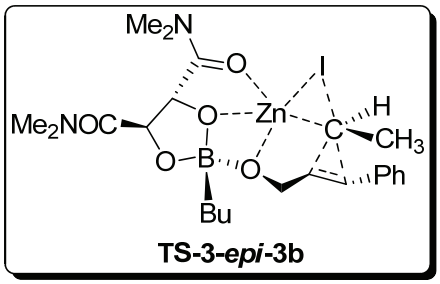
TS-*ent*-3b

Imaginary frequency: -161.6 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.833157	2.790397	1.210182
2	6	0	3.893686	1.818846	1.608932
3	6	0	4.296799	0.850373	2.547401
4	6	0	5.590788	0.844940	3.064840
5	6	0	6.510785	1.811284	2.654744
6	6	0	6.125354	2.783992	1.726294
7	6	0	2.518386	1.768680	1.102584
8	6	0	1.967915	2.540666	0.131709
9	6	0	0.504431	2.568147	-0.228439
10	8	0	-0.143157	1.393519	0.164725
11	5	0	-1.534570	1.000193	-0.249174
12	8	0	-2.400302	0.909144	0.931483
13	6	0	-2.775033	-0.394857	1.247841
14	6	0	-1.886887	-1.333949	0.354632
15	8	0	-1.325861	-0.484543	-0.623457
16	30	0	0.747894	-0.530229	-0.689816
17	53	0	1.727231	-2.499062	-2.355750
18	6	0	2.478060	0.413449	-1.136691
19	8	0	0.414524	-1.586048	1.047098
20	6	0	-0.764192	-2.003690	1.167333
21	7	0	-1.048161	-3.020314	1.999881
22	6	0	-2.370266	-3.621527	2.172796
23	6	0	0.023584	-3.662909	2.759357
24	6	0	-2.173224	1.814036	-1.488056
25	6	0	-2.747458	3.207168	-1.172563
26	6	0	-3.442754	3.877361	-2.366532
27	6	0	-4.025915	5.256720	-2.040446
28	6	0	-4.283220	-0.710718	1.027841
29	8	0	-4.606857	-1.807214	0.555284
30	7	0	-5.213019	0.206123	1.416445
31	6	0	-4.957684	1.441810	2.148280

32	6	0	-6.623964	-0.103993	1.215300
33	1	0	1.865435	1.039415	1.577565
34	1	0	-2.507799	-2.088708	-0.131495
35	1	0	-2.578722	-0.590237	2.316323
36	1	0	0.407333	2.753080	-1.310130
37	1	0	0.062477	3.450489	0.267607
38	6	0	2.915505	1.161914	-2.356067
39	1	0	3.347688	0.020969	-0.597024
40	1	0	2.567219	3.307242	-0.357324
41	1	0	-5.426228	1.388153	3.141089
42	1	0	-5.401411	2.288774	1.609546
43	1	0	-3.891924	1.626190	2.244349
44	1	0	-6.705256	-1.015473	0.625747
45	1	0	-7.114493	0.725514	0.691600
46	1	0	-7.128536	-0.249499	2.180316
47	1	0	-4.516880	5.704443	-2.912736
48	1	0	-3.243423	5.950634	-1.707343
49	1	0	-4.770446	5.192326	-1.236659
50	1	0	-4.242802	3.217429	-2.731545
51	1	0	-2.727445	3.969244	-3.196913
52	1	0	-1.956733	3.880744	-0.807972
53	1	0	-3.463723	3.118747	-0.343313
54	1	0	-2.989670	1.190745	-1.883574
55	1	0	-1.457539	1.897968	-2.323239
56	1	0	-3.136991	-3.115868	1.586448
57	1	0	-2.652510	-3.582290	3.232156
58	1	0	-2.332226	-4.674407	1.867892
59	1	0	0.966377	-3.165697	2.543205
60	1	0	0.094116	-4.719363	2.475611
61	1	0	-0.194145	-3.601445	3.832190
62	1	0	3.582403	0.095176	2.866005
63	1	0	5.880504	0.086422	3.786665
64	1	0	7.520154	1.810916	3.056501
65	1	0	6.835065	3.542866	1.408361
66	1	0	4.549269	3.562969	0.501451
67	1	0	3.819992	1.764140	-2.201113
68	1	0	3.181967	0.391981	-3.095442
69	1	0	2.126034	1.774224	-2.802685



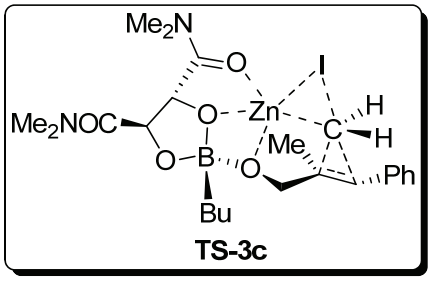
TS-3-*epi*-3b

Imaginary frequency: -259.4 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.351747	-0.014735	-0.731471
2	30	0	0.531422	-0.726897	-0.224179
3	8	0	-0.382511	-1.928009	1.136394
4	6	0	-1.611945	-2.104722	0.939932
5	7	0	-2.248191	-3.138355	1.515788
6	6	0	-1.505259	-4.073443	2.361067
7	8	0	-1.471627	-0.308165	-0.669804
8	5	0	-1.471158	1.131896	-0.107945
9	6	0	-1.574528	2.228846	-1.284699
10	6	0	-1.953593	3.653844	-0.841392
11	6	0	-2.127849	4.642551	-2.003046
12	6	0	-2.523892	6.052958	-1.552514
13	8	0	-2.619008	1.119443	0.800828
14	6	0	-3.253591	-0.119402	0.885190
15	6	0	-4.721053	-0.108726	0.368432
16	7	0	-5.539488	0.912516	0.746142
17	6	0	-6.915063	0.921497	0.261732
18	6	0	-2.382174	-1.119595	0.041359
19	8	0	-0.176075	1.118388	0.670852
20	6	0	0.777765	2.152971	0.726660
21	6	0	2.135910	1.574098	1.046672
22	6	0	3.310315	2.133424	0.649270
23	1	0	3.257652	2.925898	-0.097457
24	53	0	1.771515	-2.770486	-1.783900
25	6	0	4.663556	1.794406	1.087165
26	8	0	-5.126321	-1.044945	-0.331247
27	6	0	-5.219086	1.971238	1.696853
28	6	0	-3.662296	-3.464714	1.333911
29	1	0	-3.014172	-1.661822	-0.664578
30	1	0	-3.299355	-0.450169	1.937508
31	1	0	0.822915	2.727600	-0.208540

32	1	0	0.505475	2.860307	1.527381
33	1	0	3.238704	-0.467633	-0.287148
34	1	0	2.128834	0.814842	1.826711
35	1	0	-5.868337	1.886431	2.579590
36	1	0	-5.401235	2.950026	1.235114
37	1	0	-4.175088	1.929745	1.992396
38	1	0	-7.038934	0.120753	-0.465183
39	1	0	-7.137282	1.888384	-0.206130
40	1	0	-7.617379	0.770874	1.092934
41	1	0	-2.639343	6.732039	-2.405686
42	1	0	-1.766904	6.483967	-0.884759
43	1	0	-3.475180	6.041726	-1.005493
44	1	0	-2.887003	4.251590	-2.695686
45	1	0	-1.192694	4.692279	-2.580231
46	1	0	-1.199617	4.057802	-0.147881
47	1	0	-2.887593	3.607721	-0.263985
48	1	0	-2.343212	1.872610	-1.987016
49	1	0	-0.647112	2.268471	-1.880959
50	1	0	-4.177850	-2.743647	0.700313
51	1	0	-4.157870	-3.492554	2.312224
52	1	0	-3.748299	-4.458773	0.878755
53	1	0	-0.453764	-3.795960	2.369451
54	1	0	-1.613908	-5.088791	1.963595
55	1	0	-1.904763	-4.051346	3.382044
56	6	0	5.753927	2.418290	0.449994
57	6	0	7.065980	2.127168	0.817656
58	6	0	7.317552	1.204013	1.833900
59	6	0	6.246302	0.578633	2.481374
60	6	0	4.936110	0.870574	2.117061
61	1	0	5.562315	3.139077	-0.341566
62	1	0	7.890836	2.620034	0.310592
63	1	0	8.339033	0.974025	2.123442
64	1	0	6.435589	-0.137233	3.276498
65	1	0	4.118129	0.382930	2.639077
66	6	0	2.641850	0.756360	-1.995835
67	1	0	3.683097	1.081920	-2.093325
68	1	0	2.424694	0.101671	-2.846571
69	1	0	1.976418	1.622341	-2.098981



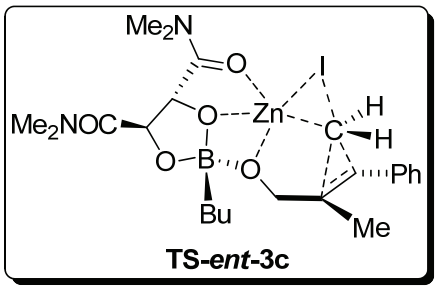
TS-3c

Imaginary frequency: -336.8 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.364956	-0.380639	-0.399899
2	30	0	0.456314	-0.867646	-0.065381
3	8	0	-0.600901	-2.053983	1.185045
4	6	0	-1.828252	-2.146363	0.918244
5	7	0	-2.561282	-3.142418	1.439097
6	6	0	-1.930897	-4.140765	2.303689
7	8	0	-1.477764	-0.352594	-0.653483
8	5	0	-1.435135	1.104521	-0.119135
9	6	0	-1.577931	2.166837	-1.321218
10	6	0	-1.799984	3.632636	-0.905953
11	6	0	-2.026788	4.587757	-2.086554
12	6	0	-2.257872	6.041992	-1.661219
13	8	0	-2.537085	1.109779	0.849888
14	6	0	-3.312392	-0.046000	0.814843
15	6	0	-4.728338	0.117264	0.187814
16	7	0	-5.460697	1.227103	0.482086
17	6	0	-6.790207	1.359919	-0.103343
18	6	0	-2.480149	-1.100543	-0.002578
19	8	0	-0.125412	1.103143	0.625383
20	6	0	0.921336	2.037479	0.477737
21	6	0	2.246342	1.452529	0.959232
22	6	0	3.391768	1.815288	0.293000
23	1	0	3.236203	2.298632	-0.671667
24	53	0	1.780403	-2.777401	-1.791071
25	6	0	4.807532	1.663959	0.642463
26	8	0	-5.178162	-0.792758	-0.519805
27	6	0	-5.115768	2.260024	1.453234
28	6	0	-3.984576	-3.362369	1.179146
29	1	0	-3.115766	-1.588248	-0.743737
30	1	0	-3.480846	-0.407558	1.843695
31	1	0	1.019796	2.377755	-0.560739

32	1	0	0.705637	2.924303	1.095332
33	1	0	2.632035	0.071133	-1.353815
34	1	0	3.230377	-0.842775	0.071785
35	1	0	-5.842417	2.250553	2.277824
36	1	0	-5.159470	3.246563	0.974657
37	1	0	-4.110151	2.115799	1.836488
38	1	0	-6.932479	0.572681	-0.841488
39	1	0	-6.887308	2.342678	-0.580303
40	1	0	-7.563674	1.274497	0.672172
41	1	0	-2.416096	6.695836	-2.527119
42	1	0	-1.398359	6.433467	-1.102089
43	1	0	-3.138663	6.130573	-1.012435
44	1	0	-2.887337	4.235461	-2.673411
45	1	0	-1.161504	4.537916	-2.763655
46	1	0	-0.945088	4.001527	-0.318808
47	1	0	-2.665204	3.686177	-0.229671
48	1	0	-2.439719	1.847559	-1.927584
49	1	0	-0.717910	2.109759	-2.009012
50	1	0	-4.418123	-2.584246	0.551193
51	1	0	-4.526113	-3.388916	2.132538
52	1	0	-4.116949	-4.331393	0.683094
53	1	0	-0.862892	-3.944289	2.364287
54	1	0	-2.098144	-5.140139	1.886726
55	1	0	-2.374024	-4.099857	3.305780
56	6	0	5.746141	1.697323	-0.411238
57	6	0	7.110401	1.568968	-0.171529
58	6	0	7.579538	1.420583	1.136360
59	6	0	6.669944	1.411122	2.195623
60	6	0	5.301954	1.531767	1.956540
61	1	0	5.388683	1.813729	-1.431577
62	1	0	7.808306	1.587008	-1.004020
63	1	0	8.644391	1.323149	1.328400
64	1	0	7.026864	1.316707	3.217694
65	1	0	4.622987	1.554836	2.799648
66	6	0	2.200919	0.833045	2.337722
67	1	0	2.999448	0.104430	2.494955
68	1	0	2.292468	1.611329	3.108158
69	1	0	1.238350	0.340048	2.493345



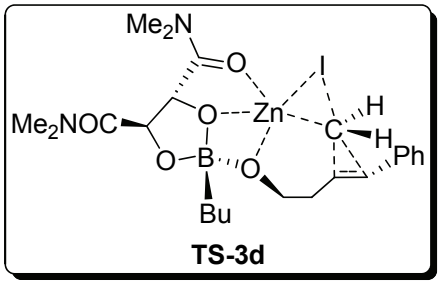
TS-*ent*-3c

Imaginary frequency: -206.2 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.494673	0.029716	-0.798789
2	30	0	0.762061	-0.854733	-0.425803
3	8	0	0.132503	-1.993387	1.143145
4	6	0	-1.097269	-2.255901	1.097657
5	7	0	-1.600687	-3.295750	1.781269
6	6	0	-0.712112	-4.156362	2.562379
7	8	0	-1.235526	-0.552619	-0.594606
8	5	0	-1.433437	0.978495	-0.250360
9	6	0	-2.248117	1.689278	-1.450289
10	6	0	-2.722819	3.127723	-1.174542
11	6	0	-3.584388	3.727567	-2.295014
12	6	0	-4.054922	5.157411	-2.005654
13	8	0	-2.152345	0.876500	1.028806
14	6	0	-2.801290	-0.344071	1.175978
15	6	0	-4.318273	-0.368099	0.821862
16	7	0	-5.108048	0.660329	1.239558
17	6	0	-6.533089	0.613273	0.931669
18	6	0	-2.017998	-1.357870	0.260298
19	8	0	-0.077667	1.472532	0.045895
20	6	0	0.654045	2.272392	-0.834613
21	6	0	2.133280	2.322186	-0.487080
22	6	0	2.570025	1.846000	0.720580
23	1	0	1.796889	1.377906	1.323449
24	53	0	2.056178	-2.653417	-2.131726
25	6	0	3.888475	1.942497	1.368154
26	8	0	-4.781584	-1.345765	0.221887
27	6	0	-4.708163	1.740512	2.135471
28	6	0	-3.005540	-3.704587	1.770021
29	1	0	-2.717905	-1.954032	-0.327571
30	1	0	-2.739210	-0.655948	2.232005

31	1	0	0.564036	1.933367	-1.878774
32	1	0	0.291985	3.315567	-0.824758
33	1	0	2.723626	0.417791	-1.793340
34	1	0	3.426265	-0.261449	-0.308955
35	1	0	-5.199183	1.621272	3.112016
36	1	0	-5.025507	2.701543	1.712585
37	1	0	-3.628707	1.763914	2.255055
38	1	0	-6.715182	-0.188874	0.218599
39	1	0	-6.849357	1.572653	0.505396
40	1	0	-7.121188	0.428604	1.841365
41	1	0	-4.669329	5.554743	-2.822351
42	1	0	-3.202699	5.835748	-1.870534
43	1	0	-4.654843	5.199299	-1.087400
44	1	0	-4.457425	3.080095	-2.461165
45	1	0	-3.016051	3.712181	-3.236347
46	1	0	-1.861102	3.791152	-1.003349
47	1	0	-3.294177	3.144232	-0.235542
48	1	0	-3.134856	1.070726	-1.661676
49	1	0	-1.671993	1.671398	-2.389828
50	1	0	-3.635196	-3.011163	1.213008
51	1	0	-3.372610	-3.761928	2.801824
52	1	0	-3.092099	-4.700970	1.319810
53	1	0	0.312975	-3.809252	2.454013
54	1	0	-0.790704	-5.187566	2.199770
55	1	0	-1.004009	-4.132083	3.618876
56	6	0	4.213246	0.967329	2.332832
57	6	0	5.434689	0.991504	2.999848
58	6	0	6.355292	2.008899	2.735703
59	6	0	6.037778	3.001399	1.806771
60	6	0	4.819243	2.971215	1.129039
61	1	0	3.496104	0.178925	2.548188
62	1	0	5.666330	0.221036	3.729955
63	1	0	7.307236	2.034361	3.258638
64	1	0	6.738171	3.809094	1.612434
65	1	0	4.580543	3.772589	0.440012
66	6	0	2.972137	3.074632	-1.490181
67	1	0	2.931562	4.154947	-1.294421
68	1	0	4.020590	2.769244	-1.467490
69	1	0	2.589632	2.921485	-2.505515



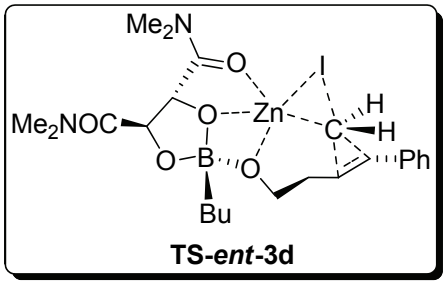
TS-3d

Imaginary frequency: -330.0 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.439992	-0.900555	0.565007
2	30	0	0.610917	-0.092565	0.626208
3	8	0	0.495824	1.805891	-0.166994
4	6	0	-0.599044	2.407102	-0.024190
5	7	0	-0.681724	3.734042	-0.218102
6	6	0	0.518180	4.499024	-0.555993
7	8	0	-1.463035	0.344751	0.860835
8	5	0	-1.925011	-0.782796	-0.075536
9	6	0	-2.982268	-1.754982	0.648896
10	6	0	-3.371267	-3.024470	-0.128116
11	6	0	-4.444597	-3.877781	0.563506
12	6	0	-4.803343	-5.153177	-0.207046
13	8	0	-2.403828	-0.040748	-1.255480
14	6	0	-2.716856	1.276322	-0.925387
15	6	0	-4.212425	1.601548	-0.637254
16	7	0	-5.198321	0.956655	-1.319564
17	6	0	-6.584960	1.296974	-1.016912
18	6	0	-1.849880	1.599947	0.351102
19	8	0	-0.606472	-1.455853	-0.377282
20	6	0	-0.298661	-1.997038	-1.651566
21	6	0	2.226714	-1.458318	-1.674055
22	6	0	3.553544	-1.762556	-1.581070
23	1	0	3.814478	-2.787718	-1.316328
24	53	0	1.904587	-0.099666	3.174356
25	6	0	4.695270	-0.880375	-1.830415
26	8	0	-4.464752	2.494335	0.182013
27	6	0	-5.028368	0.062910	-2.460841
28	6	0	-1.897036	4.533161	-0.051071
29	1	0	-2.447930	2.132213	1.091691
30	1	0	-2.432650	1.934960	-1.762194
31	1	0	-0.979348	-2.830718	-1.865255

32	1	0	-0.455129	-1.238747	-2.432205
33	1	0	2.626336	-1.917881	0.905874
34	1	0	3.356685	-0.315210	0.532648
35	1	0	1.934485	-0.471798	-2.030065
36	1	0	-5.485342	0.514308	-3.352662
37	1	0	-5.535915	-0.889660	-2.263827
38	1	0	-3.977424	-0.141335	-2.639860
39	1	0	-6.614583	1.897292	-0.109492
40	1	0	-7.164646	0.377010	-0.877232
41	1	0	-7.033563	1.867216	-1.841960
42	1	0	-5.572183	-5.737236	0.312781
43	1	0	-3.925071	-5.798865	-0.333860
44	1	0	-5.185301	-4.918204	-1.209049
45	1	0	-5.349347	-3.269657	0.709003
46	1	0	-4.095744	-4.143803	1.571439
47	1	0	-2.476782	-3.647039	-0.280963
48	1	0	-3.728506	-2.755185	-1.134696
49	1	0	-3.896975	-1.182011	0.873786
50	1	0	-2.575910	-2.051224	1.628171
51	1	0	-2.785134	3.915298	0.083155
52	1	0	-2.036812	5.156171	-0.942303
53	1	0	-1.787203	5.195996	0.816192
54	1	0	1.377032	3.831907	-0.577697
55	1	0	0.677977	5.280085	0.196107
56	1	0	0.393113	4.976479	-1.535085
57	6	0	5.994198	-1.417469	-1.747832
58	6	0	7.117410	-0.630803	-1.994350
59	6	0	6.968182	0.717386	-2.323753
60	6	0	5.685312	1.269072	-2.404225
61	6	0	4.562704	0.483311	-2.163083
62	1	0	6.116975	-2.466354	-1.488079
63	1	0	8.108857	-1.070005	-1.925478
64	1	0	7.841504	1.334937	-2.513920
65	1	0	5.560972	2.318849	-2.656320
66	1	0	3.576549	0.934088	-2.226177
67	6	0	1.140092	-2.516488	-1.700288
68	1	0	1.293225	-3.247980	-0.897203
69	1	0	1.238796	-3.071299	-2.645794



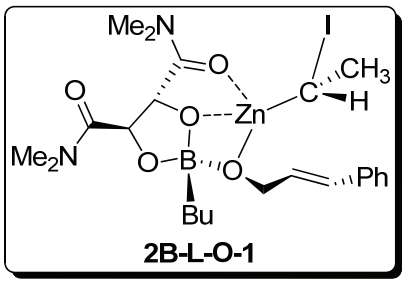
TS-*ent*-3d

Imaginary frequency: -367.2 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.395945	-0.430590	0.392740
2	30	0	0.410247	-0.594337	0.225166
3	8	0	-0.889699	-1.927639	1.064663
4	6	0	-1.921071	-2.102687	0.360214
5	7	0	-2.540001	-3.289552	0.344126
6	6	0	-1.952391	-4.419260	1.068787
7	8	0	-1.334697	-0.118654	-0.854384
8	5	0	-1.475648	1.315811	-0.312751
9	6	0	-1.150960	2.450396	-1.408976
10	6	0	-1.786348	3.831300	-1.158203
11	6	0	-1.522737	4.847983	-2.277730
12	6	0	-2.168081	6.215262	-2.025415
13	8	0	-2.848229	1.350663	0.169390
14	6	0	-3.292165	0.055320	0.476887
15	6	0	-4.809779	-0.062872	0.226285
16	7	0	-5.626830	0.751689	0.952186
17	6	0	-7.068861	0.657297	0.764516
18	6	0	-2.446578	-0.899631	-0.440514
19	8	0	-0.464763	1.204456	0.825697
20	6	0	0.106645	2.296912	1.509056
21	6	0	2.566091	1.604635	1.290919
22	6	0	3.783225	1.170512	1.743355
23	1	0	3.816341	0.754100	2.751132
24	53	0	1.859437	-2.694632	-1.271317
25	6	0	5.067752	1.197541	1.047812
26	8	0	-5.255476	-0.880371	-0.586103
27	6	0	-5.187875	1.736260	1.933280
28	6	0	-3.719634	-3.618455	-0.461285
29	1	0	-3.024963	-1.199780	-1.314164
30	1	0	-3.090475	-0.190605	1.534078
31	1	0	0.326489	3.116529	0.809888

32	1	0	-0.605474	2.684236	2.252515
33	1	0	3.054584	-0.149023	-0.423701
34	1	0	2.924337	-1.065756	1.104350
35	1	0	2.512451	2.104337	0.325004
36	1	0	-5.484120	1.430245	2.946456
37	1	0	-5.665543	2.699961	1.716693
38	1	0	-4.111899	1.882191	1.881351
39	1	0	-7.277096	-0.124493	0.035961
40	1	0	-7.468858	1.613160	0.402804
41	1	0	-7.559650	0.415662	1.716463
42	1	0	-1.963381	6.916445	-2.843287
43	1	0	-1.791477	6.666769	-1.098458
44	1	0	-3.257474	6.126350	-1.927942
45	1	0	-1.892149	4.437653	-3.228446
46	1	0	-0.437433	4.973904	-2.406061
47	1	0	-1.426494	4.255491	-0.207804
48	1	0	-2.870152	3.704828	-1.031610
49	1	0	-1.517347	2.077684	-2.377259
50	1	0	-0.062624	2.569931	-1.543071
51	1	0	-4.289510	-2.727475	-0.721007
52	1	0	-4.365806	-4.272937	0.132760
53	1	0	-3.417736	-4.160178	-1.366171
54	1	0	-1.007627	-4.113657	1.511634
55	1	0	-1.778438	-5.243123	0.368271
56	1	0	-2.641768	-4.758471	1.850646
57	6	0	6.182078	0.596131	1.664963
58	6	0	7.432851	0.600074	1.052637
59	6	0	7.598299	1.206290	-0.194137
60	6	0	6.503744	1.812813	-0.819469
61	6	0	5.254984	1.813560	-0.206943
62	1	0	6.056721	0.117895	2.633575
63	1	0	8.277105	0.127157	1.546494
64	1	0	8.571926	1.209296	-0.675882
65	1	0	6.626649	2.289989	-1.787710
66	1	0	4.421233	2.300983	-0.703731
67	6	0	1.396214	1.877149	2.218601
68	1	0	1.682671	2.704924	2.884442
69	1	0	1.200282	1.014051	2.867783

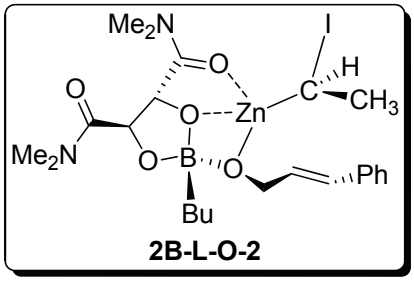


2B-L-O-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.728226	-2.625142	-2.380469
2	6	0	6.737993	-2.659362	-0.985588
3	6	0	5.535862	-2.664259	-0.279172
4	6	0	4.298376	-2.629995	-0.946449
5	6	0	4.306950	-2.603961	-2.354039
6	6	0	5.506201	-2.599102	-3.060340
7	6	0	3.063159	-2.624453	-0.147728
8	6	0	1.804118	-2.448956	-0.580076
9	6	0	0.606852	-2.484002	0.321057
10	8	0	-0.100690	-1.248368	0.232524
11	30	0	0.553417	0.674043	0.299244
12	8	0	-0.333410	1.522245	-1.353501
13	6	0	-1.562462	1.767550	-1.227631
14	7	0	-2.138627	2.738476	-1.951344
15	6	0	-1.314195	3.563254	-2.837413
16	5	0	-1.472434	-1.024713	0.900787
17	6	0	-1.589576	-1.578199	2.406332
18	6	0	-2.038064	-3.044055	2.558080
19	6	0	-2.235509	-3.481823	4.016341
20	6	0	-2.689936	-4.938425	4.160328
21	8	0	-2.558109	-1.441380	0.029982
22	6	0	-2.837922	-0.440816	-0.915171
23	6	0	-4.343923	-0.448533	-1.252589
24	7	0	-4.846377	-1.577727	-1.826206
25	6	0	-6.260450	-1.625279	-2.176419
26	6	0	-2.369360	0.901413	-0.245950
27	8	0	-1.505124	0.504293	0.807135
28	6	0	2.178180	1.528470	1.057057
29	6	0	3.441806	1.554789	0.210712
30	53	0	1.564530	3.680661	1.516626
31	8	0	-5.050500	0.538158	-1.019906
32	6	0	-4.085522	-2.782704	-2.133331

33	6	0	-3.539662	3.155686	-1.851788
34	1	0	-3.225900	1.434111	0.168396
35	1	0	-2.264592	-0.602914	-1.844459
36	1	0	0.910582	-2.682157	1.358197
37	1	0	-0.075831	-3.289534	0.014208
38	1	0	2.402818	1.183617	2.068247
39	1	0	1.591281	-2.269252	-1.633379
40	1	0	-3.984690	-2.910558	-3.220214
41	1	0	-4.618147	-3.656048	-1.737260
42	1	0	-3.105628	-2.753637	-1.663644
43	1	0	-6.718209	-0.672338	-1.916421
44	1	0	-6.759917	-2.434614	-1.628927
45	1	0	-6.378664	-1.811285	-3.251984
46	1	0	-2.822074	-5.218267	5.212313
47	1	0	-1.956561	-5.628094	3.722933
48	1	0	-3.645821	-5.107771	3.648589
49	1	0	-2.971679	-2.818708	4.492958
50	1	0	-1.295802	-3.335135	4.568827
51	1	0	-1.310014	-3.721575	2.086569
52	1	0	-2.977783	-3.187947	2.007073
53	1	0	-2.323023	-0.942448	2.925026
54	1	0	-0.643475	-1.428764	2.952233
55	1	0	-4.163177	2.377727	-1.413552
56	1	0	-3.910157	3.357626	-2.862411
57	1	0	-3.614400	4.080994	-1.266881
58	1	0	-0.274521	3.255025	-2.757214
59	1	0	-1.409764	4.615099	-2.545450
60	1	0	-1.657989	3.452963	-3.872285
61	1	0	5.549822	-2.690513	0.808088
62	1	0	3.368055	-2.596547	-2.900099
63	1	0	7.680934	-2.683144	-0.445966
64	1	0	5.489510	-2.579829	-4.146895
65	1	0	7.662465	-2.623319	-2.935199
66	1	0	3.213049	-2.778253	0.922081
67	1	0	4.268646	2.096337	0.687601
68	1	0	3.770113	0.517229	0.049083
69	1	0	3.270943	2.001758	-0.774158

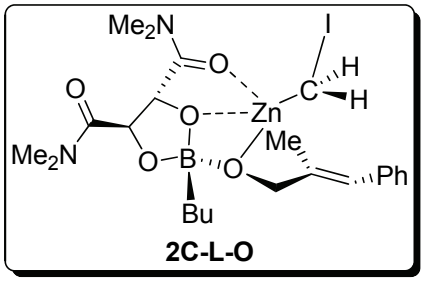


2B-L-O-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.368990	1.001479	-0.145444
2	6	0	-2.906029	-0.281343	-0.877659
3	8	0	-2.640117	-1.344522	0.000225
4	5	0	-1.511999	-1.021767	0.857528
5	8	0	-1.490243	0.512017	0.854828
6	8	0	-0.172598	-1.255186	0.133935
7	30	0	0.558092	0.639105	0.288737
8	6	0	0.503927	-2.511470	0.146294
9	6	0	2.245090	1.314591	1.090228
10	53	0	1.973173	3.566849	1.337524
11	6	0	1.689319	-2.455697	-0.769501
12	6	0	2.951467	-2.667201	-0.362991
13	6	0	-4.419109	-0.215627	-1.173427
14	8	0	-5.082848	0.779920	-0.864746
15	7	0	-4.976824	-1.290415	-1.798132
16	6	0	-4.270901	-2.504084	-2.190507
17	6	0	-6.400257	-1.268075	-2.110788
18	6	0	-2.787917	-5.070348	3.923345
19	6	0	-2.283132	-3.624964	3.849576
20	6	0	-2.106420	-3.111720	2.413533
21	6	0	-1.608456	-1.656036	2.332381
22	6	0	-1.558505	1.893718	-1.100311
23	8	0	-0.342881	1.612538	-1.276033
24	7	0	-2.116382	2.924141	-1.751646
25	6	0	-3.498951	3.382478	-1.593019
26	6	0	-1.286577	3.765317	-2.617559
27	1	0	-3.193337	1.539076	0.324519
28	1	0	-2.363337	-0.408993	-1.830479
29	1	0	0.817136	-2.771021	1.166794
30	1	0	-0.202937	-3.282791	-0.192028
31	1	0	3.077112	1.306019	0.383371
32	1	0	1.464973	-2.226055	-1.810603

33	1	0	-4.214825	-2.581216	-3.285268
34	1	0	-4.819055	-3.377592	-1.816352
35	1	0	-3.273785	-2.531530	-1.758687
36	1	0	-6.813003	-0.310397	-1.798129
37	1	0	-6.917953	-2.080387	-1.584913
38	1	0	-6.552473	-1.402639	-3.189612
39	1	0	-2.904135	-5.405411	4.960961
40	1	0	-2.092038	-5.759484	3.427741
41	1	0	-3.761914	-5.175258	3.428848
42	1	0	-2.981836	-2.964417	4.382827
43	1	0	-1.324880	-3.543769	4.383284
44	1	0	-1.415800	-3.786348	1.885038
45	1	0	-3.064122	-3.190347	1.880879
46	1	0	-2.304269	-1.026137	2.907036
47	1	0	-0.643377	-1.571547	2.858590
48	1	0	-4.137663	2.605590	-1.175335
49	1	0	-3.889087	3.646198	-2.581833
50	1	0	-3.525434	4.280155	-0.962664
51	1	0	-0.252890	3.431622	-2.567235
52	1	0	-1.354400	4.805935	-2.281581
53	1	0	-1.648618	3.705112	-3.650410
54	6	0	4.176492	-2.651482	-1.176506
55	6	0	5.419483	-2.770078	-0.530038
56	6	0	4.170341	-2.521882	-2.578295
57	6	0	6.613367	-2.749886	-1.249963
58	1	0	5.444718	-2.874341	0.552342
59	6	0	5.361263	-2.501316	-3.298288
60	1	0	3.226458	-2.443156	-3.109911
61	6	0	6.589342	-2.613879	-2.638488
62	1	0	7.561049	-2.840465	-0.725930
63	1	0	5.333170	-2.400696	-4.380119
64	1	0	7.517059	-2.598790	-3.203874
65	1	0	3.112581	-2.875404	0.696077
66	6	0	2.680927	0.728926	2.424719
67	1	0	2.882607	-0.343008	2.276015
68	1	0	3.596622	1.186873	2.819878
69	1	0	1.904043	0.814567	3.191242

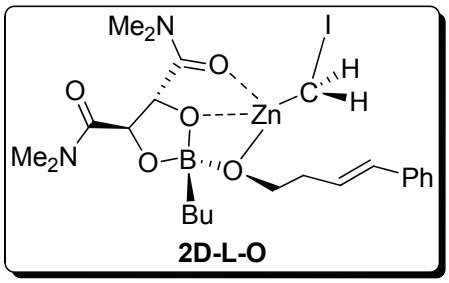


2C-L-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.348332	1.071399	-0.155520
2	6	0	-2.908644	-0.235799	-0.828697
3	8	0	-2.621882	-1.273983	0.071131
4	5	0	-1.519187	-0.911032	0.943851
5	8	0	-1.517281	0.620846	0.901019
6	8	0	-0.158823	-1.146535	0.257887
7	30	0	0.559645	0.743187	0.447395
8	6	0	0.508789	-2.408075	0.268415
9	6	0	2.174707	1.482010	1.309937
10	53	0	2.068820	3.717482	1.388820
11	6	0	1.695596	-2.377938	-0.667281
12	6	0	2.931947	-2.544337	-0.155281
13	6	0	-4.432611	-0.171816	-1.076924
14	8	0	-5.080459	0.838884	-0.784085
15	7	0	-5.015447	-1.265262	-1.642977
16	6	0	-4.330362	-2.498125	-2.012235
17	6	0	-6.449292	-1.247087	-1.905380
18	6	0	-2.794540	-4.890216	4.100431
19	6	0	-2.311204	-3.439682	3.993603
20	6	0	-2.112020	-2.966251	2.546779
21	6	0	-1.636765	-1.505302	2.433666
22	6	0	-1.490768	1.885887	-1.139656
23	8	0	-0.261180	1.623844	-1.213472
24	7	0	-2.027858	2.832004	-1.924623
25	6	0	-3.422778	3.276796	-1.890186
26	6	0	-1.164398	3.596281	-2.827946
27	1	0	-3.168917	1.661275	0.255451
28	1	0	-2.402023	-0.398168	-1.796198
29	1	0	0.826429	-2.662597	1.287545
30	1	0	-0.210023	-3.172858	-0.060760
31	1	0	2.308825	1.207623	2.356810
32	1	0	3.110241	1.297854	0.780554

33	1	0	-4.318197	-2.619632	-3.104299
34	1	0	-4.866914	-3.352706	-1.581775
35	1	0	-3.317068	-2.513987	-1.619441
36	1	0	-6.845332	-0.273012	-1.623347
37	1	0	-6.952420	-2.030267	-1.324068
38	1	0	-6.640365	-1.430693	-2.970633
39	1	0	-2.927349	-5.195817	5.145126
40	1	0	-2.077451	-5.582358	3.640606
41	1	0	-3.756155	-5.026063	3.589429
42	1	0	-3.031386	-2.775057	4.492107
43	1	0	-1.365909	-3.327031	4.544399
44	1	0	-1.398656	-3.643609	2.053370
45	1	0	-3.056866	-3.077101	1.996925
46	1	0	-2.354632	-0.871328	2.975927
47	1	0	-0.683935	-1.390376	2.976136
48	1	0	-4.067459	2.563323	-1.378686
49	1	0	-3.779265	3.381221	-2.920843
50	1	0	-3.487520	4.258231	-1.403906
51	1	0	-0.132649	3.277210	-2.700824
52	1	0	-1.251375	4.663596	-2.595419
53	1	0	-1.480101	3.436442	-3.865360
54	6	0	4.234206	-2.593271	-0.845443
55	6	0	5.364204	-2.069596	-0.188647
56	6	0	4.420454	-3.176341	-2.112320
57	6	0	6.621625	-2.089788	-0.787589
58	1	0	5.244768	-1.632577	0.800109
59	6	0	5.680688	-3.203045	-2.710049
60	1	0	3.580325	-3.640571	-2.618272
61	6	0	6.784755	-2.653906	-2.055377
62	1	0	7.475709	-1.669234	-0.263344
63	1	0	5.801241	-3.664491	-3.686810
64	1	0	7.765428	-2.675996	-2.522837
65	1	0	3.003275	-2.632309	0.929775
66	6	0	1.361631	-2.130218	-2.117863
67	1	0	2.225225	-1.785910	-2.691515
68	1	0	0.974578	-3.039160	-2.601287
69	1	0	0.573856	-1.371978	-2.188487



2D-L-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.065809	-1.899125	0.903485
2	30	0	0.722438	-0.769307	-0.015678
3	8	0	0.960269	1.267302	-0.213444
4	6	0	0.103606	1.994830	0.348655
5	7	0	0.351734	3.298675	0.561672
6	6	0	1.643231	3.867675	0.176056
7	8	0	-1.136074	-0.025790	0.772969
8	5	0	-1.960760	-0.620077	-0.361902
9	6	0	-3.013751	-1.705876	0.184024
10	6	0	-3.806613	-2.487044	-0.878135
11	6	0	-4.864073	-3.436053	-0.294858
12	6	0	-5.641618	-4.215297	-1.361347
13	8	0	-2.521972	0.563760	-1.028920
14	6	0	-2.386171	1.709491	-0.244328
15	6	0	-3.649791	2.188772	0.529119
16	7	0	-4.893678	2.000078	0.008850
17	6	0	-6.041677	2.466596	0.780153
18	6	0	-1.237656	1.379072	0.779435
19	8	0	-0.867378	-1.243905	-1.232743
20	6	0	-0.971776	-1.244822	-2.650648
21	6	0	1.470463	-0.672572	-2.989897
22	6	0	2.683573	-1.016725	-2.521797
23	1	0	2.868231	-2.072963	-2.321602
24	6	0	3.831250	-0.133645	-2.257607
25	8	0	-3.477281	2.787594	1.598713
26	6	0	-5.218271	1.530538	-1.334567
27	6	0	-0.549621	4.224869	1.248401
28	1	0	-1.510274	1.721442	1.778623
29	1	0	-2.099542	2.558826	-0.885912
30	1	0	-1.750707	-1.954741	-2.955699
31	1	0	-1.274898	-0.248146	-2.996681
32	1	0	1.859678	-2.970390	0.918287

33	1	0	3.096194	-1.743934	0.582486
34	1	0	1.245900	0.374065	-3.197062
35	1	0	-5.724924	2.331582	-1.891023
36	1	0	-5.902296	0.674908	-1.272362
37	1	0	-4.323293	1.215623	-1.861267
38	1	0	-5.717827	2.708919	1.790601
39	1	0	-6.804847	1.680165	0.808358
40	1	0	-6.482786	3.360889	0.318674
41	1	0	-6.385750	-4.883840	-0.912212
42	1	0	-4.968283	-4.830072	-1.972197
43	1	0	-6.172162	-3.535846	-2.041015
44	1	0	-5.566556	-2.856367	0.321474
45	1	0	-4.373581	-4.141523	0.390870
46	1	0	-3.112924	-3.077048	-1.495781
47	1	0	-4.303548	-1.785878	-1.566929
48	1	0	-3.726278	-1.190297	0.848640
49	1	0	-2.484276	-2.424775	0.828828
50	1	0	-1.528950	3.786422	1.441254
51	1	0	-0.682086	5.119363	0.628168
52	1	0	-0.103019	4.533499	2.201889
53	1	0	2.260421	3.095997	-0.279544
54	1	0	2.148982	4.264601	1.064107
55	1	0	1.488661	4.689384	-0.533333
56	6	0	4.991029	-0.685599	-1.685953
57	6	0	6.108429	0.102656	-1.411054
58	6	0	6.092182	1.465257	-1.708816
59	6	0	4.949228	2.029597	-2.285352
60	6	0	3.833859	1.242098	-2.557219
61	1	0	5.012054	-1.747944	-1.453761
62	1	0	6.990182	-0.349242	-0.965020
63	1	0	6.961089	2.082907	-1.499067
64	1	0	4.931907	3.088446	-2.531132
65	1	0	2.960190	1.697735	-3.013489
66	6	0	0.361548	-1.643673	-3.287726
67	1	0	0.640434	-2.653689	-2.962251
68	1	0	0.197838	-1.693054	-4.375839
69	53	0	2.152484	-1.375369	3.081026

2. Computed Energies of All Stationary Points

Table S1. Sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal correction to Enthalpy (*TCH*, in Hartree), thermal correction to Gibbs free energy (*TCGFE*, in Hartree), electronic energy (*E*, in Hartree), and total free energy in solution (E_S, in Hartree, solvent = dichloromethane)

Structure	H[a]	G[a]	TCH[a]	$TCGFE$[a]	E[b]	E_S[b]
2-M	-2253.263175	-2253.32773	0.199005	0.13445	-701.583042	-701.591911
TS-2-M	-2253.21766	-2253.277267	0.195937	0.13633	-701.531696	-701.553412
2-D	-4506.596257	-4506.703155	0.400527	0.293629	-1403.227023	-1403.227045
TS-2-D	-4506.563433	-4506.669399	0.398312	0.292346	-1403.188602	-1403.193661
2-T	-9013.264383	-9013.443432	0.803356	0.624307	-2806.503472	-2806.478574
TS-2-T	-9013.237511	-9013.414269	0.801576	0.624818	-2806.472745	-2806.452713
3-T	-9013.317553	-9013.498515	0.80537	0.624407	-2806.558674	-2806.535439
1	-906.091234	-906.170714	0.384388	0.304908	-906.737136	-906.731456
2-L-O	-3159.425046	-3159.541886	0.585558	0.468718	-1608.378685	-1608.365094
3-L-O	-3159.478321	-3159.592234	0.587922	0.47401	-1608.432038	-1608.421349
2-L-N	-3159.398686	-3159.514561	0.585183	0.469308	-1608.35179	-1608.339093
1'	-873.587411	-873.659371	0.375895	0.303935	-874.199883	-874.199454
2-L'	-3126.875062	-3126.988174	0.57664	0.463528	-1575.797892	-1575.792982
TS-3a	-3159.393242	-3159.504344	0.583822	0.472719	-1608.341597	-1608.33995
TS-*ent*-3a	-3159.385174	-3159.496527	0.583684	0.472331	-1608.334588	-1608.334415
TS-3b	-3198.676199	-3198.79199	0.613182	0.497391	-1647.666163	-1647.658915
TS-*ent*-3b	-3198.669387	-3198.785874	0.612928	0.496441	-1647.658937	-1647.65138
TS-3-*epi*-3b	-3198.672186	-3198.787197	0.613304	0.498294	-1647.661217	-1647.654863
TS-3c	-3198.675176	-3198.788678	0.613549	0.500048	-1647.663976	-1647.657698
TS-*ent*-3c	-3198.668714	-3198.783428	0.613096	0.498382	-1647.659289	-1647.653945
TS-3d	-3198.67748	-3198.792091	0.613697	0.499086	-1647.667962	-1647.661263
TS-*ent*-3d	-3198.674937	-3198.789983	0.614051	0.499005	-1647.665188	-1647.65933
2B-L-O-1	-3198.707192	-3198.827211	0.615378	0.495359	-1647.701469	-1647.685149
2B-L-O-2	-3198.707111	-3198.826942	0.615392	0.495561	-1647.701454	-1647.685375
2C-L-O	-3198.70959	-3198.829308	0.615402	0.495683	-1647.703189	-1647.684972
2D-L-O	-3198.710307	-3198.828269	0.615428	0.497465	-1647.702509	-1647.689905

[a] Computed at the B3LYP level of theory with the Ahlrichs' SVP all-electron basis set for the zinc atom and the 6-31G(d) basis set for other atoms except for the iodine atom, for which the LANL2DZ basis set was used.

[b] Computed at the B3LYP level of theory with the SDD basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms.

3. Full Citation of Reference 11

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

4. Comparison of Different Basis Sets and Atomic Radii Sets

In the initial submission of this paper, we conducted DFT calculations at the B3LYP level of theory using basis set **B1** (the Ahlrichs' SVP all-electron basis set for the zinc atom and the 6-31G(d) basis set for other atoms except for the iodine atom, for which the LANL2DZ basis set was used). A reviewer suggested that we should check the basis set dependence and compare different basis sets. During the revision, six different basis sets **B1-6** were compared. First, we conducted the comparison between experimental selectivities (enantioselectivity and diastereoselectivity) of reactions **A-D** (for details, see Scheme 2 in the paper) and DFT-calculation predicted ones using different basis sets **B1-6** (Table S2). It was found that all these calculations can repeat the experimental results in some extent. This implies that the choice of different basis sets has limited influence on understanding and predicting the selectivities (enantioselectivity and diastereoselectivity) of reactions **A-D**. Among them, the calculations using basis set **B5** (the SDD basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms) give the best results as compared with the experimental data. In addition, according to this reviewer's suggestion, the solvent effects were also computed with UAKS radii using different basis sets **B1-6** (Table S3). It was found that the results are very similar to those with UA0 radii. Therefore, we chose the basis set **B5** and the UA0 radii for the DFT calculations in the revised paper to discuss the reactions.

Table S2. Comparison between experimental selectivities of reactions **A-D** and DFT-calculation predicted ones using different basis sets **B1-6**[a] (solvent effects were computed at the B3LYP level of theory based on the gas-phase optimized structures using the CPCM model and the UA0 radii)

Reaction	Experimental Data		Predicted enantioselectivity and diastereoselectivity ($\Delta\Delta G_{DCM}$ in kcal/mol)[b]					
			B1	**B2**	**B3**	**B4**	**B5**	**B6**
A	ee	94%	100% (3.8)	100% (4.5)	99% (3.3)	100% (4.5)	99% (3.2)	100% (4.3)
B	ee	98%	100% (3.8)	100% (4.7)	100% (3.9)	100% (5.0)	100% (4.1)	100% (4.1)
	dr	>50:1	69:1 (2.5)	198:1 (3.1)	86:1 (2.6)	430:1 (3.6)	190:1 (3.1)	25:1 (1.9)
C	ee	85%	97% (2.5)	99% (3.4)	83% (1.4)	99% (3.3)	80% (1.3)	100% (3.6)
D	ee	82%	60% (0.8)	85% (1.5)	68% (1.0)	86% (1.5)	75% (1.2)	8% (0.1)

[a] **B1**: the Ahlrichs' SVP all-electron basis set for the zinc atom and the 6-31G(d) basis set for other atoms except for the iodine atom, for which the LANL2DZ basis set was used; **B2**: the LANL2DZ basis set for zinc and iodine atoms and the 6-31G(d) basis set for the other atoms; **B3**: the SDD

basis set for zinc and iodine atoms and the 6-31G(d) basis set for the other atoms; **B4**: the LANL2DZ basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms; **B5**: the SDD basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms; **B6**: the LANL2DZ basis set for the iodine atom and the 6-311G(d,p) basis set for the other atoms.
[b] $\Delta\Delta G_{DCM}$: the relative energies of two competing enantio-/diastereo-selective cyclopropanation transition states.

Table S3. Comparison between experimental selectivities of reactions **A-D** and DFT-calculation predicted ones using different basis sets **B1-6**[a] (solvent effects were computed at the B3LYP level of theory based on the gas-phase optimized structures using the CPCM model and the UAKS radii)

Reaction	Experimental Data		Predicted enantioselectivity and diastereoselectivity ($\Delta\Delta G_{DCM}$ in kcal/mol)[b]					
			B1	**B2**	**B3**	**B4**	**B5**	**B6**
A	ee	94%	100% (4.6)	100% (5.2)	100% (4.0)	100% (5.2)	100% (3.9)	100% (5.1)
B	ee	98%	100% (4.4)	100% (5.3)	100% (4.4)	100% (5.5)	100% (4.5)	100% (4.6)
	dr	>50:1	251:1 (3.3)	706:1 (3.9)	304:1 (3.4)	1344:1 (4.3)	596:1 (3.8)	73:1 (2.5)
C	ee	85%	99% (3.3)	100% (4.2)	94% (2.1)	100% (4.1)	93% (2.0)	100% (4.5)
D	ee	82%	65% (0.9)	87% (1.6)	71% (1.1)	88% (1.7)	79% (1.3)	21% (0.3)

[a] **B1**: the Ahlrichs' SVP all-electron basis set for the zinc atom and the 6-31G(d) basis set for other atoms except for the iodine atom, for which the LANL2DZ basis set was used; **B2**: the LANL2DZ basis set for zinc and iodine atoms and the 6-31G(d) basis set for the other atoms; **B3**: the SDD basis set for zinc and iodine atoms and the 6-31G(d) basis set for the other atoms; **B4**: the LANL2DZ basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms; **B5**: the SDD basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms; **B6**: the LANL2DZ basis set for the iodine atom and the 6-311G(d,p) basis set for the other atoms.
[b] $\Delta\Delta G_{DCM}$: the relative energies of two competing enantio-/diastereo-selective cyclopropanation transition states.

We then conducted the comparison of stability and reactivity between tetramer **2-T** and the chiral zinc complex **2-L-O** (for details, see Figure 3 in the paper) using different basis sets **B1-6** and radii sets (Table S4). It was found that all these calculations give similar results: the chiral zinc complex **2-L-O** is much more stable than tetramer **2-T**, and the enantioselective cyclopropanation pathway via transition state **TS-3a** is more favorable than the background reaction (via **TS-2-T**) leading to racemic products. This further indicates that the choice of different basis sets and radii sets has limited influence on understanding and predicting the reactivities of both asymmetric and racemic Simmons-Smith reactions. As suggested by this reviewer, the Ahlrichs' SVP all-electron basis set would underestimate the reaction barriers for Simmons-Smith type cyclopropanation reactions. The computed energy barriers using previously chosen basis set **B1** are 2-3 kcal/mol lower than those using basis set **B5**. Calculations with basis set **B5** showed that the background cyclopropanation requires an overall activation free energy of 16.5 kcal/mol. This result is in good agreement with the experimental observation reported by Charette and co-workers: the (*E*)-PhCH=CHCH$_2$OZnCH$_2$I was not stable for a long period of time at –20 °C, and its corresponding cyclopropane product appeared within 24 h. These computational results also support the choice of basis set **B5** to investigate the reactions in the paper.

Table S4. Comparison of stability and reactivity between tetramer **2-T** and the chiral zinc complex **2-L-O** using different basis sets **B1-6**[a] (solvent effects were computed at the B3LYP level of theory based on the gas-phase optimized structures using the CPCM model and the UA0 radii, and the results using the UAKS radii were given in the parenthesis)

Structure	ΔG_{DCM} in kcal/mol					
	B1	**B2**	**B3**	**B4**	**B5**	**B6**
2-T	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
TS-2-T	14.6 (15.9)	13.7 (14.9)	15.1 (16.1)	15.0 (16.0)	16.5 (17.4)	18.1 (19.4)
2-L-O	-5.4 (-7.0)	-6.2 (-7.8)	-7.2 (-8.8)	-3.5 (-5.0)	-3.9 (-5.4)	-4.2 (-5.7)
TS-3a	10.3 (12.6)	8.6 (10.9)	8.8 (11.0)	13.3 (15.4)	14.4 (16.4)	15.3 (17.8)

[a] **B1**: the Ahlrichs' SVP all-electron basis set for the zinc atom and the 6-31G(d) basis set for other atoms except for the iodine atom, for which the LANL2DZ basis set was used; **B2**: the LANL2DZ basis set for zinc and iodine atoms and the 6-31G(d) basis set for the other atoms; **B3**: the SDD basis set for zinc and iodine atoms and the 6-31G(d) basis set for the other atoms; **B4**: the LANL2DZ basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms; **B5**: the SDD basis set for zinc and iodine atoms and the 6-311G(d,p) basis set for the other atoms; **B6**: the LANL2DZ basis set for the iodine atom and the 6-311G(d,p) basis set for the other atoms.

5. Figure S1 and Discussion of the Entropy Overestimation in Solution

After the ASAP publication, Prof. Daniel A. Singleton from Texas A&M University pointed out to us that, mathematically, the drawing of the potential energy surfaces in the original Figures 1 and 3 should use 1 mol **2-T** as the reference point. We agree with this. The redrawn potential energy surfaces in Figure 1 using 1 mol **2-T** as the reference point were shown in Figure S1.

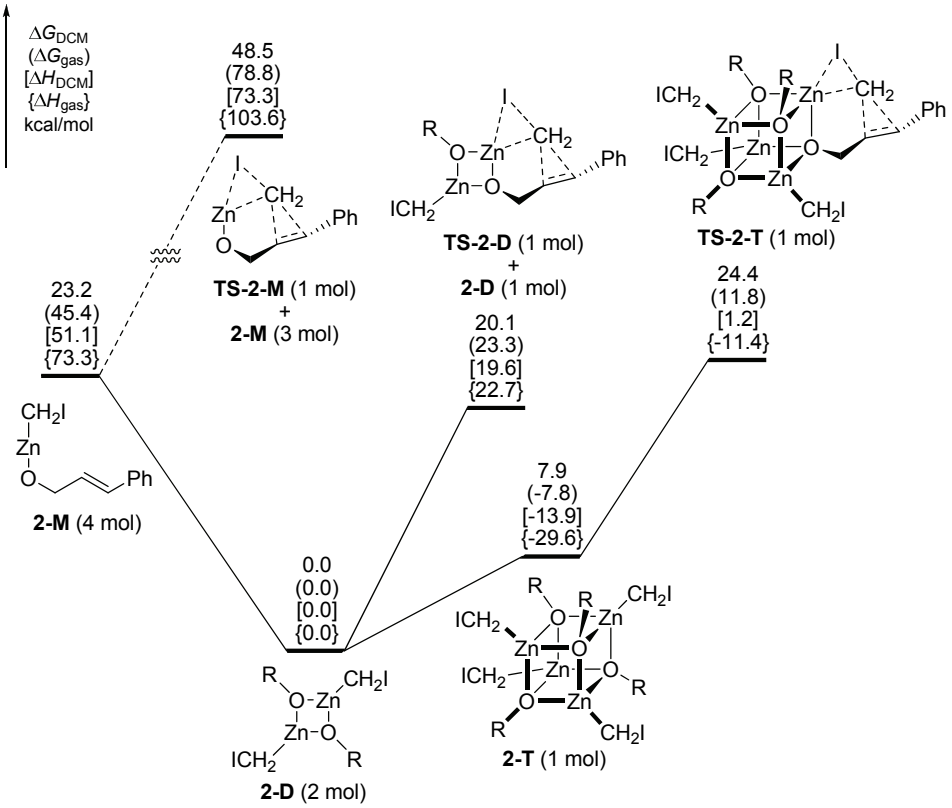
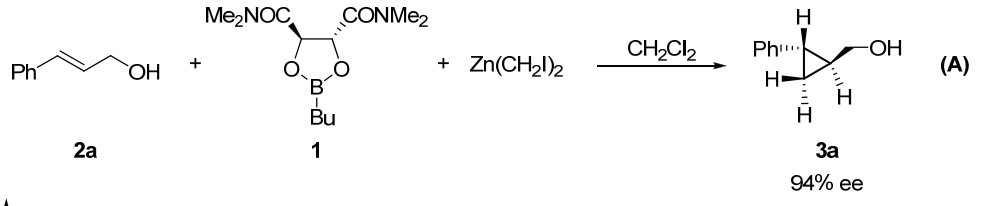


Figure S1. DFT-computed free energy surfaces for the cyclopropanation reactions of monomer **2-M**, dimer **2-D**, and tetramer **2-T** (R = (*E*)-PhCH=CHCH$_2$).

From Figure S1, we can see that, in the dimerizations of **2-M** to **2-D** and **2-D** to **2-T**, the entropy contribution parts ($-T\Delta S$) of the relative Gibbs free energies in the gas phase are 14.0 kcal/mol (2 mol **2-M** to 1 mol **2-D**) and 21.8 kcal/mol (2 mol **2-D** to 1 mol **2-T**), respectively. It is widely accepted that the entropy contributions in solution can be overestimated by 50-70% for bi- and tri-molecular processes.[1] To reduce the entropy overestimations in solution, 50% of the originally computed gas-phase entropy values from **2-M** to **2-D** and **2-D** to **2-T** are used as their entropy values in solution. Therefore in the revised Figure 1, the entropy contribution parts ($-T\Delta S$) of the relative Gibbs free energies in DCM are 7.0 kcal/mol (2 mol **2-M** to 1 mol **2-D**) and 10.9 kcal/mol (2 mol **2-D** to 1 mol **2-T**), respectively. Due to this, Figures 2 and 3 were revised correspondingly. The conclusions in the ASAP paper are not affected by these corrections. We thank Prof. Singleton for his insightful comments and help.

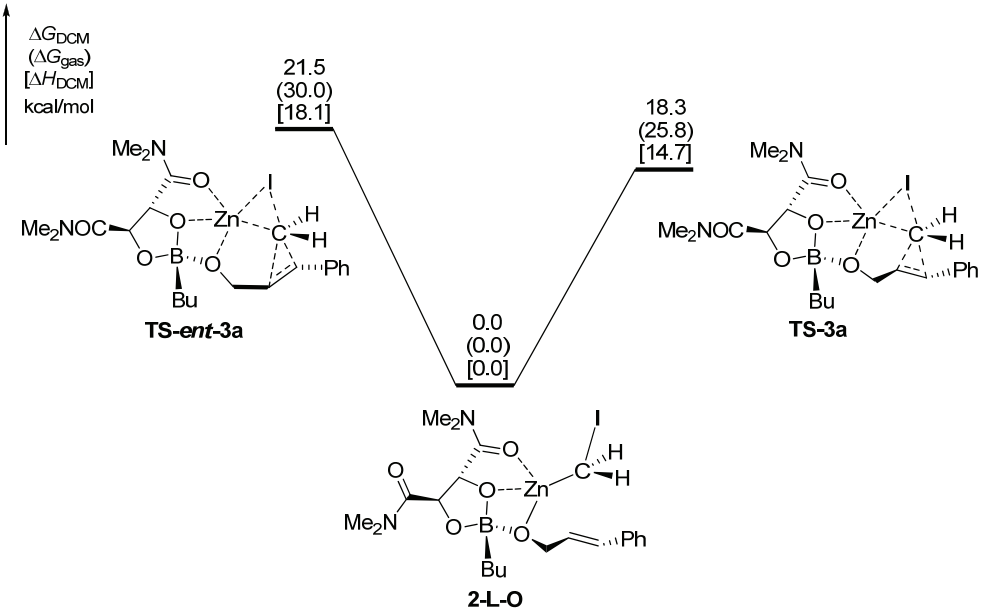
1 (a) Li, H.; Lu, G.; Jiang, J.; Huang, F.; Wang, Z.-X. *Organometallics* **2011**, *30*, 2349. (b) Kua, J.; Krizner, H. E.; De Haan, D. O. *J. Phys. Chem. A* **2011**, *115*, 1667. (c) Andrada, D. M.; Granados, A. M.; Solà, M.; Fernández, I. *Organometallics* **2011**, *30*, 466. (d) Li, H.; Zhao, L.; Lu, G.; Huang, F.; Wang, Z.-X. *Dalton Trans.* **2010**, *39*, 5519. (e) Andrada, D. M.; Jimenez-Halla, J. O. C.; Solà, M. *J. Org. Chem.* **2010**, *75*, 5821. (f) Huang, F.; Lu, G.; Zhao, L.; Li, H.; Wang, Z.-X. *J. Am. Chem. Soc.* **2010**, *132*, 12388. (g) Liang, Y.; Liu, S,; Xia, Y.; Li, Y.; Yu, Z.-X. *Chem.-Eur. J.* **2008**, *14*, 4361. (h) Yu, Z.-X.; Houk, K. N. *J. Am. Chem. Soc.* **2003**, *125*, 13825. (i) Strajbl, M.; Sham, Y. Y.; Villa, J.; Chu, Z.-T.; Warshel, A. *J. Phys. Chem. B* **2000**, *104*, 4578. (j) Hermans, J.; Wang, L. *J. Am. Chem. Soc.* **1997**, *119*, 2707. (k) Amzel, L. M. *Proteins* **1997**, *28*, 144. (l) Abraham, M. H. *J. Am. Chem. Soc.* **1981**, *103*, 6742. (m) Wertz, D. H. *J. Am. Chem. Soc.* **1980**, *102*, 5316.

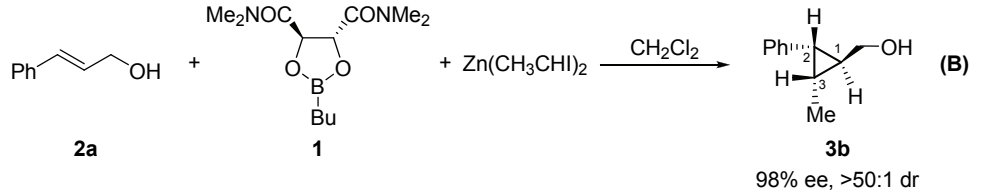
6. DFT-Computed Free Energy Surfaces for Reactions A–D



2a + **1** + $Zn(CH_2I)_2$ $\xrightarrow{CH_2Cl_2}$ **3a** (A)

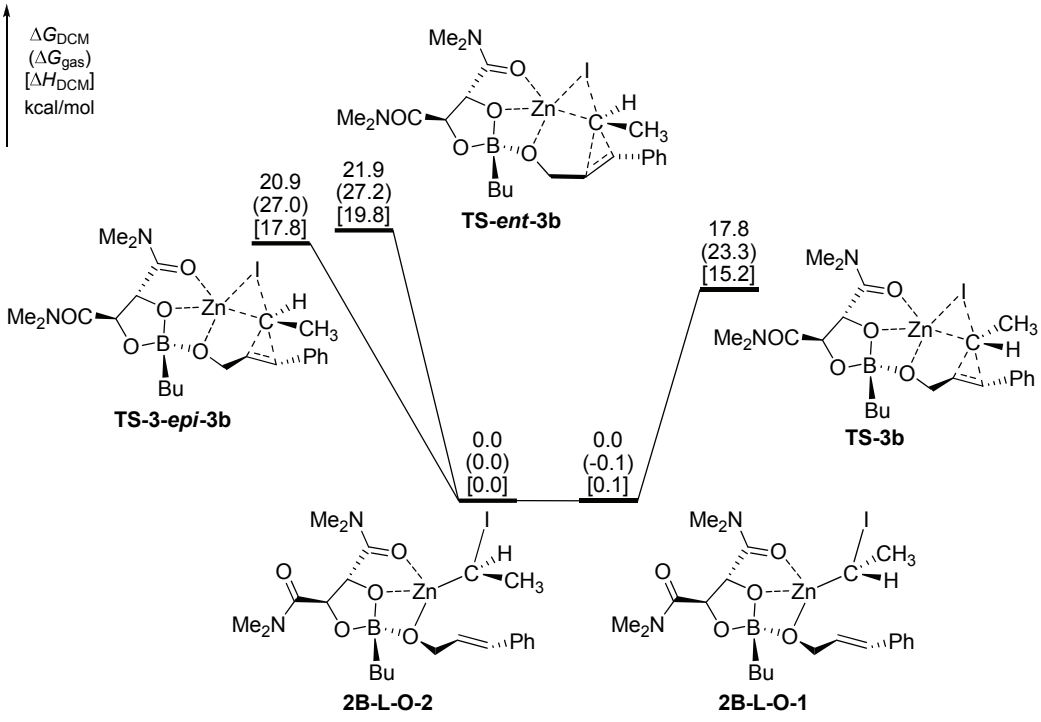
94% ee

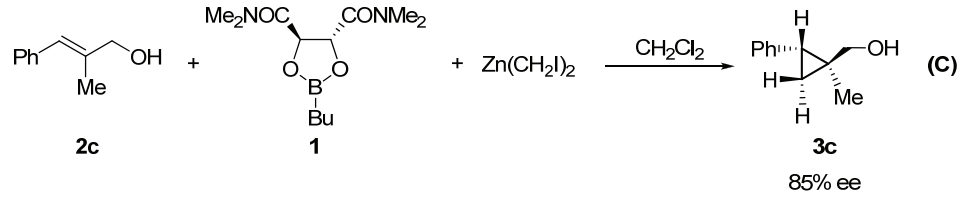




2a + **1** + $Zn(CH_3CHI)_2$ $\xrightarrow{CH_2Cl_2}$ **3b** (B)

98% ee, >50:1 dr

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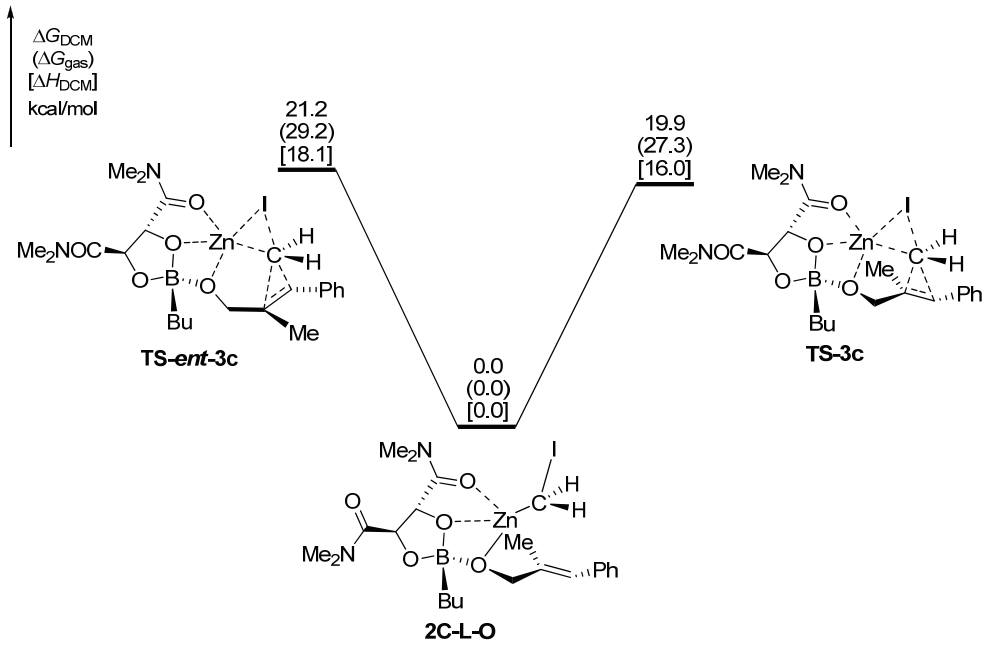
Me
2c
+
Me2NOC
CONMe2
O
B
O
Bu
1
+ Zn(CH2I)2
CH2Cl2
H
Ph
OH
H
Me
H
3c
(C)
85% ee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[ΔHDCM]
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(29.2)
[18.1]
19.9
(27.3)
[16.0]
0.0
(0.0)
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Zn
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TS-ent-3c
TS-3c
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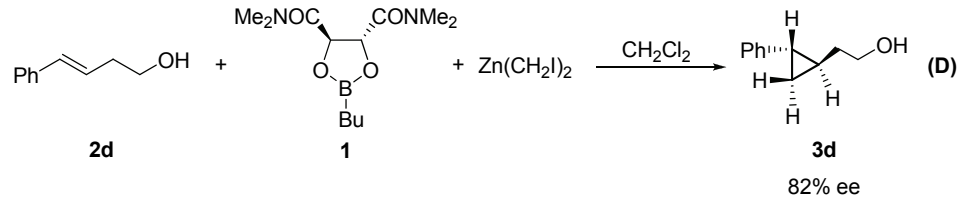
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2d
+
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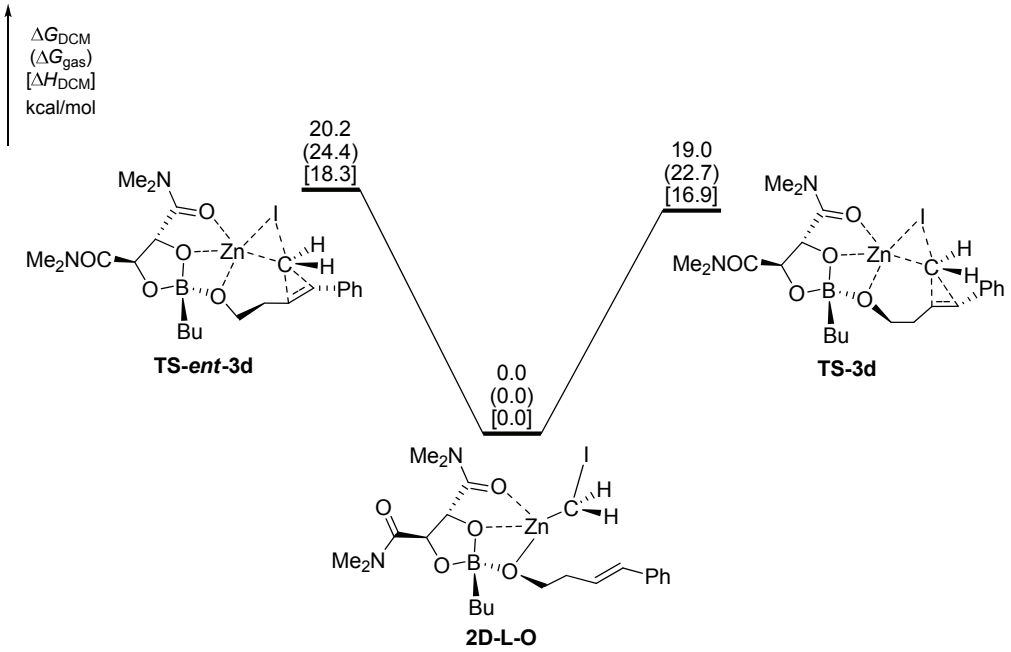
3d
(D)
82% ee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kcal/mol
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19.0
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TS-ent-3d
TS-3d
2D-L-O