Electronic Supplementary Material (ESI) for Catalysis Science & Technology

Electronic Supplementary Information

Theoretical investigation on copper hydrides catalyzed hydrosilylation reaction of 3-methylcyclohex-2-enone: Mechanism and ligands' effect

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CONTENTS:

A. Computational methods.

All the stationary points such as the transition states, reactants and products were optimized in the gas-phase at the B3LYP/[6-31G(d,p), LANL2DZ] level. Zero-point vibrational energies (ZPVE) were also applied in relative Gibbs free energies. All the transition states were characterized by one and only one imaginary frequency pertaining to the desired reaction coordinate. Considering the effect of the solvent, single-point B3LYP (PCM/toluene)/[6-311++G(d,p), SDD] calculations were performed on gas phase optimized structures at 298K. The Gibbs free energies G_{298K} in toluene including the entropy and nonelectrostatic solvation energies were obtained from these single-point energies combined with the Gibbs free energy corrections at the B3LYP/[6-31G(d,p), LANL2DZ] level in the gas phase. All energies discussed in the following refer to G_{298K}.

B. Energies and geometries.

Table 1. The relative energies (in kJ/mol) for all the species along the hydrosilylation reactions catalyzed by (Ph_3P)CuH, and (IPr)CuH at the B3LYP/[6-311++G(d,p), SDD] level.

Species	E_{total}	ΔE	Gc	ΔG
L1-COM	-1582.118872	0.0	-1582.1811	0.0
L1-TS1	-1582.106224	33.2	-1582.166499	38.3
L1-IM1	-1582.14448	30.7	-1582.207579	-69.5
L1-IM2	-2397.310178	-66.6	-2397.397978	-27.8
L1-TS2	-2397.291111	-16.6	-2397.370278	45
L2-COM	-1705.675639	0.0	-1705.751586	0.0
L2-TS1	-1705.666973	22.7	-1705.741225	27.2
L2-IM1	-1705.708921	-87.4	-1705.785572	-89.3
L2-IM2	-2520.869901	-74.4	-2520.967384	-25.0
L2-TS2	-2520.848486	-18.2	-2520.942505	40.3
Product	-1163.138636	-118.0 (L1-product) /-135.6 (L2-product)	-1163.190158	-116.2 (L1-product) /-142.2 (L2-product)

3-methylcyclohex-2-enone:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.476386	0.893117	0.257851
2	6	0	-0.333822	1.718594	-0.343719
3	6	0	1.028776	1.212975	0.146449
4	6	0	1.176594	-0.287216	0.018894
5	6	0	0.097529	-1.092918	-0.059209

6	6	0	-1.292300	-0.601931	0.017734
7	8	0	-2.246242	-1.363230	-0.067642
8	1	0	-2.454872	1.183830	-0.134066
9	1	0	-1.512104	1.043437	1.347340
10	1	0	-0.454656	2.779539	-0.100063
11	1	0	-0.369068	1.638993	-1.437508
12	1	0	1.176782	1.487456	1.203165
13	1	0	1.841382	1.707736	-0.400367
14	6	0	2.578794	-0.826958	0.000670
15	1	0	0.206905	-2.169929	-0.161068
16	1	0	3.130491	-0.500861	0.891919
17	1	0	3.132470	-0.439657	-0.864263
18	1	0	2.597499	-1.918677	-0.035969

Zero-point Energy: B3LYP/6-31G(d,p) = -347.846491 (a.u.)

Zero-point Correction = 0.155386 (a.u.) Gibbs Free Energy Correction = 0.123501 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/6-311++G(d,p) = -348.0901062 (a.u.)

TMDS:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.579454	0.268615	-0.250839
2	8	0	-0.000178	-0.008533	0.173407
3	14	0	1.581222	-0.272514	-0.251309
4	6	0	-2.385854	-1.327595	-0.835582
5	6	0	-2.474353	0.975057	1.242239
6	6	0	2.372818	1.326690	-0.848057
7	6	0	2.484114	-0.960694	1.245512
8	1	0	1.628097	-1.274486	-1.358856
9	1	0	-2.389847	-2.083636	-0.043039
10	1	0	-3.424769	-1.152385	-1.137565
11	1	0	-1.855577	-1.748445	-1.696138
12	1	0	-3.520531	1.197242	1.003369
13	1	0	-2.463292	0.267959	2.078516
14	1	0	-2.003737	1.902964	1.582379
15	1	0	3.412825	1.157881	-1.149968
16	1	0	1.838286	1.737159	-1.710988
17	1	0	2.371558	2.088219	-0.060782
18	1	0	2.020580	-1.889164	1.593721
19	1	0	3.531350	-1.177464	1.006309
20	1	0	2.469708	-0.247229	2.076312
21	1	0	-1.618342	1.263496	-1.365128

Zero-point Energy: B3LYP/6-31G(d,p) = -815.053512 (a.u.)

Zero-point Correction = 0.170680 (a.u.) Gibbs Free Energy Correction = 0.130321 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/6-311++G(d,p) = -815.3366160 (a.u.)

(Ph_3P)CuH (L1-CuH):

Standard orientation:

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

1	29	0	-0.004252	-0.006380	2.822923
2	15	0	0.000812	-0.001283	0.497558
3	1	0	-0.004694	-0.012568	4.344382
4	6	0	-1.044135	-1.323059	-0.241081
5	6	0	-1.150173	-2.534581	0.461410
6	6	0	-1.734736	-1.172806	-1.453260
7	6	0	-1.915460	-3.582780	-0.049590
8	1	0	-0.639022	-2.652273	1.413501
9	6	0	-2.504393	-2.221998	-1.958725
10	1	0	-1.680458	-0.234606	-1.996830
11	6	0	-2.593314	-3.427863	-1.260490
12	1	0	-1.990049	-4.514569	0.503189
13	1	0	-3.037852	-2.094819	-2.896403
14	1	0	-3.195927	-4.241109	-1.654487
15	6	0	-0.623811	1.568020	-0.231980
16	6	0	-0.118655	2.122865	-1.417524
17	6	0	-1.653594	2.235615	0.451428
18	6	0	-0.645368	3.315879	-1.915870
19	1	0	0.690509	1.629535	-1.946890
20	6	0	-2.181339	3.424090	-0.052617
21	1	0	-2.035571	1.827577	1.383752
22	6	0	-1.677917	3.965752	-1.237239
23	1	0	-0.245285	3.738759	-2.832987
24	1	0	-2.977031	3.930972	0.485251
25	1	0	-2.083221	4.895597	-1.625643
26	6	0	1.671397	-0.242799	-0.233941
27	6	0	2.769885	0.271222	0.474501
28	6	0	1.892986	-0.914366	-1.445856
29	6	0	4.062996	0.133407	-0.029867
30	1	0	2.611267	0.772122	1.426091
31	6	0	3.189101	-1.055551	-1.944633
32	1	0	1.056165	-1.335229	-1.994523
33	6	0	4.274126	-0.530159	-1.240167
34	1	0	4.904242	0.534538	0.527581
35	1	0	3.350717	-1.580032	-2.882068
36	1	0	5.281766	-0.644955	-1.629061

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1232.788423 (a.u.)

Zero-point Correction = 0.280905 (a.u.) Gibbs Free Energy Correction = 0.230508 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1234.4720124 (a.u.)

L1-COM:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.165351	1.477925	0.876310
2	6	0	-4.096722	0.225742	1.758757
3	6	0	-4.358715	-1.043751	0.942561
4	6	0	-3.482185	-1.135377	-0.291224
5	6	0	-2.992109	0.029763	-0.880930
6	6	0	-3.304465	1.380411	-0.380549
7	8	0	-2.947016	2.390575	-0.981381
8	1	0	-3.876095	2.385088	1.415326
9	1	0	-5.198340	1.636755	0.532689

10	1	0	-4.813511	0.302009	2.583438
11	1	0	-3.100594	0.145923	2.216082
12	1	0	-5.408612	-1.057766	0.603806
13	1	0	-4.213390	-1.937151	1.556115
14	6	0	-3.559300	-2.425514	-1.073862
15	1	0	-2.552885	-0.005162	-1.876359
16	29	0	-1.422207	-0.916278	0.348393
17	15	0	0.764168	-0.004196	0.072736
18	1	0	-1.370823	-2.210320	1.233211
19	6	0	1.833433	-0.509440	1.485064
20	6	0	1.267176	-0.529182	2.767945
21	6	0	3.181674	-0.867410	1.329255
22	6	0	2.039847	-0.872769	3.877444
23	1	0	0.212892	-0.300635	2.892059
24	6	0	3.951086	-1.218687	2.439686
25	1	0	3.628682	-0.880182	0.339644
26	6	0	3.383033	-1.216976	3.715282
27	1	0	1.588366	-0.885951	4.865238
28	1	0	4.992746	-1.497199	2.306947
29	1	0	3.982432	-1.493533	4.578021
30	6	0	1.484199	-0.903524	-1.368330
31	6	0	2.198753	-0.268758	-2.393670
32	6	0	1.259139	-2.290331	-1.446586
33	6	0	2.685083	-1.007932	-3.474972
34	1	0	2.375042	0.800997	-2.349995
35	6	0	1.751665	-3.023572	-2.525369
36	1	0	0.697964	-2.788571	-0.659893
37	6	0	2.465008	-2.383972	-3.542690
38	1	0	3.237472	-0.504723	-4.263626
39	1	0	1.575075	-4.094426	-2.572824
40	1	0	2.844675	-2.955808	-4.384636
41	6	0	1.188148	1.767599	-0.214152
42	6	0	0.253553	2.566747	-0.892299
43	6	0	2.393733	2.344358	0.218817
44	6	0	0.529183	3.911846	-1.145134
45	1	0	-0.701693	2.160405	-1.209143
46	6	0	2.661672	3.690196	-0.032851
47	1	0	3.120195	1.746704	0.759241
48	6	0	1.731652	4.475874	-0.717482
49	1	0	-0.209277	4.516199	-1.663339
50	1	0	3.596510	4.125017	0.309889
51	1	0	1.940875	5.524923	-0.907542
52	1	0	-4.561809	-2.519228	-1.517228
53	1	0	-3.392215	-3.289873	-0.427799
54	1	0	-2.831214	-2.452676	-1.888844

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1580.630503 (a.u.)

Zero-point Correction = 0.437427 (a.u.) Gibbs Free Energy Correction = 0.375199 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1582.5562987 (a.u.)

L1-TS1:

Standard orientation:

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

1	6	0	0.152769	-0.102904	-0.097754

2	6	0	0.046599	-0.128914	1.432144
3	6	0	1.431436	-0.159538	2.082066
4	6	0	2.280534	1.030203	1.655963
5	6	0	2.156107	1.433043	0.277872
6	6	0	1.153962	0.927805	-0.636803
7	8	0	1.098665	1.258856	-1.829994
8	1	0	-0.815481	0.090307	-0.570740
9	1	0	0.484460	-1.083348	-0.467959
10	1	0	-0.548904	-0.987987	1.761751
11	1	0	-0.483455	0.768218	1.786142
12	1	0	1.967631	-1.066272	1.759571
13	1	0	1.356258	-0.197834	3.173362
14	1	0	1.624933	2.070695	2.825897
15	1	0	2.963925	2.004295	-0.177193
16	6	0	3.675159	1.083713	2.257435
17	29	0	1.211822	2.932880	1.520291
18	15	0	0.192243	4.849447	0.915583
19	6	0	0.725816	5.511755	-0.716116
20	6	0	0.381546	6.244596	2.101146
21	6	0	-1.627731	4.603919	0.780899
22	6	0	-2.385398	5.096603	-0.290550
23	6	0	-3.763480	4.873318	-0.337462
24	6	0	-4.395543	4.159809	0.681471
25	6	0	-3.646287	3.663984	1.751427
26	6	0	-2.269715	3.879085	1.799323
27	6	0	1.047670	4.586873	-1.725213
28	6	0	0.822312	6.886730	-0.982773
29	6	0	1.227950	7.330920	-2.242204
30	6	0	1.536593	6.409489	-3.244936
31	6	0	1.443121	5.041218	-2.984381
32	6	0	-0.582984	7.254763	2.239657
33	6	0	-0.383950	8.298434	3.144725
34	6	0	0.777744	8.344488	3.918303
35	6	0	1.738784	7.339635	3.791404
36	6	0	1.538568	6.291568	2.892804
37	1	0	-1.900500	5.645940	-1.090971
38	1	0	-4.340815	5.255353	-1.174466
39	1	0	-5.466739	3.985010	0.640064
40	1	0	-4.131947	3.103136	2.544713
41	1	0	-1.688591	3.484442	2.629141
42	1	0	0.999490	3.514145	-1.550892
43	1	0	0.591189	7.611360	-0.208786
44	1	0	1.305289	8.396926	-2.436918
45	1	0	1.854364	6.757907	-4.223721
46	1	0	1.686524	4.314796	-3.753832
47	1	0	-1.493269	7.220164	1.648749
48	1	0	-1.138486	9.073053	3.247837
49	1	0	0.928912	9.156161	4.624102
50	1	0	2.638445	7.364371	4.399315
51	1	0	2.275163	5.496254	2.814626
52	1	0	4.270518	0.260251	1.840896
53	1	0	3.649894	0.984351	3.345904
54	1	0	4.181655	2.019780	2.006894

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1580.615796 (a.u.)

Zero-point Correction = 0.437309 (a.u.) Gibbs Free Energy Correction = 0.377034 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1582.5435334 (a.u.)

L1-IM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.312567	-1.587376	0.356847
2	6	0	5.054849	-0.602220	1.268457
3	6	0	5.428464	0.667784	0.497003
4	6	0	4.161792	1.424442	0.062361
5	6	0	3.170102	0.499441	-0.677919
6	6	0	3.308279	-0.957901	-0.618204
7	8	0	2.643320	-1.731678	-1.333844
8	1	0	3.793590	-2.366807	0.926549
9	1	0	5.030434	-2.117642	-0.283712
10	1	0	5.945612	-1.082948	1.690904
11	1	0	4.420615	-0.325513	2.122637
12	1	0	6.019697	0.396093	-0.390848
13	1	0	6.061222	1.321214	1.112145
14	1	0	3.702151	1.798888	0.989632
15	1	0	3.018360	0.791422	-1.726302
16	6	0	4.503416	2.651905	-0.791248
17	29	0	1.218827	0.495410	-0.233878
18	15	0	-1.003791	0.097900	0.013128
19	6	0	-1.604583	-0.993108	-1.337051
20	6	0	-2.107039	1.569901	-0.014507
21	6	0	-1.405030	-0.766636	1.586942
22	6	0	-2.348870	-1.800195	1.675579
23	6	0	-2.606355	-2.414084	2.903108
24	6	0	-1.926786	-2.003539	4.050938
25	6	0	-0.980802	-0.979080	3.970145
26	6	0	-0.716120	-0.368862	2.744688
27	6	0	-0.669197	-1.828357	-1.972271
28	6	0	-2.947337	-1.013308	-1.749065
29	6	0	-3.354181	-1.871342	-2.770763
30	6	0	-2.425201	-2.711201	-3.390212
31	6	0	-1.088062	-2.686597	-2.991556
32	6	0	-3.278454	1.662541	0.751288
33	6	0	-4.079074	2.804161	0.677017
34	6	0	-3.719173	3.861215	-0.160478
35	6	0	-2.551538	3.778762	-0.922480
36	6	0	-1.746270	2.642956	-0.845441
37	1	0	-2.874699	-2.132858	0.786415
38	1	0	-3.335890	-3.216852	2.959583
39	1	0	-2.126720	-2.485535	5.003496
40	1	0	-0.441293	-0.662421	4.857928
41	1	0	0.033913	0.415673	2.683554
42	1	0	0.383794	-1.806579	-1.692768
43	1	0	-3.671374	-0.353185	-1.280546
44	1	0	-4.393786	-1.879971	-3.085866
45	1	0	-2.743187	-3.375884	-4.188565
46	1	0	-0.359443	-3.327677	-3.478671
47	1	0	-3.560966	0.847948	1.410862
48	1	0	-4.982750	2.867335	1.276463
49	1	0	-4.342210	4.749259	-0.214290
50	1	0	-2.262117	4.601802	-1.569295
51	1	0	-0.830797	2.588743	-1.429080

52	1	0	5.001451	2.352757	-1.721673
53	1	0	5.169659	3.340079	-0.257792
54	1	0	3.596653	3.204880	-1.063537

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1580.658619 (a.u.)

Zero-point Correction = 0.442850 (a.u.) Gibbs Free Energy Correction = 0.379751 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1582.5873295 (a.u.)

L1-IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.078020	0.934323	0.724555
2	8	0	4.259465	-0.213504	0.463614
3	14	0	5.431471	-1.058312	-0.326197
4	6	0	2.958207	1.227875	2.573114
5	6	0	3.491189	2.520048	-0.197299
6	6	0	5.025979	-1.231174	-2.159024
7	6	0	7.105712	-0.225694	-0.096561
8	1	0	5.491774	-2.422656	0.278111
9	1	0	3.909796	1.599971	2.969343
10	1	0	2.180813	1.971092	2.769529
11	1	0	2.710925	0.305547	3.109199
12	1	0	2.699122	3.250292	-0.000672
13	1	0	4.444220	2.945495	0.136819
14	1	0	3.552391	2.359927	-1.279319
15	1	0	5.777414	-1.843493	-2.671457
16	1	0	4.050183	-1.707804	-2.299926
17	1	0	4.996973	-0.254744	-2.655506
18	1	0	7.351163	-0.120295	0.965370
19	1	0	7.903622	-0.811559	-0.567714
20	1	0	7.117377	0.775017	-0.542670
21	1	0	1.808637	0.364430	0.191921
22	15	0	-1.425823	-1.058625	-0.064067
23	6	0	-1.312781	-1.297255	1.754239
24	6	0	-0.670996	-0.309378	2.519623
25	6	0	-1.853161	-2.425003	2.394811
26	6	0	-0.558131	-0.463797	3.903472
27	1	0	-0.265001	0.585005	2.051582
28	6	0	-1.737527	-2.570755	3.776783
29	1	0	-2.373431	-3.183286	1.817160
30	6	0	-1.087110	-1.591322	4.532107
31	1	0	-0.059180	0.305656	4.484655
32	1	0	-2.159424	-3.445254	4.263782
33	1	0	-1.001011	-1.704988	5.608999
34	6	0	-3.066113	-1.744750	-0.539235
35	6	0	-3.253672	-3.084068	-0.911891
36	6	0	-4.171855	-0.879792	-0.517465
37	6	0	-4.527155	-3.549975	-1.244364
38	1	0	-2.405047	-3.760038	-0.951003
39	6	0	-5.443495	-1.349564	-0.844195
40	1	0	-4.034211	0.164116	-0.247478
41	6	0	-5.622863	-2.685861	-1.208573
42	1	0	-4.661266	-4.588256	-1.534011
43	1	0	-6.290973	-0.670689	-0.823002

44	1	0	-6.611913	-3.050182	-1.470560
45	6	0	-0.204729	-2.203166	-0.825531
46	6	0	0.011418	-2.090645	-2.209693
47	6	0	0.533845	-3.142118	-0.093131
48	6	0	0.932303	-2.916917	-2.850821
49	1	0	-0.539805	-1.352415	-2.786999
50	6	0	1.464546	-3.961238	-0.737188
51	1	0	0.391225	-3.230271	0.978630
52	6	0	1.662357	-3.854209	-2.114186
53	1	0	1.087163	-2.822937	-3.921666
54	1	0	2.036414	-4.680869	-0.158845
55	1	0	2.386340	-4.492908	-2.611585
56	29	0	-1.075049	1.117878	-0.613807
57	6	0	-1.684120	4.120758	1.299018
58	6	0	-2.811313	4.601415	0.377451
59	6	0	-2.228639	5.092588	-0.951359
60	6	0	-1.589979	3.930397	-1.730402
61	6	0	-0.668230	3.075885	-0.827692
62	6	0	-0.580143	3.310013	0.606811
63	8	0	0.340254	2.863664	1.327775
64	1	0	-2.063043	3.531399	2.142314
65	1	0	-1.172555	4.983535	1.746728
66	1	0	-3.389602	5.391426	0.871516
67	1	0	-3.515282	3.780455	0.179048
68	1	0	-1.466862	5.860548	-0.747890
69	1	0	-3.002705	5.569956	-1.565855
70	6	0	-0.826721	4.437747	-2.961552
71	1	0	0.335746	2.933139	-1.244434
72	1	0	0.011344	5.078307	-2.662050
73	1	0	-1.477524	5.019244	-3.625667
74	1	0	-0.415902	3.603458	-3.542120
75	1	0	-2.425706	3.319830	-2.104581

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -2395.709281 (a.u.)

Zero-point Correction = 0.614284 (a.u.) Gibbs Free Energy Correction = 0.526484 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -2397.9244620 (a.u.)

L1-TS2:

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.487954	-0.262873	0.102482
2	15	0	0.151696	0.070721	3.629819
3	6	0	1.398632	-0.714180	4.735584
4	6	0	2.308910	-1.614354	4.156742
5	6	0	1.481077	-0.451510	6.110730
6	6	0	3.271073	-2.250013	4.940525
7	1	0	2.262551	-1.817399	3.089654
8	6	0	2.451250	-1.083816	6.891632
9	1	0	0.793353	0.250581	6.571549
10	6	0	3.345071	-1.983971	6.309970
11	1	0	3.966817	-2.946019	4.480938
12	1	0	2.507866	-0.870287	7.955238
13	1	0	4.099732	-2.472648	6.919358
14	6	0	-0.468794	1.523571	4.576839

15	6	0	-1.623885	1.488092	5.371432
16	6	0	0.255997	2.723251	4.480884
17	6	0	-2.038457	2.628807	6.062397
18	1	0	-2.204859	0.574667	5.446052
19	6	0	-0.155168	3.857683	5.179527
20	1	0	1.142891	2.768711	3.854487
21	6	0	-1.305461	3.812723	5.970540
22	1	0	-2.937967	2.590675	6.670121
23	1	0	0.415702	4.777980	5.096972
24	1	0	-1.632518	4.698819	6.506765
25	6	0	-1.248775	-1.119372	3.580786
26	6	0	-2.051057	-1.136689	2.428178
27	6	0	-1.538806	-1.995819	4.638643
28	6	0	-3.139924	-2.006830	2.349656
29	1	0	-1.819855	-0.482558	1.591036
30	6	0	-2.624847	-2.867327	4.550045
31	1	0	-0.912571	-2.004575	5.525756
32	6	0	-3.428050	-2.871111	3.407139
33	1	0	-3.756002	-2.013145	1.455405
34	1	0	-2.840602	-3.545213	5.371052
35	1	0	-4.271523	-3.552318	3.338963
36	29	0	0.934083	0.561449	1.538765
37	6	0	4.131206	0.509183	-0.440932
38	6	0	4.981024	0.978676	0.746030
39	6	0	4.729656	2.462847	1.030186
40	6	0	3.270393	2.707188	1.450129
41	6	0	2.295876	1.970550	0.522307
42	6	0	2.715126	1.049414	-0.431432
43	8	0	1.951937	0.561780	-1.369816
44	1	0	4.076035	-0.584551	-0.495510
45	1	0	4.585161	0.830862	-1.388348
46	1	0	6.041649	0.793844	0.541217
47	1	0	4.729173	0.392308	1.640417
48	1	0	4.945326	3.045906	0.122806
49	1	0	5.406584	2.830040	1.811384
50	1	0	3.169293	2.325665	2.478630
51	1	0	1.369582	2.506118	0.291520
52	6	0	2.945999	4.208254	1.491555
53	1	0	3.039308	4.653892	0.494604
54	1	0	3.625087	4.741446	2.166816
55	1	0	1.920802	4.385380	1.837311
56	14	0	0.084326	0.386778	-1.330330
57	8	0	-1.304987	0.979994	-0.458865
58	14	0	-2.673172	1.901765	-0.522250
59	6	0	-0.281478	-1.279283	-2.156841
60	6	0	0.018096	1.683285	-2.743044
61	6	0	-2.295350	3.747402	-0.647750
62	6	0	-3.841802	1.385312	-1.914074
63	1	0	-3.393904	1.678527	0.770984
64	1	0	0.650445	-1.733902	-2.510750
65	1	0	-0.747250	-1.976112	-1.452508
66	1	0	-0.947218	-1.164384	-3.019902
67	1	0	0.727584	1.420565	-3.535196
68	1	0	-0.980427	1.751038	-3.190997
69	1	0	0.289043	2.686290	-2.390925
70	1	0	-3.215908	4.337312	-0.564618
71	1	0	-1.623484	4.067249	0.156426
72	1	0	-1.819845	3.997306	-1.601582

73	1	0	-4.060417	0.313103	-1.867085
74	1	0	-4.794243	1.923253	-1.835719
75	1	0	-3.420577	1.595720	-2.902832

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -2395.695690 (a.u.)

Zero-point Correction = 0.615278 (a.u.) Gibbs Free Energy Correction = 0.536111 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -2397.9063888 (a.u.)

(IPr)CuH (L2-CuH):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.000067	-0.000314	2.007123
2	6	0	0.000015	0.000025	0.033171
3	1	0	-0.000161	-0.001157	3.533006
4	7	0	-1.074081	0.000033	-0.811185
5	6	0	-0.678453	0.000034	-2.144954
6	6	0	0.678483	0.000024	-2.144952
7	7	0	1.074109	0.000040	-0.811182
8	6	0	-2.453458	0.000046	-0.378423
9	1	0	-1.390382	0.000034	-2.954830
10	1	0	1.390415	0.000017	-2.954827
11	6	0	2.453484	0.000051	-0.378413
12	6	0	-3.099143	1.236151	-0.178402
13	6	0	-3.099166	-1.236044	-0.178399
14	6	0	-4.435387	1.206219	0.238641
15	6	0	-5.098536	0.000073	0.445383
16	6	0	-4.435410	-1.206085	0.238644
17	1	0	-6.134216	0.000083	0.773040
18	1	0	-4.959557	-2.141163	0.410920
19	6	0	-2.392204	-2.574802	-0.365005
20	1	0	-4.959518	2.141306	0.410915
21	6	0	-2.392141	2.574891	-0.364988
22	6	0	3.099194	-1.236043	-0.178422
23	6	0	3.099163	1.236152	-0.178351
24	6	0	4.435403	1.206212	0.238703
25	6	0	5.098554	0.000062	0.445414
26	6	0	4.435434	-1.206093	0.238632
27	1	0	6.134232	0.000065	0.773080
28	1	0	4.959531	2.141295	0.411009
29	6	0	2.392161	2.574896	-0.364910
30	6	0	2.392230	-2.574795	-0.365065
31	1	0	4.959584	-2.141174	0.410884
32	6	0	-2.188204	-3.281684	0.989851
33	6	0	2.188163	-3.281674	0.989783
34	6	0	3.131122	-3.483338	-1.365828
35	6	0	3.131119	3.483612	-1.365464
36	6	0	2.187911	3.281586	0.990010
37	1	0	-1.399547	-2.378790	-0.780224
38	1	0	1.399594	-2.378772	-0.780330
39	1	0	1.399582	2.378882	-0.780316
40	1	0	3.251899	2.995321	-2.338089
41	1	0	2.570560	4.411867	-1.518850
42	1	0	1.622281	2.650397	1.682235
43	1	0	3.147317	3.521949	1.460968

44	1	0	3.147629	-3.522078	1.460598
45	1	0	1.638980	-4.219573	0.851363
46	1	0	4.128022	-3.758077	-1.005617
47	1	0	2.570609	-4.411612	-1.519259
48	1	0	-1.622659	-2.650614	1.682253
49	1	0	-3.147693	-3.522083	1.460624
50	6	0	-3.131063	-3.483335	-1.365801
51	1	0	-2.570562	-4.411623	-1.519199
52	1	0	-3.251628	-2.994917	-2.338390
53	6	0	-3.131082	3.483577	-1.365581
54	6	0	-2.187916	3.281620	0.989915
55	1	0	-1.638715	4.219516	0.851547
56	1	0	-1.622302	2.650449	1.682169
57	1	0	-3.147330	3.521999	1.460848
58	1	0	-3.251843	2.995257	-2.338195
59	1	0	-4.127926	3.758351	-1.005240
60	1	0	-2.570524	4.411829	-1.518984
61	1	0	-1.399554	2.378867	-0.780371
62	1	0	3.251746	-2.994917	-2.338408
63	1	0	1.622593	-2.650599	1.682160
64	1	0	4.127954	3.758380	-1.005095
65	1	0	1.638716	4.219487	0.851658
66	1	0	-4.127988	-3.758049	-1.005638
67	1	0	-1.639023	-4.219587	0.851452

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1356.281420 (a.u.)

Zero-point Correction = 0.577868 (a.u.) Gibbs Free Energy Correction = 0.510576 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1358.3324537 (a.u.)

L2-COM:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.103345	0.652135	1.330457
2	1	0	-0.041451	2.173445	1.702368
3	6	0	-1.932391	-1.638620	3.265547
4	6	0	-2.114212	-0.136487	3.515344
5	6	0	-0.869770	0.475546	4.166029
6	6	0	0.401611	0.154660	3.402786
7	6	0	0.483800	-1.036738	2.676315
8	6	0	-0.622908	-1.992003	2.561063
9	8	0	-0.499375	-3.070191	1.978175
10	1	0	-2.757761	-2.060460	2.683926
11	1	0	-1.920277	-2.179732	4.223452
12	1	0	-2.995889	0.038546	4.142130
13	1	0	-2.299649	0.377361	2.562663
14	1	0	-0.754186	0.080200	5.189806
15	1	0	-0.974744	1.560406	4.255667
16	6	0	1.658737	0.843971	3.881914
17	1	0	1.447682	-1.393636	2.319795
18	1	0	1.926066	0.463152	4.879117
19	1	0	1.511836	1.923403	3.958703
20	1	0	2.504545	0.654849	3.215282
21	6	0	0.094703	0.195088	-0.627924
22	7	0	1.205099	0.105703	-1.420823

23	6	0	0.875660	0.127657	-2.773032
24	6	0	-0.474921	0.224258	-2.838024
25	7	0	-0.936125	0.259519	-1.523955
26	6	0	2.546763	-0.047687	-0.909022
27	1	0	1.623245	0.068772	-3.547470
28	1	0	-1.144584	0.263924	-3.681715
29	6	0	-2.334480	0.296397	-1.159720
30	6	0	3.069953	-1.351827	-0.778430
31	6	0	3.281305	1.106342	-0.567053
32	6	0	4.363677	-1.476369	-0.256246
33	6	0	5.104013	-0.356238	0.111029
34	6	0	4.570068	0.919149	-0.050695
35	1	0	6.105316	-0.477247	0.515043
36	1	0	5.164188	1.785614	0.221867
37	6	0	2.752009	2.518007	-0.805994
38	1	0	4.796709	-2.465142	-0.140971
39	6	0	2.318327	-2.596997	-1.245348
40	6	0	-2.920512	1.536695	-0.827840
41	6	0	-3.061754	-0.912534	-1.172126
42	6	0	-4.414841	-0.853651	-0.813991
43	6	0	-5.014435	0.351413	-0.461941
44	6	0	-4.275500	1.531644	-0.474637
45	1	0	-6.064510	0.373280	-0.183676
46	1	0	-5.004590	-1.764864	-0.814468
47	6	0	-2.454403	-2.239217	-1.624819
48	6	0	-2.147560	2.849906	-0.919974
49	1	0	-4.759293	2.465792	-0.210169
50	6	0	2.892202	3.427291	0.427158
51	6	0	-2.493076	3.843354	0.200671
52	6	0	-2.358236	3.493652	-2.307253
53	6	0	-2.953882	-2.592590	-3.042527
54	6	0	-2.722371	-3.400886	-0.650870
55	1	0	1.683264	2.445043	-1.021969
56	1	0	-1.085585	2.619666	-0.807165
57	1	0	-1.369236	-2.115173	-1.678767
58	1	0	-2.735359	-1.796529	-3.761863
59	1	0	-2.476222	-3.511543	-3.398817
60	1	0	-2.272527	-3.222513	0.328858
61	1	0	-3.793750	-3.588975	-0.521936
62	1	0	-3.528132	4.198063	0.141617
63	1	0	-1.845221	4.722409	0.121457
64	1	0	-3.412879	3.744635	-2.467964
65	1	0	-1.775231	4.417202	-2.392271
66	1	0	2.337076	3.015696	1.273898
67	1	0	3.938657	3.569825	0.718510
68	6	0	3.439612	3.142499	-2.038253
69	1	0	3.026566	4.135884	-2.243954
70	1	0	3.301262	2.526481	-2.933106
71	6	0	2.969710	-3.155363	-2.528773
72	6	0	2.213104	-3.687698	-0.163419
73	1	0	1.723441	-4.573287	-0.583040
74	1	0	1.608847	-3.359351	0.686165
75	1	0	3.198082	-4.002540	0.197917
76	1	0	3.018740	-2.400533	-3.320904
77	1	0	3.991943	-3.499028	-2.335953
78	1	0	2.396105	-4.008070	-2.907286
79	1	0	1.296309	-2.302516	-1.498527
80	1	0	-2.048045	2.824606	-3.116563

81	1	0	-2.322830	3.393961	1.182063
82	1	0	-4.037523	-2.753821	-3.048185
83	1	0	-2.279417	-4.320474	-1.048552
84	1	0	4.517447	3.254252	-1.875923
85	1	0	2.476725	4.416285	0.206016

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1704.118630 (a.u.)

Zero-point Correction = 0.734647 (a.u.) Gibbs Free Energy Correction = 0.658700 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1706.4102861 (a.u.)

L2-TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.302600	0.293041	0.024994
2	6	0	0.159540	0.117318	1.541989
3	6	0	1.524725	-0.058419	2.210647
4	6	0	2.452192	1.112803	1.914372
5	6	0	2.398940	1.636838	0.578622
6	6	0	1.387183	1.295649	-0.394430
7	8	0	1.385845	1.733766	-1.555772
8	1	0	-0.642136	0.601180	-0.434351
9	1	0	0.571375	-0.665710	-0.441118
10	1	0	-0.489239	-0.736855	1.768858
11	1	0	-0.329374	1.001485	1.975761
12	1	0	2.012654	-0.964373	1.816745
13	1	0	1.419743	-0.190118	3.292430
14	6	0	3.825895	1.032546	2.559434
15	1	0	3.245253	2.208901	0.203153
16	1	0	4.395604	0.223260	2.082827
17	1	0	3.756527	0.828285	3.631537
18	1	0	4.385647	1.961484	2.420292
19	1	0	1.814837	2.098504	3.191418
20	29	0	1.482263	3.059031	1.947540
21	6	0	0.732002	4.820475	1.656514
22	7	0	1.437016	5.985402	1.543049
23	6	0	0.591063	7.085885	1.446213
24	6	0	-0.675826	6.604348	1.491802
25	7	0	-0.573838	5.221160	1.614952
26	6	0	2.877883	6.040367	1.471279
27	1	0	0.967754	8.091606	1.352293
28	1	0	-1.629072	7.105419	1.445335
29	6	0	-1.701321	4.318339	1.634820
30	6	0	3.486531	6.035373	0.198297
31	6	0	3.616623	6.085687	2.670771
32	6	0	4.886369	6.057475	0.157146
33	6	0	5.642927	6.086495	1.325533
34	6	0	5.013180	6.106370	2.566900
35	1	0	6.727733	6.100553	1.268004
36	1	0	5.612948	6.141110	3.471374
37	6	0	2.958247	6.146705	4.046150
38	1	0	5.388845	6.052546	-0.805241
39	6	0	2.689398	6.065468	-1.104531
40	6	0	-2.174781	3.849217	2.877009
41	6	0	-2.287719	3.949408	0.404828

42	6	0	-3.372431	3.064752	0.451223
43	6	0	-3.850821	2.571462	1.662051
44	6	0	-3.260741	2.964628	2.859766
45	1	0	-4.691840	1.883800	1.672354
46	1	0	-3.848952	2.761775	-0.475580
47	6	0	-1.836747	4.529343	-0.935115
48	6	0	-1.590100	4.305672	4.210664
49	1	0	-3.651570	2.585194	3.798898
50	6	0	3.390241	4.975267	4.947989
51	6	0	-1.154877	3.124821	5.097400
52	6	0	-2.584411	5.222918	4.951986
53	6	0	-2.862941	5.573640	-1.426421
54	6	0	-1.586132	3.461112	-2.015674
55	1	0	1.876899	6.062242	3.908110
56	1	0	-0.692550	4.894066	4.003225
57	1	0	-0.887741	5.049680	-0.777883
58	1	0	-3.028209	6.363678	-0.685961
59	1	0	-2.515340	6.043716	-2.352466
60	1	0	-0.761900	2.791652	-1.754036
61	1	0	-2.481392	2.861029	-2.212342
62	1	0	-2.000940	2.484337	5.369926
63	1	0	-0.714274	3.499386	6.027851
64	1	0	-3.506061	4.688161	5.206316
65	1	0	-2.143084	5.589970	5.884947
66	1	0	3.133999	4.015106	4.490176
67	1	0	4.467981	4.990979	5.143897
68	6	0	3.230051	7.504348	4.725223
69	1	0	2.709817	7.560213	5.687456
70	1	0	2.886781	8.338821	4.104781
71	6	0	2.879344	7.425445	-1.809773
72	6	0	3.031778	4.899535	-2.052166
73	1	0	2.495880	5.027935	-2.998985
74	1	0	2.733215	3.929590	-1.644326
75	1	0	4.101592	4.869113	-2.286249
76	1	0	2.609356	8.262135	-1.156265
77	1	0	3.919818	7.570731	-2.120070
78	1	0	2.253728	7.479068	-2.706941
79	1	0	1.628274	5.974863	-0.856685
80	1	0	-2.861414	6.090257	4.343522
81	1	0	-0.402548	2.514351	4.589694
82	1	0	-3.832399	5.106094	-1.631427
83	1	0	-1.316637	3.953000	-2.956789
84	1	0	4.298848	7.650225	4.915680
85	1	0	2.878693	5.037109	5.914886

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1704.108709 (a.u.)

Zero-point Correction = 0.734614 (a.u.) Gibbs Free Energy Correction = 0.660362 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1706.4015868 (a.u.)

L2-IM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.387223	-0.816800	0.195505
2	7	0	0.446654	-1.887398	0.332743

3	6	0	-0.265332	-3.080691	0.388918
4	6	0	-1.578864	-2.753809	0.280813
5	7	0	-1.633530	-1.369519	0.163968
6	6	0	1.888640	-1.787697	0.364084
7	1	0	0.223622	-4.035445	0.497327
8	1	0	-2.466784	-3.365394	0.274698
9	6	0	-2.845893	-0.603316	-0.018325
10	6	0	2.523557	-1.564321	1.601782
11	6	0	2.598399	-1.911105	-0.848039
12	6	0	3.919157	-1.451038	1.599386
13	6	0	4.647498	-1.562878	0.418330
14	6	0	3.993082	-1.794393	-0.788122
15	1	0	5.729671	-1.470256	0.438425
16	1	0	4.571415	-1.883180	-1.702415
17	6	0	1.918746	-2.198430	-2.184415
18	1	0	4.440355	-1.270170	2.534429
19	6	0	1.752380	-1.426982	2.911208
20	6	0	-3.287312	-0.343871	-1.331483
21	6	0	-3.528009	-0.137391	1.123305
22	6	0	-4.690038	0.615564	0.917518
23	6	0	-5.149767	0.891221	-0.367492
24	6	0	-4.455658	0.415413	-1.475789
25	1	0	-6.051887	1.480555	-0.505202
26	1	0	-5.236766	0.996593	1.774713
27	6	0	-3.029613	-0.393985	2.542308
28	6	0	-2.563121	-0.857352	-2.573454
29	1	0	-4.821989	0.638281	-2.473081
30	6	0	2.279121	-1.165668	-3.269704
31	6	0	-2.044635	0.292197	-3.460522
32	6	0	-3.464312	-1.818737	-3.375405
33	6	0	-4.100417	-1.072502	3.417352
34	6	0	-2.521902	0.910011	3.189664
35	1	0	0.836774	-2.140404	-2.035236
36	1	0	-1.691406	-1.431470	-2.247214
37	1	0	-2.178766	-1.079044	2.485115
38	1	0	-4.453349	-2.005992	2.967033
39	1	0	-3.690132	-1.306038	4.405590
40	1	0	-1.724659	1.360211	2.590013
41	1	0	-3.327756	1.645838	3.284372
42	1	0	-2.864116	0.940007	-3.791325
43	1	0	-1.569405	-0.119604	-4.357630
44	1	0	-4.350233	-1.306950	-3.766280
45	1	0	-2.914751	-2.226943	-4.230003
46	1	0	1.979187	-0.150200	-2.991376
47	1	0	3.353318	-1.166915	-3.486345
48	6	0	2.241053	-3.633261	-2.651883
49	1	0	1.715666	-3.856599	-3.586462
50	1	0	1.942313	-4.379436	-1.907451
51	6	0	2.224896	-2.446720	3.965078
52	6	0	1.830614	0.013581	3.453955
53	1	0	1.239456	0.109113	4.371419
54	1	0	1.445008	0.729942	2.721814
55	1	0	2.862821	0.294187	3.689837
56	1	0	2.143603	-3.473369	3.593508
57	1	0	3.267833	-2.278990	4.253548
58	1	0	1.615917	-2.364184	4.871606
59	1	0	0.698870	-1.639166	2.707559
60	1	0	-3.809443	-2.657036	-2.760482

61	1	0	-1.298148	0.909561	-2.951375
62	1	0	-4.970941	-0.425692	3.568045
63	1	0	-2.128556	0.712015	4.192901
64	1	0	3.313919	-3.758935	-2.834208
65	1	0	1.762659	-1.420692	-4.201877
66	29	0	0.067811	1.056176	-0.023615
67	6	0	2.900783	2.747612	-1.419510
68	6	0	3.334590	3.386429	-0.094574
69	6	0	2.370267	4.514672	0.284925
70	6	0	0.968225	3.957757	0.586404
71	6	0	0.503193	2.959030	-0.497954
72	6	0	1.387267	2.538874	-1.573226
73	8	0	0.986783	1.978594	-2.618124
74	1	0	3.397358	1.785403	-1.591592
75	1	0	3.193507	3.391182	-2.260047
76	1	0	4.363987	3.757431	-0.174271
77	1	0	3.337447	2.632421	0.705092
78	1	0	2.308865	5.230215	-0.549374
79	1	0	2.743750	5.072886	1.153598
80	1	0	1.044750	3.450800	1.561009
81	1	0	-0.489472	3.192497	-0.903873
82	6	0	-0.052114	5.091652	0.759147
83	1	0	-0.160929	5.660669	-0.172092
84	1	0	0.251117	5.789249	1.549653
85	1	0	-1.039916	4.695224	1.022054

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -1704.154526 (a.u.)

Zero-point Correction = 0.740057 (a.u.) Gibbs Free Energy Correction = 0.663406 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -1706.4489779 (a.u.)

L2-IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.096291	1.152050	0.299360
2	7	0	2.235512	1.334907	1.030437
3	6	0	2.326964	2.633052	1.517976
4	6	0	1.220039	3.286045	1.084454
5	7	0	0.472611	2.367068	0.355299
6	6	0	3.229100	0.312060	1.269346
7	1	0	3.161180	2.963577	2.115610
8	1	0	0.897720	4.304677	1.222919
9	6	0	-0.804621	2.671643	-0.253368
10	6	0	4.379372	0.291321	0.454463
11	6	0	3.022504	-0.602218	2.322932
12	6	0	5.336306	-0.697134	0.714443
13	6	0	5.157291	-1.618208	1.742786
14	6	0	4.015331	-1.567322	2.536992
15	1	0	5.911411	-2.378092	1.926778
16	1	0	3.890140	-2.287702	3.338956
17	6	0	1.809853	-0.540660	3.247499
18	1	0	6.230627	-0.748020	0.101105
19	6	0	4.596872	1.275608	-0.692004
20	6	0	-1.951657	2.718583	0.569664
21	6	0	-0.849089	2.936667	-1.636671

22	6	0	-2.099642	3.225825	-2.198038
23	6	0	-3.249152	3.263145	-1.415499
24	6	0	-3.172041	3.019586	-0.046291
25	1	0	-4.208613	3.491560	-1.870765
26	1	0	-2.169588	3.428299	-3.262439
27	6	0	0.393026	2.950306	-2.523049
28	6	0	-1.888653	2.516748	2.082352
29	1	0	-4.075171	3.056590	0.553350
30	6	0	1.101175	-1.899964	3.399752
31	6	0	-3.047914	1.670653	2.640911
32	6	0	-1.850958	3.879510	2.809065
33	6	0	0.643538	4.355421	-3.106719
34	6	0	0.310676	1.891604	-3.639082
35	1	0	1.083524	0.149318	2.809443
36	1	0	-0.959503	1.985423	2.312005
37	1	0	1.257896	2.697519	-1.904151
38	1	0	0.734543	5.106889	-2.315568
39	1	0	1.569480	4.364636	-3.691742
40	1	0	0.185953	0.888656	-3.219486
41	1	0	-0.529955	2.083572	-4.314288
42	1	0	-4.002171	2.205589	2.589942
43	1	0	-2.859597	1.452894	3.697772
44	1	0	-2.765629	4.447720	2.607778
45	1	0	-1.777769	3.732597	3.892024
46	1	0	0.761034	-2.300975	2.439890
47	1	0	1.750262	-2.644409	3.874078
48	6	0	2.215832	0.030216	4.622780
49	1	0	1.338523	0.117851	5.272511
50	1	0	2.670129	1.022631	4.530116
51	6	0	5.952818	1.999313	-0.586285
52	6	0	4.445886	0.576527	-2.057820
53	1	0	4.571840	1.297837	-2.872958
54	1	0	3.458880	0.115099	-2.156840
55	1	0	5.197810	-0.209520	-2.185968
56	1	0	6.065741	2.500807	0.380420
57	1	0	6.793791	1.307896	-0.702649
58	1	0	6.039042	2.756052	-1.373138
59	1	0	3.819817	2.043221	-0.634612
60	1	0	-1.003196	4.496183	2.496578
61	1	0	-3.173086	0.722992	2.113036
62	1	0	-0.170985	4.666974	-3.769181
63	1	0	1.227647	1.898955	-4.238354
64	1	0	2.939747	-0.622142	5.123338
65	1	0	0.222484	-1.783313	4.043132
66	29	0	0.651168	-0.488471	-0.658764
67	6	0	1.884563	-3.805016	-0.407030
68	6	0	2.878566	-3.567863	-1.550708
69	6	0	2.135970	-3.571199	-2.889995
70	6	0	1.169836	-2.378331	-2.990361
71	6	0	0.344037	-2.195820	-1.693003
72	6	0	0.548202	-3.062373	-0.547659
73	8	0	-0.294846	-3.222644	0.365144
74	1	0	2.316925	-3.549802	0.567276
75	1	0	1.625172	-4.870779	-0.352165
76	1	0	3.659610	-4.338218	-1.532893
77	1	0	3.388872	-2.604524	-1.417420
78	1	0	1.565557	-4.509092	-2.975493
79	1	0	2.837531	-3.555662	-3.734430

80	6	0	0.248686	-2.518642	-4.211270
81	1	0	-0.723995	-2.045830	-1.882138
82	1	0	-0.396657	-3.399512	-4.110784
83	1	0	0.824923	-2.622904	-5.139052
84	1	0	-0.401619	-1.642513	-4.318292
85	1	0	1.795520	-1.490153	-3.171867
86	14	0	-3.061603	-2.001336	0.587678
87	8	0	-4.448653	-1.056740	0.710940
88	14	0	-5.945795	-0.557387	0.245135
89	6	0	-2.838224	-2.874614	2.237481
90	6	0	-3.305010	-3.221990	-0.824630
91	6	0	-5.995457	-0.175893	-1.601358
92	6	0	-7.256043	-1.839267	0.684889
93	1	0	-6.244512	0.701655	0.994255
94	1	0	-3.728960	-3.463804	2.484723
95	1	0	-1.973027	-3.540960	2.185287
96	1	0	-2.680445	-2.157599	3.050366
97	1	0	-2.455809	-3.907681	-0.868486
98	1	0	-4.220514	-3.806328	-0.671027
99	1	0	-3.394821	-2.713673	-1.790892
100	1	0	-6.971514	0.226283	-1.897447
101	1	0	-5.230757	0.561845	-1.867113
102	1	0	-5.810143	-1.076300	-2.197533
103	1	0	-7.239036	-2.069425	1.755309
104	1	0	-8.260760	-1.478463	0.435171
105	1	0	-7.092730	-2.776028	0.140248
106	1	0	-1.987601	-1.009570	0.323866

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -2519.200230 (a.u.)

Zero-point Correction = 0.911498 (a.u.) Gibbs Free Energy Correction = 0.814015 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -2521.7813986 (a.u.)

L2-TS2:

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.165149	0.148755	0.041275
2	6	0	0.176977	0.129409	1.573628
3	6	0	1.616033	0.038070	2.091340
4	6	0	2.441246	1.272259	1.685912
5	6	0	2.187514	1.658144	0.226412
6	6	0	1.231778	1.042458	-0.561701
7	8	0	1.150472	1.155782	-1.863701
8	1	0	-0.808052	0.463196	-0.354669
9	1	0	0.333051	-0.862464	-0.354121
10	1	0	-0.425719	-0.708555	1.943069
11	1	0	-0.291318	1.045854	1.958312
12	1	0	2.087290	-0.863316	1.672960
13	1	0	1.632910	-0.076992	3.182564
14	1	0	2.144910	2.098970	2.347647
15	1	0	3.030267	2.114287	-0.296120
16	6	0	3.941077	1.033002	1.923305
17	1	0	4.311204	0.221696	1.285671
18	1	0	4.136102	0.761768	2.967468
19	1	0	4.525276	1.931675	1.698170

20	14	0	1.692036	2.526001	-2.985330
21	8	0	2.936049	3.731836	-3.069200
22	14	0	4.275188	4.266938	-3.860135
23	6	0	0.213273	2.952450	-4.100313
24	6	0	2.636610	1.187824	-3.995430
25	6	0	5.782584	3.164983	-3.571196
26	6	0	3.995478	4.490697	-5.716234
27	1	0	4.607527	5.618386	-3.303333
28	1	0	-0.573142	2.199688	-3.968654
29	1	0	-0.215296	3.929571	-3.857565
30	1	0	0.498757	2.949860	-5.158890
31	1	0	1.988660	0.330094	-4.207419
32	1	0	2.997561	1.580927	-4.953897
33	1	0	3.507497	0.804196	-3.449447
34	1	0	6.680768	3.614130	-4.012140
35	1	0	5.971228	3.026605	-2.500899
36	1	0	5.647798	2.174062	-4.016664
37	1	0	3.131287	5.135393	-5.908931
38	1	0	4.870627	4.956145	-6.185595
39	1	0	3.815679	3.534416	-6.218780
40	1	0	1.171699	3.402468	-1.719239
41	6	0	0.619643	5.270909	1.002892
42	7	0	1.177131	5.846575	2.113947
43	6	0	0.558560	7.051103	2.432747
44	6	0	-0.419132	7.239088	1.512820
45	7	0	-0.367525	6.150367	0.650420
46	6	0	2.264373	5.294142	2.888392
47	1	0	0.871395	7.651228	3.271804
48	1	0	-1.136479	8.034126	1.387989
49	6	0	-1.247603	6.005964	-0.487700
50	6	0	3.587097	5.496428	2.446303
51	6	0	1.958592	4.613382	4.086105
52	6	0	4.617926	4.970328	3.236277
53	6	0	4.346095	4.288556	4.418279
54	6	0	3.029967	4.117572	4.838899
55	1	0	5.161993	3.892478	5.016052
56	1	0	2.830426	3.590325	5.766774
57	6	0	0.529604	4.437198	4.594583
58	1	0	5.648200	5.105565	2.922126
59	6	0	3.931633	6.282598	1.184880
60	6	0	-2.430711	5.255934	-0.338527
61	6	0	-0.906701	6.658878	-1.689080
62	6	0	-1.793674	6.530295	-2.764837
63	6	0	-2.963879	5.785183	-2.650915
64	6	0	-3.276709	5.155970	-1.449689
65	1	0	-3.633738	5.694783	-3.501130
66	1	0	-1.560153	7.018761	-3.705591
67	6	0	0.356608	7.500392	-1.846199
68	6	0	-2.816371	4.570136	0.968430
69	1	0	-4.192980	4.578937	-1.369991
70	6	0	0.194444	2.968768	4.914502
71	6	0	-2.871124	3.039524	0.804176
72	6	0	-4.144725	5.119350	1.524232
73	6	0	0.005728	8.995037	-1.994481
74	6	0	1.233872	7.016383	-3.015687
75	1	0	-0.153647	4.755595	3.802252
76	1	0	-2.040643	4.787903	1.707991
77	1	0	0.950640	7.394055	-0.934098

78	1	0	-0.572401	9.362826	-1.139780
79	1	0	0.918724	9.595304	-2.069678
80	1	0	1.522095	5.968980	-2.895084
81	1	0	0.718023	7.122572	-3.976397
82	1	0	-3.640786	2.740512	0.084635
83	1	0	-3.105346	2.560329	1.761190
84	1	0	-4.980191	4.915570	0.846203
85	1	0	-4.377615	4.651133	2.486678
86	1	0	0.359147	2.324997	4.046239
87	1	0	0.800409	2.581663	5.740343
88	6	0	0.268919	5.335413	5.821141
89	1	0	-0.768419	5.234640	6.158014
90	1	0	0.449599	6.391022	5.594238
91	6	0	4.688405	7.579974	1.534094
92	6	0	4.722553	5.432944	0.173280
93	1	0	4.929063	6.013436	-0.730876
94	1	0	4.155907	4.547522	-0.128430
95	1	0	5.682423	5.102277	0.585110
96	1	0	4.112848	8.208098	2.222143
97	1	0	5.653536	7.366953	2.006196
98	1	0	4.883560	8.160170	0.626206
99	1	0	2.997131	6.572150	0.697621
100	1	0	-4.096927	6.202564	1.676224
101	1	0	-1.912339	2.650037	0.449608
102	1	0	-0.587142	9.175927	-2.897606
103	1	0	2.148486	7.616925	-3.067614
104	1	0	0.921307	5.060631	6.656974
105	1	0	-0.856163	2.879780	5.210974
106	29	0	1.173387	3.673890	-0.011621

Zero-point Energy: B3LYP/[6-31G(d,p), LANL2DZ] = -2519.182166 (a.u.)

Zero-point Correction = 0.912022 (a.u.) Gibbs Free Energy Correction = 0.818003 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/[6-311++G(d,p), SDD] = -2521.7605075 (a.u.)

Product:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.058493	1.418547	0.378584
2	8	0	-1.894111	-0.008953	0.335497
3	14	0	-2.761301	-1.063723	-0.618528
4	6	0	-2.078854	2.797817	-0.367660
5	6	0	-0.565580	1.735093	2.156861
6	6	0	-1.818294	-2.681154	-0.777175
7	6	0	-4.447707	-1.335382	0.166759
8	1	0	-2.939500	-0.462367	-1.973627
9	1	0	-3.014286	2.938609	0.184114
10	1	0	-1.531896	3.745882	-0.354157
11	1	0	-2.331994	2.573557	-1.408757
12	1	0	-0.103451	2.721862	2.265509
13	1	0	-1.439696	1.695380	2.814712
14	1	0	0.152361	0.986643	2.503826
15	1	0	-2.348477	-3.378970	-1.435141
16	1	0	-0.820657	-2.514470	-1.195226
17	1	0	-1.697721	-3.165579	0.197817

18	1	0	-5.001623	-0.395271	0.255021
19	1	0	-5.052413	-2.024781	-0.433296
20	1	0	-4.349642	-1.761659	1.170898
21	6	0	2.620301	1.251708	-1.171987
22	6	0	3.804415	0.288938	-1.332880
23	6	0	4.038108	-0.505397	-0.043265
24	6	0	2.813082	-1.362203	0.319265
25	6	0	1.528228	-0.574255	0.165371
26	6	0	1.452673	0.600935	-0.477079
27	8	0	0.305227	1.348944	-0.600577
28	1	0	2.276952	1.622356	-2.145408
29	1	0	2.919899	2.143329	-0.601769
30	1	0	4.704676	0.845911	-1.615601
31	1	0	3.595756	-0.409535	-2.153849
32	1	0	4.240417	0.194566	0.780033
33	1	0	4.923679	-1.145403	-0.137145
34	1	0	2.781394	-2.215348	-0.379594
35	1	0	0.629969	-1.003327	0.602997
36	6	0	2.935864	-1.947725	1.735554
37	1	0	2.969667	-1.149197	2.485435
38	1	0	3.847853	-2.546668	1.836416
39	1	0	2.083514	-2.593243	1.974067

Zero-point Energy: B3LYP/6-31G(d,p) = -1162.948610 (a.u.)

Zero-point Correction = 0.332265 (a.u.) Gibbs Free Energy Correction = 0.280743 (a.u.)

SCF Energy: B3LYP (PCM, toluene)/6-311++G(d,p) = -1163.4709014 (a.u.)