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Origin of Chemoselectivity of TMP-Zincate Base. Differences between TMP-Zincate and Alkyllithium Reagents: Insights from a DFT Study on Model Systems.

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Computational Methods.

All calculations were carried with a Gaussian 98 program package.[1] The molecular structures and harmonic vibrational frequencies were obtained using the hybrid density functional method based on Becke's three-parameter exchange function and the Lee-Yang-Parr nonlocal correlation functional (B3LYP).[2] We used Ahlrichs' SVP[3, 4] all-electron basis set for the zinc atom and 6-31+G* for the other atoms (denoted as 631SVP in the text). Geometry optimization and vibrational analysis were performed at the same level. All stationary points were optimized without any symmetry assumptions, and characterized by normal coordinate analysis at the same level of the theory (the number of imaginary frequency, NIMAG, 0 for minima and 1 for TSs).

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Cartesian coordinates of representative stationary points

RT *(benzonitrile)*

SCF Done: E(RB+HF-LYP) = -324.498221697 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.090619	1.218989	-0.000003
2	6	0	1.485439	1.212552	0.000002
3	6	0	2.183297	0.000035	0.000002
4	6	0	1.485497	-1.212515	0.000000
5	6	0	0.090678	-1.219019	-0.000002
6	6	0	-0.610425	-0.000032	-0.000003
7	6	0	-2.046936	-0.000049	-0.000003
8	7	0	-3.210843	0.000024	0.000005
9	1	0	-0.459210	2.155186	-0.000003
10	1	0	2.027498	2.154160	0.000003
11	1	0	3.270108	0.000061	0.000004
12	1	0	2.027601	-2.154097	0.000002
13	1	0	-0.459106	-2.155242	-0.000002

RT1 *($(MeLi)_2$…OMe_2)*

SCF Done: E(RB+HF-LYP) = -249.932648366 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.909958	1.828110	0.003128
2	3	0	-2.950867	-0.000015	0.001740
3	6	0	-1.912949	-1.826279	-0.003250
4	3	0	-0.758148	-0.000336	-0.000336
5	1	0	-1.399918	2.255905	-0.882385
6	1	0	-1.383850	2.249847	0.882278
7	1	0	-2.883545	2.358398	0.013275
8	1	0	-1.416779	-2.254517	0.889908
9	1	0	-1.373718	-2.249329	-0.873917
10	1	0	-2.886429	-2.356232	-0.030746
11	6	0	1.943115	1.194016	-0.004745
12	8	0	1.162140	-0.000626	-0.002182
13	6	0	1.943314	-1.195023	0.006073
14	1	0	1.244812	2.033142	-0.011215
15	1	0	2.578995	1.233765	-0.899475
16	1	0	2.572235	1.242188	0.894394
17	1	0	1.245346	-2.034439	0.007416
18	1	0	2.572906	-1.234695	0.905197
19	1	0	2.578735	-1.242706	-0.888672

CP1

SCF Done: E(RB+HF-LYP) = -574.440645018 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.372749	2.565010	-0.527360
2	3	0	2.209669	0.472370	0.341940
3	6	0	3.099419	0.439471	2.423310
4	3	0	3.066399	2.246641	1.403270
5	6	0	3.302690	-2.197839	-0.358190
6	8	0	3.215689	-0.843549	-0.785060
7	6	0	4.431329	-0.358899	-1.350270
8	1	0	3.221488	3.114661	-0.981860
9	1	0	1.582058	3.329780	-0.394250
10	1	0	1.993639	1.934560	-1.356270
11	1	0	2.497149	-0.489160	2.362660
12	1	0	2.866689	0.820401	3.437640
13	1	0	4.147849	0.087601	2.488190
14	1	0	2.323660	-2.473510	0.039900
15	1	0	4.061200	-2.312119	0.428540
16	1	0	3.550270	-2.852519	-1.206340
17	1	0	4.260579	0.683651	-1.623080
18	1	0	4.694819	-0.942989	-2.243820
19	1	0	5.249429	-0.419799	-0.618670
20	6	0	-3.024541	1.033589	-0.494730
21	6	0	-4.414281	1.039829	-0.604310
22	6	0	-5.158281	-0.067181	-0.181740
23	6	0	-4.513911	-1.188111	0.353050
24	6	0	-3.124731	-1.209281	0.467160
25	6	0	-2.378691	-0.095071	0.042390

26	6	0	-0.950551	-0.101690	0.158340
27	7	0	0.207599	-0.095610	0.240920
28	1	0	-2.436441	1.887039	-0.817640
29	1	0	-4.916411	1.909329	-1.018580
30	1	0	-6.241381	-0.056102	-0.268310
31	1	0	-5.093530	-2.046011	0.681620
32	1	*0*	*-2.615180*	*-2.073141*	*0.882730*

TS1-1

SCF Done: E(RB+HF-LYP) = -574.434303353 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.804764	-2.793243	0.274902
2	8	0	-3.924484	-1.385880	0.072067
3	6	0	-5.279175	-0.936203	-0.008789
4	6	0	-2.750244	1.869720	-0.318863
5	3	0	-2.459183	-0.154465	-0.060989
6	6	0	1.371475	2.256226	-0.120102
7	3	0	-0.601944	1.676453	-0.210617
8	6	0	2.754623	-0.587204	1.143448
9	6	0	4.129500	-0.809479	1.123688
10	6	0	4.738586	-1.368362	-0.005280
11	6	0	3.969543	-1.709442	-1.123444
12	6	0	2.592148	-1.500412	-1.115967
13	6	0	1.982025	-0.940521	0.022690
14	6	0	0.561340	-0.770035	0.036972
15	7	0	-0.606079	-0.836670	0.045547

16	1	0	-2.738312	-3.021469	0.324860
17	1	0	-4.261948	-3.340927	-0.560165
18	1	0	-4.290512	-3.087326	1.215042
19	1	0	-5.249969	0.144119	-0.161087
20	1	0	-5.813004	-1.165283	0.923080
21	1	0	-5.790405	-1.417267	-0.853210
22	1	0	-3.401382	1.738098	-1.206024
23	1	0	-2.347321	2.890869	-0.452713
24	1	0	-3.440842	1.980438	0.540512
25	1	0	2.097397	1.885742	-0.861496
26	1	0	1.848816	2.163422	0.871078
27	1	0	1.261368	3.340942	-0.309265
28	1	0	2.277069	-0.129898	2.002853
29	1	0	4.728897	-0.532745	1.986206
30	1	0	5.813019	-1.530273	-0.017014
31	1	0	4.443237	-2.136566	-2.002853
32	1	0	1.988068	-1.758453	-1.980377

TS1-2

SCF Done: E(RB+HF-LYP) = -574.409263551 A.U.

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

1	6	0	-1.577897	1.611629	1.693559
2	3	0	-2.008872	-0.041907	0.493244
3	3	0	-0.006169	1.850877	0.343336
4	6	0	0.525510	2.591602	-1.552331
5	6	0	2.116245	0.625197	-0.133980

6	6	0	3.461529	0.992019	0.025596
7	6	0	4.470144	0.049437	0.250215
8	6	0	4.165046	-1.318919	0.306697
9	6	0	2.847507	-1.737231	0.146215
10	6	0	1.851012	-0.763209	-0.069814
11	6	0	0.477914	-1.151541	-0.179869
12	7	0	-0.667264	-1.367987	-0.241406
13	6	0	-4.904542	0.424283	0.286997
14	8	0	-3.815398	-0.456271	0.005398
15	6	0	-4.192179	-1.595658	-0.769624
16	1	0	-2.096591	0.952412	2.418895
17	1	0	-2.292784	2.432335	1.497163
18	1	0	-0.799240	2.072837	2.334770
19	1	0	-0.280051	2.168408	-2.177348
20	1	0	1.362301	2.807964	-2.231510
21	1	0	0.168760	3.578904	-1.198111
22	1	0	3.729440	2.046997	-0.039542
23	1	0	5.501358	0.373257	0.377830
24	1	0	4.950972	-2.050426	0.473648
25	1	0	2.589051	-2.792506	0.191349
26	1	0	-4.504489	1.252883	0.873872
27	1	0	-5.679096	-0.099455	0.863074
28	1	0	-5.337025	0.807208	-0.646927
29	1	0	-3.287899	-2.183632	-0.933681
30	1	0	-4.609149	-1.279256	-1.735059
31	1	0	-4.935832	-2.195302	-0.227743
32	1	0	1.317692	1.540886	-0.725731

PD1-1

SCF Done: E(RB+HF-LYP) = -574.490739763 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.284894	-0.400886	1.081486
2	6	0	2.059413	-1.546171	1.273035
3	6	0	3.164334	-1.793323	0.449383
4	6	0	3.492100	-0.874536	-0.551390
5	6	0	2.726313	0.283866	-0.722861
6	6	0	1.599305	0.533256	0.079317
7	6	0	0.721524	1.761570	-0.099907
8	7	0	-0.527386	1.736085	0.113900
9	3	0	-2.049960	0.511808	0.227408
10	6	0	-1.417409	-2.179413	-0.892918
11	8	0	-2.391646	-1.321893	-0.296665
12	6	0	-3.707858	-1.874981	-0.308280
13	1	0	0.426962	-0.202385	1.719047
14	1	0	1.807425	-2.243620	2.069139
15	1	0	3.767820	-2.686251	0.593203
16	1	0	4.349023	-1.054831	-1.196560
17	1	0	3.005786	0.990465	-1.499431
18	1	0	-0.454261	-1.671700	-0.826046
19	1	0	-1.669390	-2.368926	-1.945367
20	1	0	-1.367559	-3.134020	-0.351648
21	1	0	-4.372187	-1.137834	0.145549
22	1	0	-3.733666	-2.808910	0.269757
23	1	0	-4.029783	-2.074840	-1.339535
24	3	0	-2.071788	2.782926	0.340291
25	6	0	-3.841475	1.713121	0.603356

26	1	0	-4.091209	1.013488	1.426286
27	1	0	-4.446516	1.381726	-0.261955
28	1	0	-4.339735	2.650525	0.923744
29	6	0	1.476541	3.020562	-0.550615
30	1	0	1.809507	2.938498	-1.595119
31	1	0	0.809004	3.884076	-0.479455
32	1	0	2.372793	3.204494	0.057690

PD1-2

SCF Done: E(RB+HF-LYP) = -574.465684989 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.652527	0.175903	1.120926
2	3	0	1.790878	0.868484	-0.660507
3	3	0	0.665146	-0.244293	1.617783
4	6	0	-1.397263	-0.384872	1.528152
5	6	0	-2.374527	-0.867188	2.431335
6	6	0	-3.747910	-0.865265	2.161469
7	6	0	-4.240646	-0.370087	0.943619
8	6	0	--3.344757	0.123154	0.002319
9	6	0	--1.968338	0.103470	0.315582
10	6	0	-1.005905	0.601471	-0.618484
11	7	0	-0.120255	0.976196	-1.284195
12	6	0	4.411957	1.612549	-1.859894
13	8	0	2.992126	1.559906	-2.002457
14	6	0	2.531555	2.071869	-3.254959
15	1	0	3.182327	1.142365	1.227600

16	1	0	3.338516	-0.479660	0.550446
17	1	0	2.710220	-0.244492	2.145569
18	1	0	-2.053864	-1.265472	3.395203
19	1	0	-4.447891	-1.251755	2.901077
20	1	0	-5.307892	-0.371460	0.737564
21	1	0	-3.695175	0.514069	-0.950623
22	1	0	4.653748	1.200928	-0.878540
23	1	0	4.763672	2.651108	-1.923294
24	1	0	- 4.896957	1.013900	-2.642715
25	1	0	- 1.444138	1.988403	-3.252594
26	1	0	- 2.950287	1.484253	-4.083115
27	1	0	2.826477	3.123900	-3.366898
28	6	0	- 0.517365	-4.389160	1.165955
29	1	0	1.545746	-4.015182	1.134918
30	1	0	0.316116	-4.972427	0.262024
31	1	0	0.388779	-5.027176	2.045883
32	1	0	-0.180008	-3.547684	1.219437

RT2 *(methylbenzoate)*

SCF Done: E(RB+HF-LYP) = -460.139577117 A.U.

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

1	6	0	2.133670	-1.379157	-0.000007
2	6	0	3.000679	-0.281366	0.000190
3	6	0	2.483601	1.019022	0.000186
4	6	0	1.103656	1.221582	-0.000013
5	6	0	0.230900	0.122616	-0.000220

6	6	0	0.751781	-1.180965	-0.000205
7	6	0	-1.235598	0.394304	-0.000458
8	8	0	-1.976967	-0.738157	-0.000027
9	8	0	-1.731122	1.507201	-0.000037
10	6	0	-3.402984	-0.553576	0.000344
11	1	0	2.533811	-2.389658	-0.000005
12	1	0	4.076375	-0.438566	0.000347
13	1	0	3.155617	1.873156	0.000338
14	1	0	0.684432	2.222831	-0.000024
15	1	0	0.075656	-2.028887	-0.000359
16	1	0	-3.823812	-1.559684	0.000441
17	1	0	-3.716032	-0.003138	-0.891025
18	1	0	-3.715569	-0.003179	0.891903

CP2

SCF Done: E(RB+HF-LYP) = -710.084279106 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.532229	-0.096076	-0.031281
2	6	0	4.407325	-1.476862	0.157567
3	6	0	3.139427	-2.065746	0.214803
4	6	0	1.997200	-1.277394	0.081179
5	6	0	2.119436	0.108174	-0.108313
6	6	0	3.392861	0.698230	-0.161956
7	6	0	0.876212	0.910169	-0.245558
8	8	0	1.093864	2.228348	-0.304202
9	8	0	-0.246640	0.418671	-0.307936

10	6	0	-0.066420	3.079019	-0.457302
11	6	0	-1.864106	-0.657017	2.609540
12	3	0	-2.020499	0.105529	0.477709
13	6	0	-3.422227	1.945514	0.468736
14	3	0	-3.007491	1.037750	2.286457
15	6	0	-2.870398	-1.167894	-2.101800
16	8	0	-2.799906	-1.316773	-0.689527
17	6	0	-3.867293	-2.092239	-0.151080
18	1	0	5.516973	0.361311	-0.074819
19	1	0	5.297062	-2.092553	0.262183
20	1	0	3.041371	-3.136930	0.368016
21	1	0	1.006946	-1.718246	0.130773
22	1	0	3.483755	1.769422	-0.305219
23	1	0	0.316227	4.095477	-0.366306
24	1	0	-0.808976	2.862860	0.312935
25	1	0	-0.512555	2.922432	-1.442814
26	1	0	-2.543502	-1.241051	3.262834
27	1	0	-1.051228	-0.320374	3.282319
28	1	0	-1.381894	-1.430904	1.979973
29	1	0	-3.073045	1.799553	-0.572953
30	1	0	-3.278558	3.029349	0.646768
31	1	0	-4.521305	1.820310	0.397578
32	1	0	-2.002339	-0.579171	-2.405718
33	1	0	-3.791802	-0.644688	-2.394764
34	1	0	-2.836791	-2.150384	-2.594535
35	1	0	-3.715034	-2.130786	0.928913
36	1	0	-3.847999	-3.109380	-0.568129
37	1	0	-4.837360	-1.625314	-0.373431

TS2-1

SCF Done: E(RB+HF-LYP) = -710.078077649 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.047494	-0.885639	-0.086750
2	6	0	3.713504	-2.104236	0.513407
3	6	0	2.369801	-2.436134	0.721870
4	6	0	1.365312	-1.551910	0.333245
5	6	0	1.696546	-0.328991	-0.273027
6	6	0	3.046122	0.000372	-0.482574
7	6	0	0.610001	0.584448	-0.690065
8	8	0	1.009768	1.556787	-1.506795
9	8	0	-0.592671	0.390916	-0.433834
10	6	0	0.064751	2.597317	-1.808045
11	6	0	-2.452180	1.119159	2.367831
12	3	0	-2.151331	0.215887	0.531477
13	6	0	1.394857	2.534485	1.591675
14	3	0	-0.477724	1.705970	1.778539
15	6	0	-3.378214	-1.549556	-1.523636
16	8	0	-3.520013	-0.869869	-0.277204
17	6	0	-4.794165	-1.069777	0.338198
18	1	0	5.090361	-0.621150	-0.239031
19	1	0	4.497122	-2.791506	0.821920
20	1	0	2.107397	-3.381160	1.190008
21	1	0	0.321484	-1.800006	0.497157
22	1	0	3.300281	0.952996	-0.932468
23	1	0	0.580070	3.259583	-2.503915
24	1	0	-0.180550	3.124920	-0.880445
25	1	0	-0.836266	2.181208	-2.265903

26	1	0	-2.081291	1.745043	3.202084
27	1	0	-2.758192	0.182903	2.874954
28	1	0	-3.397685	1.619779	2.080017
29	1	0	1.805547	2.980399	0.671708
30	1	0	2.163883	1.841353	1.975294
31	1	0	1.331565	3.358916	2.327477
32	1	0	-2.376036	-1.329673	-1.896514
33	1	0	-4.128077	-1.192794	-2.242689
34	1	0	-3.492346	-2.633234	-1.384965
35	1	0	-4.788766	-0.510723	1.275502
36	1	0	-4.955670	-2.136606	0.542831
37	1	0	-5.595324	-0.695721	-0.313173

TS2-2

SCF Done: E(RB+HF-LYP) = -710.049751598 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.533539	-1.093063	1.664078
2	6	0	-1.622910	-1.557495	2.433380
3	6	0	-1.382004	-2.152664	3.666992
4	6	0	-0.061310	-2.309372	4.117493
5	6	0	1.006226	-1.885086	3.322876
6	6	0	0.806595	-1.247528	2.088318
7	6	0	-0.764511	-0.395981	0.392166
8	8	0	0.113449	0.218994	-0.237808
9	6	0	2.548920	2.328033	0.461655
10	3	0	1.129013	1.671097	-0.901428
11	3	0	2.071548	0.271042	0.817993

12	8	0	-2.024078	-0.460754	-0.067963
13	6	0	-2.323349	0.210846	-1.299545
14	6	0	3.018005	-1.592316	0.255951
15	6	0	0.705902	1.718658	-3.881561
16	8	0	1.076828	2.403915	-2.686829
17	6	0	1.883209	3.561661	-2.934662
18	1	0	-2.640274	-1.439514	2.072266
19	1	0	-2.213333	-2.498215	4.275986
20	1	0	0.125015	-2.770355	5.085861
21	1	0	2.026215	-2.059860	3.666061
22	1	0	3.481857	2.509583	-0.103867
23	1	0	2.895600	2.172775	1.503159
24	1	0	2.051041	3.317856	0.526489
25	1	0	1.822693	-1.320526	1.265121
26	1	0	-3.386017	0.037079	-1.470734
27	1	0	-1.733536	-0.212875	-2.117325
28	1	0	-2.123444	1.283112	-1.213974
29	1	0	2.610977	-1.927246	-0.712494
30	1	0	3.404709	-2.485794	0.767900
31	1	0	3.897339	-0.957321	0.038620
32	1	0	0.123779	0.843094	-3.587143
33	1	0	1.598358	1.393127	-4.432266
34	1	0	0.096634	2.369492	-4.523102
35	1	0	2.152695	3.980042	-1.963821
36	1	0	1.316437	4.298050	-3.519485
37	1	0	2.795471	3.280792	-3.476486

PD2-1

SCF Done: E(RB+HF-LYP) = -710.139880102 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.380403	-1.174712	-0.598737
2	6	0	3.297813	-1.995207	0.531593
3	6	0	2.320813	-1.736309	1.496352
4	6	0	1.432986	-0.667490	1.329378
5	6	0	1.506304	0.158395	0.201421
6	6	0	2.494060	-0.106457	-0.760010
7	6	0	0.553799	1.363014	0.056298
8	8	0	0.211938	1.351072	-1.369604
9	8	0	-0.568182	1.239621	0.820572
10	6	0	-0.615619	2.409595	-1.821468
11	6	0	-3.410019	0.584984	2.141727
12	3	0	-1.990400	0.077269	0.570468
13	6	0	1.316885	2.663140	0.399456
14	3	0	-1.657361	1.715269	2.103112
15	6	0	-1.506050	-1.695519	-1.744216
16	8	0	-2.376735	-1.336782	-0.665631
17	6	0	-3.470507	-2.235818	-0.494574
18	1	0	4.135486	-1.368010	-1.357516
19	1	0	3.988345	-2.825571	0.658519
20	1	0	2.246862	-2.366045	2.380249
21	1	0	0.671549	-0.468345	2.077518
22	1	0	2.555427	0.519994	-1.644692
23	1	0	-0.957095	2.131422	-2.823486
24	1	0	-0.068144	3.360868	-1.893453
25	1	0	-1.490148	2.548789	-1.171288

26	1	0	-3.790354	1.213372	2.971770
27	1	0	-3.458833	-0.439742	2.558453
28	1	0	-4.227061	0.640648	1.395783
29	1	0	2.170973	2.822175	-0.268166
30	1	0	1.691306	2.599912	1.427041
31	1	0	0.646124	3.527426	0.333836
32	1	0	-0.730151	-0.929665	-1.798145
33	1	0	-2.070136	-1.726501	-2.686564
34	1	0	-1.053621	-2.678146	-1.555394
35	1	0	-4.064431	-1.867237	0.344329
36	1	0	-3.105025	-3.248130	-0.273451
37	1	0	-4.089177	-2.261818	-1.402089

PD2-2

SCF Done: E(RB+HF-LYP) = -710.104609544 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.85488	-0.58673	-0.29038
2	6	0	-2.97093	-1.42871	-0.05540
3	6	0	-4.24380	-0.95952	-0.34805
4	6	0	-4.39247	0.33751	-0.86906
5	6	0	-3.27327	1.14543	-1.08909
6	6	0	-1.94808	0.73387	-0.81518
7	6	0	-0.50739	-1.08096	0.01597
8	8	0	0.55128	-0.43789	-0.15136
9	6	0	1.80036	2.50201	-1.22460
10	3	0	2.09906	0.58241	-0.44159

11	3	0	-0.07789	1.53552	-0.98131
12	8	0	-0.45527	-2.32994	0.51481
13	6	0	0.82676	-2.87544	0.83956
14	6	0	4.46534	-1.11576	0.46094
15	8	0	3.95280	0.07780	-0.12485
16	6	0	4.98365	1.00450	-0.48628
17	1	0	-2.83826	-2.42888	0.34761
18	1	0	-5.11403	-1.58846	-0.17621
19	1	0	-5.39038	0.70939	-1.10030
20	1	0	-3.44617	2.14376	-1.49475
21	1	0	2.39451	3.04363	-0.46288
22	1	0	1.05587	3.26077	-1.53921
23	1	0	2.46015	2.42165	-2.11041
24	1	0	0.62629	-3.87983	1.21489
25	1	0	1.31587	-2.27514	1.61304
26	1	0	1.46187	-2.92512	-0.05033
27	1	0	3.61289	-1.75406	0.69901
28	1	0	5.01955	-0.88638	1.38122
29	1	0	5.12819	-1.63677	-0.24323
30	1	0	4.49362	1.87766	-0.91780
31	1	0	5.65812	0.55037	-1.22419
32	1	0	5.55589	1.29948	0.40322
33	6	0	-1.77578	3.11727	2.91863
34	1	0	-1.96559	2.52996	2.01544
35	1	0	-1.97982	2.50544	3.80314
36	1	0	-2.42891	3.99550	2.92645
37	1	0	-0.73069	3.44280	2.93284

TS3-1

SCF Done: E(RB+HF-LYP) = -2480.66882419 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.606863	-1.225171	-0.251502
2	6	0	-4.994817	-1.384221	-0.268380
3	6	0	-5.832004	-0.303914	0.022409
4	6	0	-5.274348	0.943182	0.329969
5	6	0	-3.890449	1.106533	0.343805
6	6	0	-3.041970	0.019254	0.052330
7	6	0	-1.595129	0.270542	0.081056
8	7	0	-0.800634	1.154275	0.230361
9	3	0	1.149563	1.281184	0.258955
10	6	0	0.638629	3.976611	-0.765228
11	8	0	1.667090	3.038097	-0.433772
12	6	0	2.975815	3.536955	-0.697113
13	1	0	-2.946983	-2.055609	-0.471628
14	1	0	-5.421256	-2.355060	-0.507773
15	1	0	-6.911693	-0.430782	0.011281
16	1	0	-5.919447	1.787793	0.559320
17	1	0	-3.446565	2.068703	0.580998
18	1	0	-0.311636	3.496469	-0.529066
19	1	0	0.682112	4.224192	-1.834735
20	1	0	0.758902	4.894071	-0.172853
21	1	0	3.685762	2.759042	-0.413092
22	1	0	3.167766	4.443557	-0.106559
23	1	0	3.090885	3.769231	-1.765025
24	30	0	1.853729	-1.783799	-0.222523
25	6	0	2.821523	-3.211776	-1.231191

26	1	0	3.886297	-2.979037	-1.361765
27	1	0	2.379627	-3.354108	-2.225820
28	1	0	2.752783	-4.172165	-0.703101
29	6	0	-0.457564	-1.580069	-0.228769
30	1	0	-0.789522	-2.594241	-0.441097
31	1	0	-0.116558	-0.997162	-1.076450
32	1	0	-0.186866	-1.351734	0.793767
33	6	0	2.171240	-0.291509	2.269732
34	7	0	2.437602	-0.158270	0.831358
35	6	0	3.868642	0.093787	0.643815
36	1	0	1.106025	-0.482927	2.453552
37	1	0	2.438519	0.629511	2.822082
38	1	0	2.743836	-1.111436	2.744845
39	1	0	4.105090	0.203818	-0.422365
40	1	0	4.507649	-0.718729	1.038483
41	1	0	4.192988	1.018971	1.158378

TS3-2

SCF Done: E(RB+HF-LYP) = -2480.67328839 A.U.

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

1	3	0	2.208678	0.534996	-0.000007
2	6	0	-0.591724	1.659071	-0.000004
3	7	0	0.575790	1.633635	-0.000006
4	6	0	-4.144299	2.737032	0.000001
5	6	0	-4.765746	1.477761	0.000003
6	6	0	-4.001614	0.305824	0.000003

7	6	0	-2.589068	0.296476	0.000001
8	6	0	-2.020737	1.597784	-0.000001
9	6	0	-2.756643	2.805268	-0.000001
10	30	0	0.811385	-1.472061	0.000005
11	6	0	1.684304	-1.086190	-1.819606
12	6	0	1.684293	-1.086180	1.819617
13	6	0	4.002916	2.834770	-0.000002
14	8	0	3.905583	1.407883	-0.000002
15	6	0	5.174148	0.752772	0.000001
16	1	0	-4.738504	3.647185	0.000000
17	1	0	-5.853604	1.419891	0.000004
18	1	0	-4.536630	-0.645383	0.000004
19	1	0	-2.246744	3.766727	-0.000003
20	1	0	0.983346	-0.602080	-2.512922
21	1	0	1.941352	-2.061795	-2.258826
22	1	0	2.623556	-0.506547	-1.874729
23	1	0	1.941364	-2.061779	2.258837
24	1	0	0.983321	-0.602087	2.512931
25	1	0	2.623529	-0.506512	1.874742
26	1	0	2.983676	3.224395	-0.000004
27	1	0	4.533403	3.179169	-0.897399
28	1	0	4.533400	3.179169	0.897397
29	1	0	4.984761	-0.322619	0.000003
30	1	0	5.745218	1.025245	0.897277
31	1	0	5.745220	1.025242	-0.897274
32	6	0	-1.564246	-2.796389	-1.212828
33	7	0	-1.137767	-2.082854	-0.000003
34	6	0	-1.564251	-2.796401	1.212812
35	1	0	-1.304229	-2.205416	-2.096732
36	1	0	-2.654308	-2.956979	-1.216746
37	1	0	-1.078106	-3.778503	-1.298273
38	1	0	-1.304238	-2.205437	2.096723
39	1	0	-1.078113	-3.778517	1.298249

40	1	0	-2.654314	-2.956990	1.216724
41	1	0	-1.735760	-1.047673	0.000000

CP3

SCF Done: E(RB+HF-LYP) = -2480.71633132 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	1.715878	0.711204	-0.026136
2	6	0	2.816806	3.326772	-1.020362
3	8	0	2.917753	2.245578	-0.098850
4	6	0	4.008846	2.373927	0.810081
5	30	0	0.908322	-1.673528	-0.616898
6	6	0	-0.460171	-3.133613	-0.342070
7	6	0	1.503717	-0.502464	-2.215049
8	1	0	1.959248	3.123716	-1.664853
9	1	0	3.726294	3.397447	-1.632734
10	1	0	2.660527	4.274633	-0.486553
11	1	0	3.990211	1.495603	1.457215
12	1	0	3.898915	3.284729	1.415068
13	1	0	4.961693	2.410532	0.264197
14	1	0	-0.971555	-3.056810	0.629222
15	1	0	0.026822	-4.120026	-0.356845
16	1	0	-1.227225	-3.153418	-1.130339
17	1	0	2.272327	0.281217	-2.084745
18	1	0	0.648044	-0.028672	-2.718807
19	1	0	1.942430	-1.194281	-2.950160
20	6	0	-3.274419	-0.434874	0.004940

21	6	0	-4.643896	-0.694579	0.034166
22	6	0	-5.557752	0.354451	0.180764
23	6	0	-5.107319	1.674226	0.300929
24	6	0	-3.741853	1.951863	0.275413
25	6	0	-2.826464	0.894021	0.127272
26	6	0	-1.418709	1.153277	0.098126
27	7	0	-0.269008	1.320251	0.067177
28	1	0	-2.555579	-1.240905	-0.109246
29	1	0	-4.995529	-1.717935	-0.058644
30	1	0	-6.623673	0.144059	0.201725
31	1	0	-5.819660	2.486378	0.414572
32	1	0	-3.380799	2.971598	0.368592
33	6	0	1.424570	-1.146276	2.318408
34	7	0	2.003763	-0.921626	1.002756
35	6	0	3.367885	-1.432945	0.981204
36	1	0	0.394780	-0.767313	2.357055
37	1	0	1.993590	-0.630782	3.119540
38	1	0	1.389459	-2.217688	2.601634
39	1	0	3.823982	-1.279972	-0.007752
40	1	0	3.435484	-2.517218	1.208727
41	1	0	4.020179	-0.930381	1.726819

TS4-1

SCF Done: E(RB+HF-LYP) = -2616.31292229 A.U.

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

1	3	0	1.007376	1.278679	0.090187

2	30	0	1.873348	-1.935640	-0.024688
3	6	0	2.880586	-3.661093	0.028414
4	6	0	3.765240	0.237928	-0.055894
5	7	0	2.415557	-0.030913	-0.561139
6	6	0	2.438512	0.058058	-2.026018
7	6	0	-4.683663	-1.223857	-0.628291
8	6	0	-4.659020	-0.595681	-1.879206
9	6	0	-3.624112	0.293108	-2.183189
10	6	0	-2.619478	0.548086	-1.245940
11	6	0	-2.634725	-0.085257	0.004414
12	6	0	-3.680395	-0.971326	0.307889
13	6	0	-1.538884	0.215756	0.989882
14	8	0	-1.982454	-0.012705	2.273420
15	8	0	-0.697432	1.145799	0.775975
16	6	0	-1.126213	0.396686	3.332451
17	6	0	0.250589	4.117324	0.370598
18	8	0	1.281807	3.229045	-0.071819
19	6	0	2.403923	3.917388	-0.616072
20	1	0	3.912859	-3.550410	-0.327354
21	1	0	2.385981	-4.416006	-0.596280
22	1	0	2.916544	-4.056836	1.051953
23	1	0	3.784304	0.186176	1.041228
24	1	0	4.126257	1.244980	-0.341183
25	1	0	4.521545	-0.476885	-0.433038
26	1	0	1.445768	-0.163903	-2.443205
27	1	0	3.157327	-0.641040	-2.496212
28	1	0	2.721313	1.069452	-2.377830
29	1	0	-5.488164	-1.912560	-0.381659
30	1	0	-5.441111	-0.795683	-2.607361
31	1	0	-3.601149	0.793673	-3.148342
32	1	0	-1.822779	1.250490	-1.471553
33	1	0	-3.699462	-1.459773	1.276360
34	1	0	-1.680146	0.201355	4.252922

35	1	0	-0.879551	1.459861	3.255798
36	1	0	-0.198037	-0.190708	3.335365
37	1	0	-0.561295	3.493397	0.744951
38	1	0	-0.102588	4.734387	-0.467127
39	1	0	0.630394	4.771012	1.168136
40	1	0	3.125994	3.165070	-0.936669
41	1	0	2.863053	4.567380	0.141982
42	1	0	2.100170	4.526245	-1.479087
43	6	0	-0.247739	-1.517941	0.602920
44	1	0	-0.763974	-2.453127	0.785413
45	1	0	-0.261102	-1.101254	-0.394176
46	1	0	0.313302	-1.067927	1.412663

TS4-2

SCF Done: E(RB+HF-LYP) = -2616.31620254 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.208535	-1.982102	0.314430
2	6	0	-3.144315	-2.892494	0.298347
3	6	0	-1.835604	-2.440237	0.092701
4	6	0	-1.511219	-1.080970	-0.091523
5	6	0	-2.617976	-0.193860	-0.057759
6	6	0	-3.946787	-0.627409	0.130776
7	6	0	-2.334630	1.250444	-0.196103
8	8	0	-3.406375	2.027315	-0.407119
9	8	0	-1.202117	1.745585	-0.117645
10	6	0	-3.171530	3.443910	-0.519988

11	3	0	0.248411	0.601650	0.322910
12	30	0	2.751077	0.261777	-0.440066
13	6	0	4.264722	-1.018498	-0.156383
14	6	0	2.233479	2.225076	-0.348298
15	6	0	1.601145	1.154463	2.958900
16	8	0	0.957849	0.199607	2.112380
17	6	0	0.851247	-1.090743	2.719640
18	6	0	0.668682	-0.153894	-2.588031
19	7	0	0.957572	-0.774717	-1.283925
20	6	0	1.329114	-2.185551	-1.481759
21	1	0	-5.227983	-2.326570	0.468585
22	1	0	-3.339858	-3.954159	0.440579
23	1	0	-1.041013	-3.186541	0.066241
24	1	0	-4.759575	0.092850	0.143907
25	1	0	-4.156499	3.884201	-0.677143
26	1	0	-2.514207	3.653730	-1.367475
27	1	0	-2.716506	3.828924	0.396309
28	1	0	4.581296	-1.493233	-1.095673
29	1	0	3.988625	-1.830593	0.532117
30	1	0	5.145500	-0.516604	0.265503
31	1	0	2.885763	2.739348	0.371460
32	1	0	1.205846	2.553659	-0.133999
33	1	0	2.470060	2.653112	-1.334578
34	1	0	1.622024	2.103731	2.422918
35	1	0	2.628590	0.837037	3.180235
36	1	0	1.039535	1.266095	3.896175
37	1	0	0.290355	-1.724349	2.031991
38	1	0	0.307858	-1.017422	3.671269
39	1	0	1.850177	-1.510687	2.896188
40	1	0	0.399990	0.899549	-2.454723
41	1	0	-0.168090	-0.659854	-3.099144
42	1	0	1.539382	-0.197891	-3.259991
43	1	0	1.521498	-2.659841	-0.513670

44	1	0	2.243192	-2.281621	-2.083206
45	1	0	0.528257	-2.746294	-1.992414
46	1	0	-0.166391	-0.870682	-0.701346

CP4

SCF Done: E(RB+HF-LYP) = -2616.35709140 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.549650	-0.764580	-0.342409
2	6	0	-5.214700	-1.912720	0.384101
3	6	0	-3.900810	-2.108100	0.823281
4	6	0	-2.921990	-1.156200	0.541091
5	6	0	-3.255420	-0.002770	-0.187119
6	6	0	-4.574550	0.190050	-0.630609
7	6	0	-2.184830	0.987070	-0.464879
8	8	0	-2.587461	2.019540	-1.213449
9	8	0	-1.034410	0.889710	-0.047889
10	6	0	-1.599591	3.028430	-1.522309
11	3	0	0.820100	0.452491	0.291471
12	30	0	2.956510	-0.504839	-0.928199
13	6	0	4.743120	-1.390769	-1.188029
14	6	0	2.024660	1.192661	-1.695199
15	6	0	0.839750	-2.420039	-0.237519
16	7	0	1.564570	-1.338179	0.414571
17	6	0	2.182250	-1.845209	1.630461
18	6	0	2.656569	2.198641	1.968261
19	8	0	1.328620	1.712621	1.783751

20	6	0	0.611320	1.583521	3.007291
21	1	0	-6.569730	-0.614630	-0.685179
22	1	0	-5.976550	-2.655900	0.604841
23	1	0	-3.638330	-3.002540	1.381241
24	1	0	-1.897050	-1.301390	0.866671
25	1	0	-4.828150	1.080470	-1.195339
26	1	0	-2.123281	3.754300	-2.143969
27	1	0	-0.758881	2.585501	-2.060489
28	1	0	-1.240141	3.494020	-0.601159
29	1	0	4.653240	-2.485079	-1.239089
30	1	0	5.422250	-1.166889	-0.351499
31	1	0	5.243260	-1.055909	-2.107109
32	1	0	2.787230	1.693461	-2.307089
33	1	0	1.625149	1.982781	-1.035929
34	1	0	1.210540	0.916491	-2.385259
35	1	0	0.361560	-2.067359	-1.163269
36	1	0	0.035820	-2.834479	0.406551
37	1	0	1.484710	-3.281129	-0.509759
38	1	0	2.739660	-1.048999	2.144101
39	1	0	2.897510	-2.671729	1.445301
40	1	0	1.432270	-2.236109	2.349691
41	1	0	3.116689	2.259881	0.980581
42	1	0	3.236660	1.515071	2.603601
43	1	0	2.636749	3.196101	2.429401
44	1	0	-0.388820	1.223381	2.757541
45	1	0	0.534269	2.556861	3.512391
46	1	0	1.105030	0.863881	3.675021

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