Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Origins of Enantioselectivity in the Chiral Diphosphine-Ligated CuH-Catalyzed Asymmetric Hydrosilylation of Ketones

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CONTENTS:

Part I: Model System

S1: The summarize energies of all optimized stationary points over model reaction system……2

S2. Cartesian coordinates and energies of all optimized stationary points of model reaction system at the B3LYP/6-31+G(d, p) level.....3

S3. Cartesian coordinates and energies of all optimized stationary points of model reaction system at theB3LYP/6-311++G(2d, 2p) level.....7

Part II: Actual System

S4: The summarize energies of all species over L_1-CuH (L_1=BDPP) reaction system.....11

S5. Cartesian coordinates and energies of all optimized structures over L_1-CuH reaction system at the B3LYP/6-31+G(d, p):3-21G level.。。。.....12**

S6. Cartesian coordinates and energies of all optimized catalyst and TS structures over L_n-CuH (n=2-3*) reaction systems at the B3LYP/6-31+G(d, p):3-21G level….....26**

S7. Reference 18 details.....36

Part I: Model system

S1: The summarize energies properties of all optimized stationary points over model reaction system.

Table a. ZPE-corrected total energies at the B3LYP/6-31+G(d,p) and B3LYP/6-311++G(2d,2p) levels

spices	B3LYP/6-31+G(d, p)				B3LYP/6-311++G(2d,2p)	
	SCF	ZPE	E_{ZPE}	ΔE_{ZPE}	E_{ZPE}	ΔE_{ZPE}
SiH_4	−291.888023	0.031280	−291.856743		−291.883092	
acetophenone	−384.916696	0.137875	−384.778821		−384.878288	
CuH	−1640.915718	0.004280	−1640.911438		−1641.069495	
Reactant*			−2317.547002	0.0	−2317.830875	0.0
COM1	−2025.870223	0.145245	−2025.724978		−2025.980711	
COM1 + SiH_4			−2317.581721	−91.2	−2317.863803	−86.5
TS1	−2025.798453	0.143605	−2025.654847		−2025.912412	
TS1 + SiH4			−2317.511590	93.0	−2317.795504	92.9
IM1	−2025.844538	0.149712	−2025.694826		−2025.950952	
IM1 + SiH_4			−2317.551569	−12.0	−2317.834044	−8.3
IM2	−2317.765757	0.183457	−2317.582301	−92.7	−2317.867399	−95.9
TS2	−2317.733488	0.182644	−2317.550844	−10.1	−2317.836547	−14.9
Product	−676.8438566	0.176480	−676.667377		−676.797122	
Product + CuH			−2317.578815	−83.5	−2317.866617	−93.8

* Reactant= CuH + acetophenone + SiH_4

Table b. Relative energies at the B3LYP/6-31+G(d,p) level in the gas-phase and toluene. (ΔG_{RT} presents the relative Gibbs free energies in the gas-phase; ΔG_{solv} presents the energies in toluene.)

spices	B3LYP/6-31+G(d, p)				B3LYP(PCM)/6-31+G(d,p)		
	SCF	*Gc*	G_{RT}	ΔG_{RT}	SCF_{PCM}	G_{solv}	ΔG_{solv}
SiH_4	−291.888023	0.009718	−291.878305		−291.889907	−291.880189	
acetophenone	−384.916696	0.105094	−384.811602		−384.926171	−384.8210768	
CuH	−1640.915718	−0.014699	−1640.930417		−1640.92061	−1640.935312	
Reactant*			−2317.620324	0.0		−2317.636613	0.0
COM1	−2025.870223	0.107219	−2025.763004		−2025.885852	−2025.778633	
COM1 + SiH_4			−2317.641309	−55.1		−2317.658822	−58.3
TS1	−2025.798453	0.107234	−2025.691219		−2025.811468	−2025.704234	
TS1 + SiH4			−2317.569524	133.4		−2317.584423	137.0
IM1	−2025.844538	0.111777	−2025.732761		−2025.858411	−2025.746634	
IM1 + SiH_4			−2317.611066	24.3		−2317.626823	25.7
IM2	−2317.765757	0.139526	−2317.626231	−15.5	−2317.780665	−2317.641139	−11.9
TS2	−2317.733488	0.140450	−2317.593038	71.6	−2317.747449	−2317.606999	77.8
Product	−676.843857	0.138760	-676.705097		−676.853636	−676.714859	
Product + CuH			−2317.635518	−39.9		−2317.650188	−35.6

* Reactant= CuH + acetophenone + SiH_4

S2. Cartesian coordinates and energies of all optimized stationary points of model reaction system at the B3LYP/6-31+G(d, p) level.

Acetophenone

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.579817	-1.222873	0.000119
2	6	0	-1.970090	-1.138078	0.000232
3	6	0	-2.596089	0.114044	0.000033
4	6	0	0.205453	-0.057371	-0.000064
5	6	0	-0.431209	1.194628	-0.000154
6	6	0	-1.825125	1.279308	-0.000186
7	6	0	1.699635	-0.201568	-0.000103
8	6	0	2.563045	1.047797	0.000342
9	8	0	2.218366	-1.310523	-0.000361
10	1	0	-0.075366	-2.183419	0.000228
11	1	0	-2.568165	-2.044704	0.000425
12	1	0	-3.680373	0.180360	0.000014
13	1	0	0.153948	2.108468	-0.000244
14	1	0	-2.307548	2.252322	-0.000369
15	1	0	2.362531	1.663720	0.884248
16	1	0	2.361934	1.665008	-0.882511
17	1	0	3.611292	0.747101	-0.000217

Zero-point correction= 0.137875 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.105094
Sum of electronic and zero-point Energies= −384.778821(a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −384.9261708 (a.u.)

CuH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	0.049336
2	1	0	0.000000	0.000000	-1.430756

Zero-point correction= 0.004280 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= −0.014699
Sum of electronic and zero-point Energies= −1640.911438 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −1640.9206128 (a.u.)

SiH_4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.000004	0.000006	-0.000007
2	1	0	1.079914	0.501317	-0.887445
3	1	0	-0.914516	-0.873860	-0.777966
4	1	0	-0.762536	1.149536	0.549815
5	1	0	0.597079	-0.777075	1.115690

Zero-point correction= 0.031280 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.009718
Sum of electronic and zero-point Energies= −291.856743 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −291.8899074 (a.u.)

COM1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.240697	1.149365	0.000106
2	6	0	3.579607	0.759776	0.000275
3	6	0	3.911919	-0.597966	0.000195
4	6	0	2.902593	-1.568117	-0.000052
5	6	0	1.219397	0.181794	-0.000140
6	6	0	1.565259	-1.183162	-0.000216
7	6	0	-0.213363	0.561355	-0.000275
8	6	0	-0.621079	2.013627	-0.000188
9	1	0	1.996836	2.206257	0.000195
10	1	0	4.361470	1.512887	0.000477
11	1	0	4.955076	-0.900267	0.000335
12	1	0	3.161634	-2.622418	-0.000100
13	1	0	0.772433	-1.922964	-0.000417
14	1	0	-1.709810	2.086303	-0.000663
15	1	0	-0.224688	2.525626	0.883632
16	1	0	-0.223899	2.526003	-0.883423
17	8	0	-1.072694	-0.336016	-0.000428
18	29	0	-3.017636	-0.353093	0.000153
19	1	0	-4.506242	-0.383646	0.000708

Zero-point correction= 0.145245 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.107219
Sum of electronic and zero-point Energies= −2025.724978(a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −2025.885852 (a.u.)

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	2.234518	-0.539409	-0.572551
2	1	0	1.189646	0.636462	-0.999915
3	6	0	0.675913	0.560379	0.474622
4	8	0	1.346240	-0.329487	1.192021
5	6	0	0.942499	2.021849	0.833583
6	1	0	2.017862	2.189676	0.922820
7	1	0	0.521686	2.728610	0.114501
8	1	0	0.482069	2.199814	1.814078
9	6	0	-0.773314	0.222160	0.166119
10	6	0	-1.579103	1.027431	-0.654544
11	6	0	-1.332351	-0.917524	0.760615
12	6	0	-2.918060	0.701925	-0.871764
13	1	0	-1.156525	1.900185	-1.144344
14	6	0	-2.674770	-1.242292	0.545290
15	1	0	-0.699408	-1.528154	1.395613
16	6	0	-3.471534	-0.434983	-0.270531
17	1	0	-3.529687	1.331635	-1.512045
18	1	0	-3.097729	-2.125309	1.016773
19	1	0	-4.514520	-0.687828	-0.439995

Zero-point correction= 0.143605 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.107234
Sum of electronic and zero-point Energies= −2025.654847(a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −2025.8114682 (a.u.)

IM1

Standard orientation:

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

1	6	0	-1.463210	-1.045238	0.329127
2	6	0	-2.801894	-1.442408	0.400537
3	6	0	-3.821094	-0.565439	0.017243
4	6	0	-3.490723	0.712132	-0.445486
5	6	0	-1.124743	0.236007	-0.124003
6	6	0	-2.151566	1.105180	-0.518667
7	6	0	0.331204	0.705045	-0.159451
8	6	0	0.663025	1.501979	1.117256
9	1	0	-0.666271	-1.726982	0.606401
10	1	0	-3.049045	-2.441234	0.751206
11	1	0	-4.861020	-0.875857	0.070916
12	1	0	-4.273489	1.399358	-0.755959
13	1	0	-1.902817	2.097718	-0.889650
14	1	0	0.429782	1.390803	-1.019372
15	1	0	1.691769	1.884711	1.061110
16	1	0	-0.012124	2.355011	1.248827
17	1	0	0.578318	0.853332	1.995928
18	8	0	1.170978	-0.414768	-0.327302
19	29	0	2.960382	-0.305595	-0.143115

Zero-point correction= 0.149712 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.111777
Sum of electronic and zero-point Energies= −2025.694826 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −2025.8584106 (a.u.)

IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.400552	-0.284451	-0.610909
2	6	0	-2.259672	-1.054001	0.359645
3	6	0	-3.571440	-1.540086	0.355399
4	6	0	-4.611168	-0.765636	-0.166614
5	6	0	-4.328149	0.500830	-0.689319
6	6	0	-1.968891	0.216733	-0.150717
7	6	0	-3.017185	0.983476	-0.681583
8	6	0	-0.544526	0.774359	-0.122088
9	6	0	-0.417252	1.871208	0.954662
10	1	0	-1.442932	-1.654263	0.745629
11	1	0	-3.780170	-2.529347	0.755236
12	1	0	-5.629306	-1.145433	-0.172928
13	1	0	-5.126107	1.109159	-1.107449
14	1	0	-2.806714	1.966479	-1.099161
15	1	0	-0.368251	1.250156	-1.104343
16	1	0	0.589685	2.307649	0.925004
17	1	0	-1.144387	2.677539	0.806127
18	1	0	-0.579131	1.436573	1.947149
19	8	0	0.377412	-0.264510	0.086253
20	29	0	2.145625	-0.142377	0.310896
21	1	0	3.633436	-0.145226	0.777585
22	1	0	5.748088	-0.344346	0.001192
23	1	0	4.097892	-1.543200	-1.325616
24	1	0	4.267442	0.920287	-1.458012

Zero-point correction= 0.183457 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.139526
Sum of electronic and zero-point Energies= −2317.582301 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −2317.7806649 (a.u.)

TS2

Standard orientation:

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

1	14	0	-2.025003	0.641939	1.650514
2	6	0	1.475786	-1.007613	0.090545
3	6	0	2.683394	-1.692085	0.264810
4	6	0	3.890612	-0.991286	0.307812
5	6	0	3.880869	0.401948	0.180989
6	6	0	1.455530	0.384590	-0.047915
7	6	0	2.673378	1.080555	0.005908
8	6	0	0.159450	1.157133	-0.282814
9	6	0	0.044277	1.648735	-1.733272
10	1	0	0.538397	-1.553815	0.082157
11	1	0	2.677874	-2.773315	0.374502
12	1	0	4.828221	-1.521779	0.447614
13	1	0	4.812302	0.959850	0.225440
14	1	0	2.677444	2.165171	-0.081344
15	1	0	0.168896	2.038809	0.377240
16	1	0	-0.867136	2.242755	-1.854976
17	1	0	0.904656	2.264273	-2.014439
18	1	0	0.004509	0.792031	-2.416511
19	8	0	-0.995466	0.392155	0.037609
20	29	0	-2.341388	-0.862412	-0.643174
21	1	0	-2.909299	-0.571500	0.896034
22	1	0	-3.001444	0.361158	2.778143
23	1	0	-0.762185	0.568559	2.443325
24	1	0	-2.437995	2.021498	1.270409

Zero-point correction= 0.182644 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.140450
Sum of electronic and zero-point Energies= −2317.550844 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −2317.7474493 (a.u.)

product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.525489	-1.293436	0.212596
2	6	0	-1.035710	2.356220	-0.334780
3	6	0	-0.931331	0.952566	0.265489
4	6	0	0.465496	0.364767	0.127028
5	1	0	-1.173818	1.011200	1.337785
6	8	0	-1.914750	0.139324	-0.392692
7	6	0	0.926341	-0.102299	-1.112989
8	6	0	1.325740	0.313335	1.230856
9	6	0	2.221270	-0.607164	-1.243662
10	6	0	2.625918	-0.186344	1.101824
11	6	0	3.076725	-0.648400	-0.136820
12	1	0	0.261023	-0.079243	-1.971328
13	1	0	2.564064	-0.969850	-2.208899
14	1	0	4.084192	-1.041577	-0.239619
15	1	0	3.280290	-0.220944	1.968503
16	1	0	0.977371	0.663842	2.200162
17	1	0	-0.818426	2.325705	-1.407056
18	1	0	-2.047256	2.749610	-0.195040
19	1	0	-0.320904	3.032559	0.144812
20	1	0	-1.541639	-2.406565	0.151834
21	1	0	-3.698969	-1.616311	-0.630789
22	1	0	-2.937784	-1.110993	1.633152

Zero-point correction= 0.176480 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.138760
Sum of electronic and zero-point Energies= −676.667377 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −676.853636 (a.u.)

S3. Cartesian coordinates and energies of all optimized stationary points of model reaction system at the B3LYP/6-311++G(2d, 2p) level.

Acetophonone

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.580185	-1.217761	-0.000095
2	6	0	-1.963947	-1.132117	0.000001
3	6	0	-2.585913	0.115288	0.000055
4	6	0	0.203321	-0.058308	-0.000160
5	6	0	-0.429695	1.188404	-0.000107
6	6	0	-1.817490	1.274421	0.000005
7	6	0	1.695826	-0.203850	-0.000282
8	6	0	2.555373	1.044739	0.000132
9	8	0	2.210027	-1.305336	0.000258
10	1	0	-0.079623	-2.175168	-0.000133
11	1	0	-2.560680	-2.033968	0.000038
12	1	0	-3.665420	0.182253	0.000138
13	1	0	0.154256	2.097394	-0.000148
14	1	0	-2.297253	2.243454	0.000050
15	1	0	2.352243	1.657833	0.879622
16	1	0	2.352711	1.658074	-0.879295
17	1	0	3.599811	0.747915	0.000379

Zero-point correction= 0.137577 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.104766
Sum of electronic and zero-point Energies= −384.878288 (a.u.)

CuH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	0.049486
2	1	0	0.000000	0.000000	-1.435094

Zero-point correction= 0.004256 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= −0.014729
Sum of electronic and zero-point Energies= −1641.069495 (a.u.)

SiH_4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.000001	-0.000002	0.000003
2	1	0	1.043141	-0.911988	0.531125
3	1	0	-0.617717	0.751092	1.120797
4	1	0	-1.042126	-0.793372	-0.697509
5	1	0	0.616685	0.954295	-0.954450

Zero-point correction= 0.031186 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.009626
Sum of electronic and zero-point Energies= −291.883092 (a.u.)

COM1

Standard orientation:

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

1	6	0	2.234024	1.143405	0.000135
2	6	0	3.568454	0.759861	0.000195
3	6	0	3.903055	-0.590581	0.000129
4	6	0	2.900938	-1.559523	0.000005
5	6	0	1.219475	0.177882	0.000015
6	6	0	1.568619	-1.180152	-0.000051
7	6	0	-0.212480	0.553399	-0.000036
8	6	0	-0.617223	2.002845	-0.000028
9	1	0	1.987770	2.194821	0.000188
10	1	0	4.344981	1.511714	0.000293
11	1	0	4.942530	-0.888752	0.000173
12	1	0	3.162392	-2.608397	-0.000047
13	1	0	0.782287	-1.920072	-0.000143
14	1	0	-1.701131	2.077134	-0.000160
15	1	0	-0.219883	2.511455	0.879624
16	1	0	-0.219649	2.511562	-0.879511
17	8	0	-1.065165	-0.339437	-0.000129
18	29	0	-3.015138	-0.349819	-0.000057
19	1	0	-4.508154	-0.372047	0.000099

Zero-point correction= 0.145047 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.107289
Sum of electronic and zero-point Energies= −2025.980711 (a.u.)

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	2.222266	-0.550357	-0.572860
2	1	0	1.187537	0.637154	-0.993527
3	6	0	0.676014	0.567528	0.480672
4	8	0	1.345312	-0.309034	1.200876
5	6	0	0.931222	2.029908	0.825464
6	1	0	2.000268	2.207739	0.912387
7	1	0	0.504374	2.722510	0.103507
8	1	0	0.470909	2.212639	1.800093
9	6	0	-0.769136	0.224885	0.168707
10	6	0	-1.559494	0.998764	-0.685679
11	6	0	-1.336987	-0.885291	0.793673
12	6	0	-2.890184	0.671099	-0.906944
13	1	0	-1.129324	1.847296	-1.200408
14	6	0	-2.672644	-1.210744	0.577032
15	1	0	-0.717128	-1.473368	1.454219
16	6	0	-3.452677	-0.435528	-0.273464
17	1	0	-3.488786	1.274887	-1.575591
18	1	0	-3.103097	-2.069782	1.074093
19	1	0	-4.489653	-0.690170	-0.445606

Zero-point correction= 0.143391 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.107011
Sum of electronic and zero-point Energies= −2025.912412(a.u.)

IM1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.473994	-1.040897	0.346032
2	6	0	-2.808876	-1.430969	0.404603
3	6	0	-3.815299	-0.559766	0.000029
4	6	0	-3.476142	0.705051	-0.471237
5	6	0	-1.126419	0.227778	-0.114948
6	6	0	-2.141311	1.091275	-0.530207

7	6	0	0.328156	0.691655	-0.139097
8	6	0	0.639313	1.530454	1.109910
9	1	0	-0.688055	-1.719867	0.642038
10	1	0	-3.062888	-2.420092	0.762636
11	1	0	-4.852099	-0.864928	0.043387
12	1	0	-4.249172	1.387709	-0.798585
13	1	0	-1.886112	2.074352	-0.907715
14	1	0	0.439478	1.342743	-1.017457
15	1	0	1.661527	1.915547	1.053558
16	1	0	-0.039395	2.379271	1.204400
17	1	0	0.548797	0.913039	2.004149
18	8	0	1.168253	-0.431458	-0.252678
19	29	0	2.966528	-0.304952	-0.158466

Zero-point correction= 0.149534 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.111706
Sum of electronic and zero-point Energies= −2025.950952 (a.u.)

IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.378625	-0.340160	0.670800
2	6	0	2.271983	-1.008653	-0.455933
3	6	0	3.572443	-1.505171	-0.423336
4	6	0	4.583660	-0.789418	0.208982
5	6	0	4.283492	0.428296	0.813403
6	6	0	1.963949	0.214018	0.137486
7	6	0	2.983885	0.921567	0.777148
8	6	0	0.550150	0.786220	0.079701
9	6	0	0.469615	1.914893	-0.961445
10	1	0	1.478014	-1.567656	-0.928486
11	1	0	3.794739	-2.456843	-0.888382
12	1	0	5.592779	-1.177982	0.237614
13	1	0	5.059115	0.989595	1.317666
14	1	0	2.759176	1.865898	1.259045
15	1	0	0.349524	1.229284	1.066270
16	1	0	-0.525210	2.366500	-0.943918
17	1	0	1.204325	2.698068	-0.768874
18	1	0	0.648598	1.509561	-1.957913
19	8	0	-0.373474	-0.233753	-0.193532
20	29	0	-2.154363	-0.113426	-0.329520
21	1	0	-3.664720	-0.103831	-0.721417
22	1	0	-5.744887	-0.345693	0.112813
23	1	0	-4.058304	-1.646405	1.273227
24	1	0	-4.203131	0.790601	1.599434

Zero-point correction= 0.183248 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.139057
Sum of electronic and zero-point Energies= −2317.867399 (a.u.)

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.067627	0.049951	-0.047436
2	6	0	0.097448	-0.002287	4.073036
3	6	0	0.854727	0.011952	5.241519
4	6	0	1.166871	-1.177166	5.890059
5	6	0	0.720546	-2.383625	5.357919
6	6	0	-0.362162	-1.203054	3.537626
7	6	0	-0.035432	-2.393197	4.191916

8	6	0	-1.232086	-1.250754	2.288865
9	6	0	-2.701784	-1.507386	2.632616
10	1	0	-0.122983	0.923057	3.561637
11	1	0	1.207026	0.954050	5.640020
12	1	0	1.759503	-1.166543	6.794539
13	1	0	0.967679	-3.316598	5.846380
14	1	0	-0.367575	-3.338978	3.781078
15	1	0	-0.879195	-2.080519	1.665728
16	1	0	-3.288083	-1.598298	1.718225
17	1	0	-2.816803	-2.422169	3.213368
18	1	0	-3.095348	-0.680302	3.226547
19	8	0	-1.142185	-0.059980	1.514794
20	29	0	-2.024761	1.639911	1.026367
21	1	0	-0.836366	1.553576	-0.117162
22	1	0	0.651987	0.637062	-1.241614
23	1	0	1.130740	-0.346101	0.737955
24	1	0	-0.780155	-1.073452	-0.707942

Zero-point correction= 0.182386 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.140281
Sum of electronic and zero-point Energies= −2317.836547 (a.u.)

product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.548226	-1.254146	0.254951
2	6	0	-1.020285	2.330945	-0.393684
3	6	0	-0.922527	0.942685	0.231494
4	6	0	0.471908	0.354227	0.112669
5	1	0	-1.170266	1.021003	1.295668
6	8	0	-1.903760	0.117251	-0.413700
7	6	0	0.924956	-0.173768	-1.097883
8	6	0	1.336978	0.367197	1.205634
9	6	0	2.216694	-0.673243	-1.210944
10	6	0	2.633269	-0.128167	1.094308
11	6	0	3.076534	-0.649392	-0.115690
12	1	0	0.257172	-0.202471	-1.947877
13	1	0	2.553479	-1.082837	-2.153760
14	1	0	4.081347	-1.039102	-0.204636
15	1	0	3.291067	-0.112871	1.952747
16	1	0	0.995046	0.763797	2.153800
17	1	0	-0.798783	2.278407	-1.459353
18	1	0	-2.026700	2.728343	-0.266431
19	1	0	-0.309067	3.011548	0.073886
20	1	0	-1.587190	-2.381206	0.274967
21	1	0	-3.709717	-1.605427	-0.584041
22	1	0	-2.976303	-0.982058	1.649888

Zero-point correction= 0.176289 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.138565
Sum of electronic and zero-point Energies= −676.797122 (a.u.)

Part II: Actual system

S4: The summarize energies properties of all species over actual reaction system.

Species	B3LYP/gen			B3LYP(PCM)/6-31+G**		
	ZPE(a.u.)	E_{ZPE}(a.u.)	G_c[a](a.u.)	SCF[b](a.u.)	G_{solv}[c](a.u.)	ΔG_{solv}[d] (kJ/mol)
SiH_4	0.031280	−291.856743	0.009718	−291.8899074	−291.880189	
acetophenone	0.137875	−384.778821	0.105094	−384.9261708	−384.821077	
BDPP-CuH	0.522908	−3440.305606	0.457003	−3446.908070	−3446.451067	
*Reactant	0.692063	−3825.084427	0.571815	−4123.724148	−4123.152333	0.0
L_1-CuH-**COM**-*re*	0.661315	−3825.099212	0.580612	−3831.832691	−3831.252079	52.7[d]
L_1-CuH-**TS1**-*re*	0.661272	−3825.088855	0.584742	−3831.822553	−3831.237811	90.2[d]
L_1-CuH-**IM1**-*re*	0.666732	−3825.122575	0.588774	−3831.863610	−3831.274836	−7.1[d]
L_1-CuH-**TS2**-*re*	0.701972	−4116.973020	0.622295	−4123.748279	−4123.125984	69.2
S-product +BDPP-CuH	0.176479	−4116.972983	0.595759	−4123.761684	−4123.165925	−35.7
L_1-CuH-**COM**-*si*	0.661960	−3825.098695	0.581709	−3831.834069	−3831.252360	52.0[d]
L_1-CuH-**TS1**-*si*	0.661668	−3825.088431	0.585188	−3831.821551	−3831.236363	94.0[d]
L_1-CuH-**IM1**-*si*	0.666824	−3825.123708	0.587719	−3831.863804	−3831.276085	−10.3[d]
L_1-CuH- **TS2**-*si*	0.701659	−4116.979511	0.621961	−4123.750683	−4123.128722	62.0
R-product +BDPP-CuH	0.176480	−4116.972983	0.595763	−4123.761706	−4123.165943	−35.7

* Reactant= BDPP-CuH + acetophenone +SiH_4

a: G_c = Thermal correction to Gibbs Free Energy

b: SCF = electronic energies in solvent.

c: G_{solv} =SCF + G_c

d: $\Delta G_{solv} = G_{solv} + G_{solv\,(SiH4)} - G_{solv\,(reactant)}$

S5. Cartesian coordinates and energies of all optimized structures over L_1-CuH reaction (L_1=BDPP) system at the B3LYP/6-31+G(d, p):3-21G level**

L_1-CuH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.972365	0.497348	1.439037
2	6	0	0.026059	-0.499448	2.109062
3	6	0	1.146321	-1.182239	1.247316
4	29	0	0.013904	-0.723718	-1.643481
5	15	0	1.769380	-0.132155	-0.202050
6	15	0	-1.682135	-0.159633	-0.178503
7	6	0	2.218448	-1.795424	2.188954
8	6	0	-2.006496	0.957821	2.500151
9	1	0	-0.395997	1.372729	1.127988
10	1	0	-0.550769	-1.304797	2.574472
11	1	0	0.509432	0.052633	2.920168
12	1	0	0.678867	-2.017697	0.713398
13	1	0	1.734410	-2.478724	2.892285
14	1	0	2.966326	-2.352044	1.625156
15	1	0	2.733074	-1.028325	2.769969
16	1	0	-1.486349	1.436401	3.334311
17	1	0	-2.710785	1.678148	2.081583
18	1	0	-2.563046	0.106032	2.892454
19	6	0	-2.800124	-1.528004	0.327697
20	6	0	-2.795575	1.200497	-0.714788
21	6	0	3.422666	-0.843738	-0.583808
22	6	0	2.153056	1.543829	0.462114
23	6	0	4.621827	-0.394536	-0.002943
24	6	0	5.834554	-1.003990	-0.336291
25	6	0	5.862684	-2.066375	-1.245078
26	6	0	4.676006	-2.508771	-1.836984
27	6	0	3.460955	-1.895698	-1.519891
28	6	0	2.566829	1.822142	1.778867
29	6	0	2.800511	3.139890	2.185397
30	6	0	2.638226	4.195054	1.283364
31	6	0	2.237152	3.931643	-0.029904
32	6	0	1.989386	2.618222	-0.436433
33	6	0	-2.434559	-2.830926	-0.057923
34	6	0	-3.202638	-3.928841	0.342767
35	6	0	-4.347714	-3.736435	1.119134
36	6	0	-4.733445	-2.442578	1.486922
37	6	0	-3.966989	-1.342761	1.095087
38	6	0	-2.340416	2.534347	-0.675259
39	6	0	-3.130653	3.567254	-1.183863
40	6	0	-4.377237	3.287723	-1.751643
41	6	0	-4.827036	1.966313	-1.815111
42	6	0	-4.044057	0.927710	-1.304267
43	1	0	4.611730	0.433760	0.691633
44	1	0	6.802905	-2.535517	-1.499050
45	1	0	4.695764	-3.315727	-2.556182
46	1	0	2.544076	-2.202751	-2.009271
47	1	0	2.708810	1.019535	2.486317
48	1	0	3.113389	3.340221	3.200961
49	1	0	2.822886	5.211687	1.600320
50	1	0	2.112972	4.743789	-0.732642
51	1	0	1.665854	2.417687	-1.450137
52	1	0	-1.568638	-2.970278	-0.693532
53	1	0	-2.913813	-4.925027	0.038189
54	1	0	-4.943761	-4.584724	1.425105
55	1	0	-5.629249	-2.290990	2.073160
56	1	0	-4.283735	-0.346237	1.365537
57	1	0	-1.368983	2.769620	-0.261188
58	1	0	-2.770864	4.585980	-1.141057
59	1	0	-4.985992	4.088526	-2.146517

60	1	0	-5.784299	1.740813	-2.264166
61	1	0	-4.398705	-0.091334	-1.366915
62	1	0	6.753362	-0.648495	0.109586
63	1	0	0.136971	-1.680429	-2.862798

Zero-point correction= 0.522908 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.457003
Sum of electronic and zero-point Energies= −3440.305606(a.u.)
SCF- Energy: B3LYP (PCM, toluene)/6-31+G(d, p) = −3446.9080697 (a.u.)

L_1-CuH-**COM**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.320213	3.151335	0.223724
2	8	0	0.900823	2.356201	1.062320
3	6	0	0.410018	4.232917	-0.320421
4	1	0	0.794059	5.229100	-0.069778
5	1	0	0.343157	4.157148	-1.410464
6	1	0	-0.581956	4.108484	0.115241
7	6	0	2.732183	3.062606	-0.266947
8	6	0	3.326284	4.086081	-1.022869
9	6	0	3.478805	1.909074	0.025313
10	6	0	4.647215	3.966114	-1.459593
11	1	0	2.764695	4.980802	-1.270896
12	6	0	4.785732	1.774949	-0.436127
13	1	0	3.010672	1.113483	0.590999
14	6	0	5.377523	2.810118	-1.168577
15	1	0	5.101811	4.768704	-2.033562
16	1	0	5.339708	0.864415	-0.229321
17	1	0	6.400502	2.711120	-1.521713
18	1	0	0.379766	1.214768	-2.330601
19	6	0	-0.170408	-2.581255	-0.660219
20	6	0	-1.474358	-2.755902	0.194674
21	6	0	-2.106396	-1.517318	0.912901
22	15	0	-2.216363	-0.005706	-0.204459
23	15	0	1.002453	-1.258924	0.024098
24	6	0	-3.427914	-1.957890	1.595342
25	6	0	0.430068	-3.976698	-0.979126
26	1	0	-0.465976	-2.133391	-1.615534
27	1	0	-1.268910	-3.488699	0.980804
28	1	0	-2.230384	-3.195466	-0.463836
29	1	0	-1.407183	-1.205437	1.692963
30	1	0	-3.222149	-2.762210	2.306871
31	1	0	-3.888151	-1.132383	2.140462
32	1	0	-4.138025	-2.332805	0.856781
33	1	0	-0.312890	-4.578430	-1.510909
34	1	0	1.316432	-3.891221	-1.607697
35	1	0	0.703774	-4.515987	-0.070887
36	6	0	1.182964	-1.606367	1.826845
37	6	0	2.654777	-1.688143	-0.670632
38	6	0	-2.982317	1.269991	0.871086
39	6	0	-3.510450	-0.433897	-1.437876
40	6	0	-2.531429	1.435703	2.195948
41	6	0	-3.006188	2.491527	2.978496
42	6	0	-3.923197	3.405392	2.449626
43	6	0	-4.363095	3.258727	1.130664
44	6	0	-3.897523	2.200944	0.343893
45	6	0	-4.868365	-0.623647	-1.114185
46	6	0	-5.782603	-0.995811	-2.102589
47	6	0	-5.356221	-1.182430	-3.422203
48	6	0	-4.015258	-0.979463	-3.756739
49	6	0	-3.096630	-0.599974	-2.772692
50	6	0	1.241522	-2.895383	2.392388
51	6	0	1.354268	-3.058884	3.776761
52	6	0	1.421524	-1.941283	4.614688

53	6	0	1.372713	-0.656925	4.065603
54	6	0	1.248325	-0.486472	2.682339
55	6	0	2.919839	-1.264059	-1.989301
56	6	0	4.161290	-1.521430	-2.577317
57	6	0	5.162017	-2.178655	-1.851851
58	6	0	4.916159	-2.577092	-0.533883
59	6	0	3.668857	-2.337633	0.055759
60	1	0	-1.798137	0.759693	2.613204
61	1	0	-4.286856	4.222674	3.056039
62	1	0	-5.067788	3.964360	0.712771
63	1	0	-4.241340	2.101172	-0.676308
64	1	0	-5.211887	-0.461516	-0.102919
65	1	0	-6.823535	-1.135740	-1.845379
66	1	0	-6.067207	-1.470692	-4.183773
67	1	0	-3.685707	-1.101540	-4.779137
68	1	0	-2.064092	-0.401511	-3.033285
69	1	0	1.204779	-3.769839	1.760389
70	1	0	1.394269	-4.054329	4.197662
71	1	0	1.511601	-2.072321	5.683943
72	1	0	1.427053	0.211793	4.707371
73	1	0	1.195733	0.509740	2.262104
74	1	0	2.168010	-0.697468	-2.525975
75	1	0	4.351495	-1.192097	-3.589569
76	1	0	6.124068	-2.371928	-2.305847
77	1	0	5.689497	-3.075630	0.034775
78	1	0	3.493953	-2.641080	1.078242
79	1	0	-2.653494	2.602828	3.994444
80	29	0	-0.141275	0.512002	-1.039938

Zero-point correction= 0.661315 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.580612
Sum of electronic and zero-point Energies= −3825.099212(a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −3831.8326911(a.u.)

L1-CuH-**TS1**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.727116	2.656170	-1.196780
2	8	0	0.277974	2.653399	0.006981
3	6	0	-0.000475	3.541220	-2.204250
4	1	0	0.269689	4.583481	-1.980999
5	1	0	0.272589	3.325274	-3.238832
6	1	0	-1.078828	3.426391	-2.082414
7	6	0	2.225800	2.503583	-1.389664
8	6	0	2.805345	2.220328	-2.636150
9	6	0	3.067012	2.701712	-0.285766
10	6	0	4.189947	2.136237	-2.775146
11	1	0	2.164843	2.023869	-3.490933
12	6	0	4.456219	2.624381	-0.424342
13	1	0	2.617588	2.925444	0.675326
14	6	0	5.023307	2.338181	-1.667825
15	1	0	4.621259	1.899051	-3.744144
16	1	0	5.093062	2.783304	0.442293
17	1	0	6.102314	2.267270	-1.776214
18	1	0	0.253606	1.121190	-2.143592
19	6	0	-0.031365	-2.380483	0.744664
20	6	0	-1.184582	-2.087639	1.765722
21	6	0	-1.939339	-0.715314	1.737725
22	15	0	-2.213458	-0.042111	-0.002550
23	15	0	1.126098	-0.909460	0.499974
24	6	0	-3.169003	-0.789128	2.683725
25	6	0	0.630722	-3.729810	1.133489
26	1	0	-0.488080	-2.501789	-0.242525
27	1	0	-0.775510	-2.194161	2.775162
28	1	0	-1.920891	-2.885710	1.630483

29	1	0	-1.262225	0.037114	2.153312
30	1	0	-2.830737	-1.020168	3.697567
31	1	0	-3.704673	0.159699	2.709379
32	1	0	-3.866443	-1.572059	2.382497
33	1	0	-0.116428	-4.527285	1.087349
34	1	0	1.446410	-3.985491	0.457165
35	1	0	1.015645	-3.695100	2.153599
36	6	0	1.707392	-0.463783	2.185792
37	6	0	2.582202	-1.633307	-0.353656
38	6	0	-3.508576	1.240320	0.212919
39	6	0	-2.995777	-1.376191	-0.994819
40	6	0	-3.066723	2.528327	0.581133
41	6	0	-3.994781	3.553002	0.788931
42	6	0	-5.360609	3.314002	0.606966
43	6	0	-5.800195	2.046972	0.211900
44	6	0	-4.881314	1.010359	0.017741
45	6	0	-3.925993	-2.310505	-0.500461
46	6	0	-4.440869	-3.307047	-1.335610
47	6	0	-4.043486	-3.378997	-2.673987
48	6	0	-3.125890	-2.453130	-3.178454
49	6	0	-2.600195	-1.461804	-2.345316
50	6	0	2.380004	-1.347473	3.052298
51	6	0	2.741138	-0.935574	4.338187
52	6	0	2.439144	0.359496	4.773351
53	6	0	1.783198	1.248304	3.917398
54	6	0	1.420430	0.843179	2.627684
55	6	0	2.366763	-2.270998	-1.593323
56	6	0	3.442977	-2.765216	-2.331597
57	6	0	4.750907	-2.614532	-1.856545
58	6	0	4.974950	-1.962699	-0.641783
59	6	0	3.899307	-1.472441	0.108503
60	1	0	-2.004671	2.729810	0.661152
61	1	0	-6.075148	4.110985	0.757833
62	1	0	-6.854085	1.864853	0.052588
63	1	0	-5.229401	0.036727	-0.298376
64	1	0	-4.252190	-2.264563	0.527239
65	1	0	-5.152084	-4.020773	-0.943065
66	1	0	-4.445329	-4.149841	-3.316417
67	1	0	-2.815709	-2.504092	-4.212918
68	1	0	-1.871509	-0.755844	-2.724527
69	1	0	2.637198	-2.342714	2.720091
70	1	0	3.257724	-1.620882	4.996023
71	1	0	2.720206	0.673195	5.768955
72	1	0	1.558002	2.253727	4.245683
73	1	0	0.936177	1.535826	1.949301
74	1	0	1.363142	-2.361181	-1.989099
75	1	0	3.263055	-3.255459	-3.278400
76	1	0	5.583789	-2.993560	-2.431629
77	1	0	5.983720	-1.829948	-0.275672
78	1	0	4.087079	-0.958177	1.040061
79	1	0	-3.648298	4.536883	1.073497
80	29	0	-0.139190	0.611479	-0.686894

Zero-point correction= 0.661272 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.584742
Sum of electronic and zero-point Energies= −3825.088855 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −3825.8225533(a.u.)

L_1-CuH-**IM1**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.145953	3.121125	-1.646534
2	8	0	0.106596	2.575126	-0.900038
3	6	0	1.024604	4.661147	-1.630624
4	1	0	1.114730	5.029405	-0.602020

5	1	0	1.797160	5.141898	-2.243370
6	1	0	0.039281	4.947607	-2.014331
7	6	0	2.548464	2.709625	-1.181091
8	6	0	3.602530	2.583314	-2.097576
9	6	0	2.819134	2.478134	0.174370
10	6	0	4.891878	2.243947	-1.675492
11	1	0	3.408341	2.745530	-3.156396
12	6	0	4.100374	2.119938	0.603489
13	1	0	2.003230	2.569703	0.884280
14	6	0	5.146698	2.011726	-0.319633
15	1	0	5.694235	2.154998	-2.404295
16	1	0	4.284268	1.926987	1.657115
17	1	0	6.145663	1.741146	0.013005
18	1	0	1.074925	2.807913	-2.708648
19	6	0	-0.248956	-2.348580	0.881342
20	6	0	-1.211379	-1.866635	2.019560
21	6	0	-1.927656	-0.471658	1.920130
22	15	0	-2.280490	0.093733	0.154286
23	15	0	0.992291	-1.035198	0.364848
24	6	0	-3.092793	-0.416057	2.946230
25	6	0	0.381022	-3.699890	1.315768
26	1	0	-0.857686	-2.510482	-0.013208
27	1	0	-0.655563	-1.869856	2.962434
28	1	0	-1.981646	-2.638325	2.106613
29	1	0	-1.201272	0.285961	2.233777
30	1	0	-2.704672	-0.625909	3.946836
31	1	0	-3.558417	0.568909	2.957108
32	1	0	-3.864682	-1.155437	2.727563
33	1	0	-0.409869	-4.424146	1.529946
34	1	0	1.021204	-4.115113	0.537017
35	1	0	0.977580	-3.569130	2.220304
36	6	0	2.125894	-0.933955	1.809103
37	6	0	1.973181	-1.836531	-0.963814
38	6	0	-3.497380	1.455553	0.317872
39	6	0	-3.199966	-1.252320	-0.696500
40	6	0	-2.997935	2.768203	0.195269
41	6	0	-3.866759	3.856398	0.334441
42	6	0	-5.227327	3.647438	0.573076
43	6	0	-5.730835	2.344745	0.666475
44	6	0	-4.871761	1.250818	0.540293
45	6	0	-3.952761	-2.256573	-0.059419
46	6	0	-4.586806	-3.251870	-0.810800
47	6	0	-4.488555	-3.252937	-2.204644
48	6	0	-3.747952	-2.257459	-2.850119
49	6	0	-3.102279	-1.269820	-2.103756
50	6	0	3.197377	-1.822398	2.011144
51	6	0	4.009628	-1.701575	3.142513
52	6	0	3.755249	-0.704925	4.090894
53	6	0	2.689571	0.180839	3.901641
54	6	0	1.885652	0.073587	2.762181
55	6	0	1.402734	-2.788324	-1.830725
56	6	0	2.123408	-3.265776	-2.930438
57	6	0	3.414976	-2.798418	-3.184257
58	6	0	3.982988	-1.839765	-2.338585
59	6	0	3.268902	-1.353740	-1.241410
60	1	0	-1.951352	2.931024	-0.045076
61	1	0	-5.895986	4.491279	0.671645
62	1	0	-6.786935	2.182570	0.832816
63	1	0	-5.268936	0.246389	0.597532
64	1	0	-4.046397	-2.269942	1.015449
65	1	0	-5.158661	-4.019704	-0.307956
66	1	0	-4.981785	-4.022176	-2.781763
67	1	0	-3.666788	-2.254460	-3.928158
68	1	0	-2.514286	-0.511553	-2.605258
69	1	0	3.406069	-2.589832	1.279339
70	1	0	4.836101	-2.384160	3.283773
71	1	0	4.383752	-0.617004	4.965896
72	1	0	2.493467	0.958582	4.626818
73	1	0	1.086876	0.785551	2.600105

74	1	0	0.399140	-3.154420	-1.664162
75	1	0	1.673235	-3.999648	-3.584643
76	1	0	3.969090	-3.169368	-4.034726
77	1	0	4.975124	-1.458429	-2.536259
78	1	0	3.710789	-0.589639	-0.616370
79	1	0	-3.479589	4.861315	0.239227
80	29	0	-0.119801	0.772032	-0.409342

Zero-point correction= 0.666732 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.588774
Sum of electronic and zero-point Energies= −3825.122575 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −3825.8636098(a.u.)

L_1-CuH-**TS2**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542227	-2.598322	0.957119
2	6	0	-1.369738	-1.874396	2.079732
3	6	0	-1.794159	-0.372654	1.948766
4	15	0	-2.262390	0.136416	0.191997
5	15	0	0.791510	-1.588258	0.079968
6	6	0	-2.795854	-0.024899	3.084292
7	6	0	-0.064035	-3.961083	1.528611
8	1	0	-1.231364	-2.796954	0.129403
9	1	0	-0.824449	-1.966111	3.023820
10	1	0	-2.277428	-2.472605	2.197553
11	1	0	-2.346354	-0.263880	4.052301
12	1	0	-3.046603	1.035433	3.074873
13	1	0	-3.722182	-0.595030	2.998333
14	1	0	-0.906654	-4.480540	1.992969
15	1	0	0.331701	-4.601523	0.742020
16	1	0	0.706596	-3.815078	2.288647
17	6	0	2.216829	-1.435336	1.231839
18	6	0	1.368043	-2.762665	-1.216315
19	6	0	-3.300802	1.643789	0.368900
20	6	0	-3.417029	-1.133437	-0.464754
21	6	0	-4.655908	1.618566	0.745571
22	6	0	-5.377940	2.809996	0.851069
23	6	0	-4.759452	4.035353	0.578863
24	6	0	-3.419263	4.068718	0.185509
25	6	0	-2.692280	2.878875	0.074061
26	6	0	-4.313111	-1.896532	0.307978
27	6	0	-5.142132	-2.844847	-0.299959
28	6	0	-5.097575	-3.035755	-1.683829
29	6	0	-4.218075	-2.278194	-2.462802
30	6	0	-3.379342	-1.338522	-1.859140
31	6	0	3.539022	-1.531251	0.751571
32	6	0	4.622267	-1.277089	1.598187
33	6	0	4.410627	-0.901171	2.928326
34	6	0	3.103474	-0.780711	3.409720
35	6	0	2.015884	-1.042854	2.571074
36	6	0	0.967017	-2.507201	-2.540478
37	6	0	1.330216	-3.377754	-3.573203
38	6	0	2.108513	-4.503900	-3.297879
39	6	0	2.529045	-4.757894	-1.987760
40	6	0	2.162379	-3.896118	-0.951271
41	1	0	-5.149719	0.675786	0.935547
42	1	0	-5.323592	4.953902	0.658329
43	1	0	-2.942552	5.009886	-0.050648
44	1	0	-1.663451	2.900462	-0.259529
45	1	0	-4.369311	-1.759225	1.377397
46	1	0	-5.822602	-3.428058	0.305080
47	1	0	-5.741340	-3.768107	-2.149911
48	1	0	-4.179597	-2.421354	-3.533585
49	1	0	-2.687899	-0.763754	-2.461969

50	1	0	3.721380	-1.797255	-0.279861
51	1	0	5.629971	-1.366721	1.215644
52	1	0	5.251139	-0.700161	3.577234
53	1	0	2.927841	-0.481362	4.433860
54	1	0	1.016079	-0.927762	2.963221
55	1	0	0.393361	-1.615810	-2.759128
56	1	0	1.018592	-3.165319	-4.586150
57	1	0	2.396475	-5.172703	-4.096681
58	1	0	3.142943	-5.621919	-1.774055
59	1	0	2.510971	-4.092203	0.052441
60	1	0	-6.420286	2.781887	1.137060
61	1	0	-0.901831	0.240516	2.114774
62	1	0	0.011489	0.850189	-2.379034
63	14	0	0.577191	2.377529	-2.579425
64	6	0	3.666164	2.105020	0.271670
65	6	0	5.052892	2.179246	0.133453
66	6	0	5.664372	3.371148	-0.271147
67	6	0	4.873236	4.487272	-0.551218
68	6	0	2.862585	3.217639	-0.019396
69	6	0	3.482415	4.405243	-0.426508
70	6	0	1.344708	3.149976	0.115786
71	6	0	0.917652	2.867719	1.561575
72	1	0	3.209124	1.170916	0.577706
73	1	0	5.659681	1.304635	0.351010
74	1	0	6.744946	3.425061	-0.373979
75	1	0	5.333990	5.417020	-0.874708
76	1	0	2.868180	5.269841	-0.667059
77	1	0	0.946500	4.133143	-0.181751
78	1	0	-0.173112	2.882941	1.651685
79	1	0	1.329331	3.626598	2.236384
80	1	0	1.287459	1.890584	1.889646
81	8	0	0.787102	2.163927	-0.746833
82	29	0	-0.185436	0.293414	-0.767930
83	1	0	0.384373	3.863814	-2.317982
84	1	0	-0.263000	2.378123	-3.854795
85	1	0	1.955751	2.151952	-3.097520

Zero-point correction= 0.701972 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.622295
Sum of electronic and zero-point Energies= −4116.973020 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4123.7482788(a.u.)

S-Product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.527116	-1.292094	0.214245
2	6	0	1.035063	2.355621	-0.337155
3	6	0	0.930955	0.952448	0.264307
4	6	0	-0.465860	0.364445	0.126586
5	1	0	1.173669	1.011979	1.336503
6	8	0	1.914243	0.138723	-0.393461
7	6	0	-0.926351	-0.105048	-1.112635
8	6	0	-1.326492	0.315404	1.230225
9	6	0	-2.221344	-0.609913	-1.242740
10	6	0	-2.626714	-0.184290	1.101751
11	6	0	-3.077195	-0.648740	-0.136123
12	1	0	-0.260702	-0.083875	-1.970760
13	1	0	-2.563869	-0.974481	-2.207364
14	1	0	-4.084703	-1.041925	-0.238477
15	1	0	-3.281382	-0.217042	1.968278
16	1	0	-0.978390	0.667773	2.198953
17	1	0	0.818804	2.323869	-1.409604
18	1	0	2.046231	2.749795	-0.196869
19	1	0	0.319377	3.031987	0.141082

20	1	0	2.941152	-1.106006	1.633820
21	1	0	3.699729	-1.615884	-0.629993
22	1	0	1.544149	-2.406222	0.157389

Zero-point correction= 0.176479 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.138756
Sum of electronic and zero-point Energies= −676.667377 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −676.8536145 (a.u.)

L_1-CuH-**COM** -*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.720101	-2.584680	-1.164825
2	8	0	1.287652	-1.646059	-0.489957
3	6	0	0.811344	-3.250796	-2.168988
4	1	0	0.238570	-2.451353	-2.657197
5	1	0	1.334914	-3.850149	-2.915275
6	1	0	0.094492	-3.889683	-1.638480
7	6	0	3.134605	-3.022275	-0.971178
8	6	0	3.632598	-4.226398	-1.497194
9	6	0	3.991464	-2.190600	-0.226415
10	6	0	4.956251	-4.605662	-1.265077
11	1	0	2.987269	-4.881002	-2.073547
12	6	0	5.313850	-2.567563	-0.006341
13	1	0	3.602544	-1.262501	0.174367
14	6	0	5.799996	-3.774866	-0.522307
15	1	0	5.328423	-5.543933	-1.666478
16	1	0	5.968676	-1.916090	0.564817
17	1	0	6.832118	-4.066132	-0.347064
18	1	0	-0.318556	-0.172271	-2.806766
19	6	0	-2.732688	1.404574	0.060496
20	6	0	-2.013439	2.267530	1.153772
21	6	0	-0.520532	1.984850	1.532154
22	15	0	0.579973	1.698997	0.029275
23	15	0	-2.166408	-0.402097	0.016841
24	6	0	-0.057731	3.084376	2.525349
25	6	0	-4.260554	1.670964	0.124702
26	1	0	-2.383392	1.756928	-0.915474
27	1	0	-2.581145	2.177563	2.084824
28	1	0	-2.090301	3.310779	0.831382
29	1	0	-0.495075	1.021848	2.048847
30	1	0	-0.700445	3.072228	3.410055
31	1	0	0.971028	2.925745	2.851198
32	1	0	-0.133835	4.071533	2.067276
33	1	0	-4.448423	2.740495	-0.006540
34	1	0	-4.788769	1.130285	-0.660240
35	1	0	-4.682066	1.376665	1.087369
36	6	0	-2.218887	-1.008601	1.758046
37	6	0	-3.554880	-1.285142	-0.810057
38	6	0	2.253562	1.489174	0.766472
39	6	0	0.651419	3.335586	-0.808433
40	6	0	2.432149	0.726443	1.938948
41	6	0	3.714894	0.468699	2.432903
42	6	0	4.841442	0.953357	1.757700
43	6	0	4.677313	1.686186	0.576848
44	6	0	3.395902	1.951622	0.083289
45	6	0	1.247118	4.482873	-0.248390
46	6	0	1.216635	5.698537	-0.935953
47	6	0	0.595282	5.784692	-2.187070
48	6	0	0.018706	4.648173	-2.758961
49	6	0	0.051227	3.426487	-2.078439
50	6	0	-3.195066	-0.660601	2.711424
51	6	0	-3.117034	-1.151226	4.018985
52	6	0	-2.072504	-2.003449	4.390359
53	6	0	-1.099716	-2.361824	3.452450

54	6	0	-1.167271	-1.863473	2.147921
55	6	0	-3.582077	-1.233656	-2.219328
56	6	0	-4.601029	-1.875552	-2.927202
57	6	0	-5.587620	-2.595329	-2.245064
58	6	0	-5.550514	-2.673943	-0.850149
59	6	0	-4.542647	-2.020686	-0.132421
60	1	0	1.577018	0.323113	2.463266
61	1	0	5.832456	0.765853	2.148170
62	1	0	5.542426	2.057010	0.044133
63	1	0	3.281686	2.519103	-0.829800
64	1	0	1.749261	4.421155	0.706226
65	1	0	1.678750	6.573683	-0.500029
66	1	0	0.574407	6.727739	-2.715277
67	1	0	-0.442369	4.705591	-3.735212
68	1	0	-0.355527	2.530038	-2.532113
69	1	0	-4.013915	-0.012267	2.438224
70	1	0	-3.870745	-0.872550	4.742772
71	1	0	-2.017717	-2.382632	5.401156
72	1	0	-0.289486	-3.019972	3.734776
73	1	0	-0.399239	-2.115404	1.427725
74	1	0	-2.785060	-0.719946	-2.744295
75	1	0	-4.613552	-1.827335	-4.007438
76	1	0	-6.369562	-3.099790	-2.795285
77	1	0	-6.301932	-3.242700	-0.319629
78	1	0	-4.519996	-2.095043	0.945632
79	1	0	3.832404	-0.107931	3.340640
80	29	0	-0.235174	-0.055535	-1.236792

Zero-point correction= 0.661960 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.581709
Sum of electronic and zero-point Energies= −3825.098695 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −3831.8340689(a.u.)

L_1-CuH-**TS1**-*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660725	2.864037	0.287679
2	8	0	-0.483593	2.093249	1.302192
3	6	0	0.408920	3.924147	0.035634
4	1	0	1.389847	3.493462	0.242071
5	1	0	0.403354	4.311398	-0.984991
6	1	0	0.239731	4.755582	0.734595
7	6	0	-2.091048	3.206536	-0.084804
8	6	0	-2.416949	4.315004	-0.880722
9	6	0	-3.131867	2.417234	0.428355
10	6	0	-3.750533	4.631390	-1.154993
11	1	0	-1.633568	4.940343	-1.295359
12	6	0	-4.462740	2.732900	0.155206
13	1	0	-2.882888	1.570395	1.054625
14	6	0	-4.780258	3.841251	-0.637717
15	1	0	-3.982551	5.497249	-1.769831
16	1	0	-5.254241	2.111213	0.564641
17	1	0	-5.817818	4.087344	-0.847862
18	1	0	-0.343940	1.994200	-1.250322
19	6	0	2.040700	-1.749646	-0.929135
20	6	0	1.280339	-2.817339	-0.071125
21	6	0	0.047619	-2.401891	0.800294
22	15	0	-1.124691	-1.214272	-0.078053
23	15	0	2.162089	-0.060036	-0.095529
24	6	0	-0.583891	-3.688544	1.397818
25	6	0	3.357965	-2.373085	-1.464628
26	1	0	1.413568	-1.524448	-1.797698
27	1	0	1.997644	-3.274797	0.616971
28	1	0	0.956487	-3.599844	-0.764751
29	1	0	0.419856	-1.795410	1.630867

30	1	0	0.149511	-4.188957	2.035995
31	1	0	-1.461633	-3.459554	2.002835
32	1	0	-0.868698	-4.387026	0.609544
33	1	0	3.123408	-3.260089	-2.059831
34	1	0	3.901503	-1.669802	-2.095496
35	1	0	4.014767	-2.685376	-0.651364
36	6	0	2.757189	-0.338586	1.619744
37	6	0	3.553110	0.770357	-0.964709
38	6	0	-2.572450	-1.147039	1.050207
39	6	0	-1.692523	-2.095466	-1.584975
40	6	0	-2.355797	-0.670942	2.361358
41	6	0	-3.428975	-0.497353	3.237667
42	6	0	-4.734850	-0.774066	2.814906
43	6	0	-4.959720	-1.224881	1.510921
44	6	0	-3.886995	-1.410866	0.630073
45	6	0	-2.328462	-3.352653	-1.576258
46	6	0	-2.688088	-3.969338	-2.777341
47	6	0	-2.424134	-3.340352	-3.998956
48	6	0	-1.808627	-2.086520	-4.018791
49	6	0	-1.446601	-1.465046	-2.819649
50	6	0	3.737204	-1.278100	1.994346
51	6	0	4.089405	-1.434326	3.338560
52	6	0	3.477461	-0.650682	4.322035
53	6	0	2.508998	0.290191	3.960968
54	6	0	2.143368	0.445549	2.619903
55	6	0	3.262056	1.367219	-2.208140
56	6	0	4.265800	2.012742	-2.933984
57	6	0	5.563508	2.093669	-2.418216
58	6	0	5.852817	1.530074	-1.172604
59	6	0	4.855988	0.868183	-0.447383
60	1	0	-1.359158	-0.400010	2.682552
61	1	0	-5.566133	-0.634476	3.491649
62	1	0	-5.966970	-1.431365	1.175832
63	1	0	-4.076785	-1.746394	-0.379385
64	1	0	-2.559040	-3.837343	-0.639356
65	1	0	-3.176410	-4.933908	-2.759870
66	1	0	-2.705028	-3.821261	-4.925384
67	1	0	-1.616856	-1.590199	-4.959860
68	1	0	-0.984944	-0.485188	-2.825998
69	1	0	4.227358	-1.884469	1.247256
70	1	0	4.840266	-2.161616	3.615456
71	1	0	3.754535	-0.773729	5.359673
72	1	0	2.034336	0.899974	4.717227
73	1	0	1.375990	1.159950	2.341826
74	1	0	2.246252	1.349288	-2.582951
75	1	0	4.031103	2.466001	-3.887067
76	1	0	6.337065	2.603467	-2.974932
77	1	0	6.850306	1.606807	-0.762383
78	1	0	5.088547	0.445999	0.520010
79	1	0	-3.247724	-0.130831	4.238615
80	29	0	0.035637	0.741016	-0.310711

Zero-point correction= 0.661668 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.585188
Sum of electronic and zero-point Energies= −3825.088431 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −3831.8215511(a.u.)

L_1-CuH-**IM1**-*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.340326	2.699501	-1.783943
2	8	0	-0.093962	2.070002	-1.727844
3	6	0	-1.271759	3.911175	-2.732854
4	1	0	-0.954378	3.574634	-3.726109
5	1	0	-2.242006	4.415821	-2.822707

6	1	0	-0.534284	4.634326	-2.366275
7	6	0	-1.830206	3.113736	-0.391038
8	6	0	-3.121478	2.801338	0.052315
9	6	0	-0.968394	3.789100	0.490108
10	6	0	-3.547233	3.145408	1.339923
11	1	0	-3.794732	2.263481	-0.611681
12	6	0	-1.392778	4.150533	1.770436
13	1	0	0.041783	4.016065	0.160335
14	6	0	-2.685479	3.827050	2.202273
15	1	0	-4.544713	2.870290	1.671616
16	1	0	-0.715027	4.680849	2.435696
17	1	0	-3.012467	4.097161	3.203170
18	1	0	-2.118534	2.016449	-2.188578
19	6	0	-0.242058	-2.412511	0.786721
20	6	0	0.967660	-2.886611	-0.091058
21	6	0	1.860772	-1.842810	-0.849498
22	15	0	2.112177	-0.215060	0.078180
23	15	0	-1.278212	-1.075525	-0.044749
24	6	0	3.126896	-2.552955	-1.401685
25	6	0	-1.008001	-3.667187	1.285968
26	1	0	0.170225	-1.896365	1.659401
27	1	0	0.583909	-3.573867	-0.851468
28	1	0	1.610800	-3.472408	0.571998
29	1	0	1.285954	-1.502328	-1.717330
30	1	0	2.824246	-3.390298	-2.036465
31	1	0	3.730115	-1.870153	-1.999446
32	1	0	3.752676	-2.950636	-0.601492
33	1	0	-0.346449	-4.276669	1.907817
34	1	0	-1.878699	-3.392472	1.882270
35	1	0	-1.334364	-4.281997	0.446088
36	6	0	-1.873850	-1.794542	-1.627104
37	6	0	-2.760790	-0.918346	1.026015
38	6	0	3.537091	0.584752	-0.755281
39	6	0	2.699549	-0.611404	1.773459
40	6	0	3.225755	1.523667	-1.760664
41	6	0	4.257063	2.155498	-2.463601
42	6	0	5.592210	1.877737	-2.157990
43	6	0	5.903769	0.967707	-1.141855
44	6	0	4.882192	0.319993	-0.442072
45	6	0	3.429870	-1.760276	2.130716
46	6	0	3.804481	-1.977370	3.460751
47	6	0	3.466230	-1.048612	4.448680
48	6	0	2.746916	0.100418	4.105821
49	6	0	2.360016	0.315215	2.781131
50	6	0	-2.634277	-2.976644	-1.719955
51	6	0	-3.018854	-3.470287	-2.969272
52	6	0	-2.654387	-2.790932	-4.137222
53	6	0	-1.913622	-1.609335	-4.055708
54	6	0	-1.525545	-1.108069	-2.808286
55	6	0	-2.578762	-0.637776	2.395758
56	6	0	-3.679110	-0.394052	3.219994
57	6	0	-4.974642	-0.411567	2.690700
58	6	0	-5.162585	-0.670438	1.330327
59	6	0	-4.065062	-0.921121	0.499355
60	1	0	2.190108	1.777158	-1.965876
61	1	0	6.386122	2.375928	-2.696825
62	1	0	6.936664	0.765749	-0.893612
63	1	0	5.129572	-0.372659	0.351027
64	1	0	3.708794	-2.484578	1.381130
65	1	0	4.362245	-2.866204	3.721921
66	1	0	3.759178	-1.218759	5.474982
67	1	0	2.482246	0.822269	4.865854
68	1	0	1.788743	1.197471	2.521204
69	1	0	-2.941215	-3.494882	-0.823404
70	1	0	-3.603705	-4.377623	-3.031134
71	1	0	-2.954979	-3.176809	-5.101233
72	1	0	-1.642578	-1.073086	-4.954425
73	1	0	-0.967728	-0.179373	-2.743572
74	1	0	-1.582082	-0.593166	2.816158

75	1	0	-3.525158	-0.183693	4.269334
76	1	0	-5.824813	-0.223539	3.331269
77	1	0	-6.160230	-0.679463	0.913082
78	1	0	-4.222226	-1.112246	-0.552758
79	1	0	4.013344	2.873741	-3.233981
80	29	0	0.093732	0.694508	-0.425962

Zero-point correction= 0.666824 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.587719
Sum of electronic and zero-point Energies= −3825.123708 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −3831.8638037(a.u.)

L_1-CuH-**TS2**-*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.295714	-2.199326	-1.996385
2	6	0	0.191798	-2.671075	-1.897756
3	6	0	1.300425	-1.573568	-2.079215
4	15	0	1.801077	-0.902229	-0.388461
5	15	0	-1.798880	-1.019835	-0.591500
6	6	0	2.476923	-2.143539	-2.917100
7	6	0	-1.626770	-1.675798	-3.419959
8	1	0	-1.898987	-3.095038	-1.821942
9	1	0	0.329388	-3.410881	-2.692932
10	1	0	0.347627	-3.206207	-0.957015
11	1	0	0.866611	-0.725348	-2.616723
12	1	0	2.117810	-2.413374	-3.913496
13	1	0	3.285315	-1.420096	-3.028932
14	1	0	2.881388	-3.038620	-2.443153
15	1	0	-1.347613	-2.429572	-4.160734
16	1	0	-2.691076	-1.461914	-3.526647
17	1	0	-1.095470	-0.750873	-3.646706
18	6	0	-2.360665	0.519558	-1.436152
19	6	0	-3.350156	-1.771489	0.047691
20	6	0	3.005652	0.438872	-0.754906
21	6	0	2.855445	-2.238946	0.310230
22	6	0	3.841118	0.880376	0.294345
23	6	0	4.717898	1.949621	0.101739
24	6	0	4.771321	2.603215	-1.136242
25	6	0	3.934862	2.186880	-2.175720
26	6	0	3.052331	1.115729	-1.987715
27	6	0	4.188519	-2.446555	-0.094256
28	6	0	4.934623	-3.494827	0.449115
29	6	0	4.361608	-4.350484	1.396413
30	6	0	3.044123	-4.146630	1.811973
31	6	0	2.295063	-3.092076	1.279342
32	6	0	-1.380517	1.486950	-1.735684
33	6	0	-1.735037	2.694309	-2.342694
34	6	0	-3.074838	2.957842	-2.646019
35	6	0	-4.056598	2.012191	-2.335935
36	6	0	-3.705343	0.798976	-1.733773
37	6	0	-4.295114	-2.420802	-0.770116
38	6	0	-5.460034	-2.956479	-0.214022
39	6	0	-5.696547	-2.849214	1.160369
40	6	0	-4.762846	-2.211706	1.981188
41	6	0	-3.593127	-1.679204	1.430067
42	1	0	3.802424	0.386055	1.256379
43	1	0	5.455975	3.426208	-1.287162
44	1	0	3.968897	2.689320	-3.132859
45	1	0	2.415376	0.813951	-2.806997
46	1	0	4.644736	-1.781916	-0.813900
47	1	0	5.959355	-3.640981	0.136829
48	1	0	4.943479	-5.158825	1.816266

49	1	0	2.603450	-4.789502	2.560825
50	1	0	1.291673	-2.908730	1.640188
51	1	0	-0.348755	1.318963	-1.456177
52	1	0	-0.972696	3.433220	-2.546012
53	1	0	-3.351766	3.897122	-3.103226
54	1	0	-5.095423	2.219046	-2.552787
55	1	0	-4.477180	0.087507	-1.476848
56	1	0	-4.130011	-2.510445	-1.835461
57	1	0	-6.178725	-3.454548	-0.850043
58	1	0	-6.598184	-3.265411	1.587028
59	1	0	-4.935323	-2.135613	3.045541
60	1	0	-2.860943	-1.201453	2.066654
61	1	0	5.352997	2.273173	0.914694
62	1	0	-0.023071	-1.167730	2.451585
63	14	0	0.079618	-0.095531	3.673656
64	6	0	-2.516437	2.183922	2.084354
65	6	0	-1.017915	2.292677	2.414923
66	6	0	-0.312942	3.360849	1.579921
67	1	0	-0.929562	2.592113	3.471941
68	8	0	-0.400683	1.025129	2.274489
69	29	0	-0.105971	-0.528778	0.843889
70	6	0	-0.808500	4.675215	1.538157
71	6	0	0.858628	3.074360	0.870986
72	6	0	-0.161296	5.665753	0.796849
73	6	0	1.507631	4.059381	0.118612
74	6	0	1.001131	5.360025	0.080431
75	1	0	-1.704124	4.934761	2.096525
76	1	0	-0.560848	6.676736	0.784388
77	1	0	1.506860	6.131512	-0.494826
78	1	0	2.414686	3.808675	-0.420298
79	1	0	1.263722	2.072234	0.920277
80	1	0	-2.660905	1.878640	1.044461
81	1	0	-2.979167	1.439055	2.739600
82	1	0	-3.036911	3.135356	2.236024
83	1	0	1.537112	0.206232	3.798514
84	1	0	-0.045452	-1.327260	4.574143
85	1	0	-0.707904	0.806478	4.604215

Zero-point correction= 0.701659 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.621961
Sum of electronic and zero-point Energies= −4116.979511 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4123.7506827 (a.u.)

R-Product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.525489	-1.293436	0.212596
2	6	0	-1.035710	2.356220	-0.334780
3	6	0	-0.931331	0.952566	0.265489
4	6	0	0.465496	0.364767	0.127028
5	1	0	-1.173818	1.011200	1.337785
6	8	0	-1.914750	0.139324	-0.392692
7	6	0	0.926341	-0.102299	-1.112989
8	6	0	1.325740	0.313335	1.230856
9	6	0	2.221270	-0.607164	-1.243662
10	6	0	2.625918	-0.186344	1.101824
11	6	0	3.076725	-0.648400	-0.136820
12	1	0	0.261023	-0.079243	-1.971328
13	1	0	2.564064	-0.969850	-2.208899
14	1	0	4.084192	-1.041577	-0.239619
15	1	0	3.280290	-0.220944	1.968503
16	1	0	0.977371	0.663842	2.200162
17	1	0	-0.818426	2.325705	-1.407056
18	1	0	-2.047256	2.749610	-0.195040
19	1	0	-0.320904	3.032559	0.144812

20	1	0	-1.541639	-2.406565	0.151834
21	1	0	-3.698969	-1.616311	-0.630789
22	1	0	-2.937784	-1.110993	1.633152

Zero-point correction= 0.176480 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.138760
Sum of electronic and zero-point Energies= −676.667377 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −676.853636 (a.u.)

S6. Cartesian coordinates and energies of all optimized catalyst and TS structures over L_x-CuH(x=2-3*) reaction system at the B3LYP/6-31+G(d, p):3-21G level.**

L_2-CuH system

L_2-CuH-**TS1**-*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.285827	1.961826	-1.205966
2	6	0	1.319676	-2.359893	-3.259936
3	6	0	2.635486	-2.023097	-2.850573
4	6	0	2.833960	-1.464417	-1.546142
5	6	0	1.701763	-1.234268	-0.685784
6	6	0	0.418175	-1.584139	-1.122531
7	6	0	0.249216	-2.150065	-2.424978
8	6	0	1.992765	-0.726875	0.706630
9	6	0	2.542424	-1.678474	1.637851
10	6	0	2.873441	-1.262296	2.967937
11	6	0	2.679660	0.095179	3.330297
12	6	0	2.178223	0.999159	2.425684
13	6	0	1.822919	0.606219	1.097793
14	6	0	3.756698	-2.250156	-3.696456
15	6	0	2.775112	-3.041191	1.284143
16	6	0	3.402219	-2.208159	3.889782
17	6	0	4.168721	-1.166665	-1.140112
18	15	0	-1.103152	-1.092164	-0.188441
19	15	0	0.935963	1.832637	0.027266
20	1	0	1.168885	-2.793075	-4.240023
21	1	0	-0.744060	-2.415737	-2.754007
22	1	0	2.939212	0.414483	4.331049
23	1	0	2.040361	2.027834	2.721911
24	29	0	-1.217382	1.184225	-0.295647
25	6	0	1.120867	3.424989	0.936111
26	6	0	2.143095	4.353933	0.676897
27	6	0	0.148176	3.722727	1.913495
28	6	0	2.202373	5.552165	1.396706
29	1	0	2.877257	4.152721	-0.089900
30	6	0	0.223425	4.917111	2.636488
31	1	0	-0.677057	3.039710	2.076286
32	6	0	1.249764	5.832210	2.380484
33	1	0	2.988697	6.263682	1.185590
34	1	0	-0.525859	5.134710	3.385185
35	1	0	1.300596	6.759104	2.934465
36	6	0	1.976858	2.056798	-1.461157
37	6	0	1.323660	2.308064	-2.680666
38	6	0	3.381410	2.034223	-1.420377
39	6	0	2.068378	2.547444	-3.838908
40	1	0	0.241481	2.307326	-2.711406
41	6	0	4.120122	2.272509	-2.581722
42	1	0	3.888919	1.816814	-0.490728
43	6	0	3.465044	2.532627	-3.789510
44	1	0	1.560133	2.738978	-4.773662
45	1	0	5.200109	2.244602	-2.546365
46	1	0	4.040017	2.713903	-4.686763
47	6	0	-2.469015	-1.997950	-1.033764
48	6	0	-2.917730	-3.271411	-0.644529
49	6	0	-3.112346	-1.338849	-2.099948
50	6	0	-3.974009	-3.884577	-1.326494
51	1	0	-2.462897	-3.771971	0.197817
52	6	0	-4.157955	-1.962328	-2.786148
53	1	0	-2.807830	-0.334014	-2.364233
54	6	0	-4.588635	-3.236744	-2.402630
55	1	0	-4.315261	-4.862436	-1.015717

56	1	0	-4.644451	-1.447433	-3.602784
57	1	0	-5.402833	-3.714684	-2.929420
58	6	0	-1.005564	-1.877930	1.462227
59	6	0	-1.508468	-1.137899	2.549034
60	6	0	-0.500419	-3.171417	1.677445
61	6	0	-1.524940	-1.700397	3.829529
62	1	0	-1.875246	-0.132344	2.383104
63	6	0	-0.517761	-3.724901	2.960043
64	1	0	-0.076813	-3.730013	0.854396
65	6	0	-1.035570	-2.993821	4.034038
66	1	0	-1.911123	-1.126900	4.660864
67	1	0	-0.115960	-4.715156	3.122350
68	1	0	-1.045738	-3.426383	5.024745
69	6	0	5.234817	-1.403619	-1.979379
70	6	0	5.030705	-1.948499	-3.272454
71	6	0	3.294856	-3.932051	2.197109
72	6	0	3.610052	-3.516027	3.515566
73	1	0	3.586596	-2.670499	-4.678585
74	1	0	2.541004	-3.366064	0.282627
75	1	0	3.642237	-1.875712	4.890762
76	1	0	4.331670	-0.754518	-0.156852
77	1	0	6.238951	-1.174980	-1.650840
78	1	0	5.878481	-2.127935	-3.918244
79	1	0	3.467603	-4.959053	1.907317
80	1	0	4.016385	-4.228196	4.219622
81	6	0	-3.178835	2.276737	0.365066
82	6	0	-3.234384	3.780336	0.108611
83	1	0	-3.928210	4.214799	0.842553
84	1	0	-2.246044	4.213868	0.265079
85	1	0	-3.582265	4.036471	-0.893335
86	8	0	-2.498690	1.885339	1.378714
87	6	0	-4.408727	1.471006	-0.008242
88	6	0	-5.199680	1.772851	-1.128229
89	6	0	-4.806841	0.420711	0.831351
90	6	0	-6.357955	1.045142	-1.401101
91	1	0	-4.897402	2.565221	-1.806197
92	6	0	-5.961435	-0.315367	0.554194
93	1	0	-4.206153	0.197503	1.705527
94	6	0	-6.742141	-0.006960	-0.561741
95	1	0	-6.957317	1.292738	-2.273573
96	1	0	-6.249287	-1.131483	1.211639
97	1	0	-7.639450	-0.580242	-0.778625

Zero-point correction= 0.776411 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.691934
Sum of electronic and zero-point Energies= −4394.650235
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4404.6657092(a.u.)

L_2-CuH-**TS1**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.529796	1.342769	-1.213026
2	6	0	-2.516782	0.402543	-3.543827
3	6	0	-2.860198	-0.929562	-3.198081
4	6	0	-2.645065	-1.371684	-1.852612
5	6	0	-2.065640	-0.473739	-0.886449
6	6	0	-1.719132	0.827931	-1.269442
7	6	0	-1.963716	1.249361	-2.614561
8	6	0	-1.994310	-0.970723	0.537276
9	6	0	-3.236905	-1.000908	1.266042
10	6	0	-3.265879	-1.521266	2.599933
11	6	0	-2.068504	-2.031306	3.163502
12	6	0	-0.893431	-2.010673	2.452010
13	6	0	-0.831269	-1.471360	1.129404
14	6	0	-3.429521	-1.820878	-4.149396

15	6	0	-4.458857	-0.522705	0.705249
16	6	0	-4.490057	-1.530683	3.324989
17	6	0	-3.027286	-2.703895	-1.514813
18	15	0	-0.650194	1.915681	-0.220166
19	15	0	0.815711	-1.311698	0.291936
20	1	0	-2.697791	0.747399	-4.553419
21	1	0	-1.704440	2.256847	-2.902075
22	1	0	-2.091645	-2.442169	4.164249
23	1	0	0.006514	-2.400830	2.901457
24	29	0	1.349154	0.842945	-0.221373
25	6	0	1.989612	-2.028759	1.519150
26	6	0	2.653368	-3.249726	1.317209
27	6	0	2.311344	-1.251724	2.652802
28	6	0	3.611373	-3.691857	2.238818
29	1	0	2.437066	-3.846314	0.443089
30	6	0	3.255493	-1.705704	3.576122
31	1	0	1.856465	-0.280530	2.784178
32	6	0	3.910949	-2.925989	3.369341
33	1	0	4.119021	-4.631865	2.071026
34	1	0	3.495206	-1.097532	4.437358
35	1	0	4.650400	-3.272281	4.077996
36	6	0	0.798510	-2.547067	-1.060219
37	6	0	1.504763	-2.236802	-2.235316
38	6	0	0.156434	-3.792424	-0.944966
39	6	0	1.577753	-3.167829	-3.275658
40	1	0	1.986507	-1.271200	-2.325185
41	6	0	0.228556	-4.715962	-1.990324
42	1	0	-0.399952	-4.032234	-0.048939
43	6	0	0.941367	-4.405847	-3.153543
44	1	0	2.124041	-2.923935	-4.176056
45	1	0	-0.271118	-5.670410	-1.899709
46	1	0	0.994335	-5.123227	-3.960506
47	6	0	-0.720450	3.560621	-1.050129
48	6	0	-1.627753	4.571133	-0.689811
49	6	0	0.222258	3.814123	-2.066303
50	6	0	-1.602447	5.806043	-1.346449
51	1	0	-2.335248	4.402159	0.109230
52	6	0	0.233256	5.044972	-2.728136
53	1	0	0.950453	3.051724	-2.313625
54	6	0	-0.678766	6.042699	-2.368535
55	1	0	-2.299689	6.579960	-1.056858
56	1	0	0.958111	5.227097	-3.509515
57	1	0	-0.662742	6.998497	-2.873126
58	6	0	-1.484191	2.212529	1.379281
59	6	0	-0.642769	2.392318	2.494268
60	6	0	-2.876175	2.313812	1.535512
61	6	0	-1.194254	2.683589	3.745356
62	1	0	0.430324	2.299058	2.373347
63	6	0	-3.420078	2.593629	2.791843
64	1	0	-3.528967	2.152126	0.689642
65	6	0	-2.580904	2.784247	3.894229
66	1	0	-0.544270	2.824410	4.597717
67	1	0	-4.492987	2.650727	2.909975
68	1	0	-3.006314	3.001686	4.863968
69	6	0	-3.576104	-3.543724	-2.458263
70	6	0	-3.780187	-3.102235	-3.789973
71	6	0	-5.629014	-0.545756	1.431984
72	6	0	-5.648239	-1.051512	2.756881
73	1	0	-3.582806	-1.469097	-5.160775
74	1	0	-4.454712	-0.142907	-0.304341
75	1	0	-4.491258	-1.924463	4.332451
76	1	0	-2.878859	-3.046639	-0.503081
77	1	0	-3.857184	-4.550429	-2.182957
78	1	0	-4.213036	-3.774712	-4.516819
79	1	0	-6.544438	-0.179944	0.988527
80	1	0	-6.575191	-1.063080	3.312386
81	6	0	3.389435	1.923679	0.228376
82	6	0	3.343133	3.399789	-0.158395
83	1	0	2.350977	3.793774	0.062795

84	1	0	4.074576	3.937245	0.461453
85	1	0	3.570574	3.582138	-1.210651
86	8	0	2.754870	1.587662	1.292497
87	6	0	4.650894	1.153732	-0.120957
88	6	0	4.849940	-0.119618	0.433924
89	6	0	5.651433	1.691237	-0.944860
90	6	0	6.015262	-0.836262	0.164559
91	1	0	4.090013	-0.530063	1.083054
92	6	0	6.821109	0.973752	-1.212762
93	1	0	5.528145	2.673985	-1.386985
94	6	0	7.008430	-0.294974	-0.659335
95	1	0	6.149486	-1.821311	0.603238
96	1	0	7.585735	1.410203	-1.850294
97	1	0	7.916950	-0.854646	-0.865569

Zero-point correction= 0.776728 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.690626
Sum of electronic and zero-point Energies= −4394.647724 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4404.6620811(a.u.)

L_3-CuH system

L_3-CuH-**TS1**-*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.100924	-3.144248	-3.083428
2	6	0	1.141344	-3.535176	-2.584500
3	6	0	1.548089	-3.094576	-1.323528
4	6	0	0.732860	-2.236087	-0.557487
5	6	0	-0.517770	-1.839852	-1.076116
6	6	0	-0.928833	-2.305265	-2.341177
7	6	0	1.226796	-1.914390	0.824482
8	6	0	1.075494	-2.936726	1.783899
9	6	0	1.562640	-2.780015	3.082391
10	6	0	2.228315	-1.605105	3.431409
11	6	0	2.398465	-0.584648	2.498769
12	6	0	1.896222	-0.728927	1.189943
13	15	0	-1.488907	-0.528776	-0.215667
14	15	0	1.918392	0.702095	0.024583
15	1	0	-0.422412	-3.495239	-4.054327
16	1	0	-1.884646	-2.001698	-2.739912
17	1	0	2.614404	-1.486651	4.434424
18	1	0	2.904630	0.325505	2.781349
19	6	0	2.964753	1.950137	0.884627
20	6	0	4.323871	2.157206	0.600135
21	6	0	2.323556	2.759808	1.841455
22	6	0	5.044348	3.154794	1.270859
23	1	0	4.817048	1.558027	-0.152191
24	6	0	3.039020	3.750079	2.527551
25	1	0	1.260674	2.644030	2.018404
26	6	0	4.394963	3.939313	2.232856
27	1	0	4.948242	4.715502	2.747684
28	6	0	2.946273	0.153932	-1.389695
29	6	0	2.598791	0.612257	-2.668163
30	6	0	4.088530	-0.649394	-1.219884
31	6	0	3.387339	0.281944	-3.780175
32	1	0	1.710416	1.220193	-2.790772
33	6	0	4.896288	-0.963948	-2.317394
34	1	0	4.337275	-1.029680	-0.238718
35	6	0	4.533261	-0.496126	-3.590197
36	1	0	5.154788	-0.742621	-4.442542
37	6	0	-3.084467	-0.477288	-1.138433
38	6	0	-4.238596	-1.176455	-0.747459

39	6	0	-3.127362	0.345105	-2.277831
40	6	0	-5.416508	-1.078387	-1.498490
41	1	0	-4.229102	-1.779308	0.149631
42	6	0	-4.296896	0.443680	-3.043279
43	1	0	-2.255202	0.930906	-2.542823
44	6	0	-5.430926	-0.275140	-2.647480
45	1	0	-6.339402	-0.198876	-3.232604
46	6	0	-1.927736	-1.224029	1.422362
47	6	0	-1.874497	-0.354026	2.521774
48	6	0	-2.352133	-2.553922	1.597707
49	6	0	-2.258598	-0.799798	3.795748
50	1	0	-1.530279	0.663821	2.378571
51	6	0	-2.762060	-2.999430	2.858613
52	1	0	-2.350651	-3.235836	0.758268
53	6	0	-2.709534	-2.114602	3.947316
54	1	0	-3.022498	-2.459217	4.925576
55	8	0	2.753731	-3.455354	-0.738920
56	8	0	0.414684	-4.075540	1.345445
57	6	0	0.294841	-5.198827	2.272492
58	1	0	1.773801	-4.179571	-3.174025
59	1	0	1.432053	-3.557157	3.818411
60	1	0	-0.207796	-5.978682	1.705863
61	1	0	-0.305821	-4.932222	3.144620
62	1	0	1.276310	-5.553117	2.598060
63	6	0	3.613943	-4.388134	-1.463639
64	1	0	3.956441	-3.960068	-2.408218
65	1	0	4.464588	-4.554215	-0.807473
66	1	0	3.103241	-5.335728	-1.653117
67	6	0	-3.301910	-4.411585	3.045693
68	1	0	-2.938354	-4.856499	3.974476
69	1	0	-4.394563	-4.401978	3.091473
70	1	0	-3.008457	-5.056252	2.216165
71	6	0	-2.153636	0.136533	4.990806
72	1	0	-2.768432	-0.211899	5.822098
73	1	0	-1.117626	0.196926	5.335722
74	1	0	-2.472709	1.145383	4.722772
75	6	0	-6.661957	-1.851922	-1.087370
76	1	0	-7.555331	-1.230351	-1.173088
77	1	0	-6.802319	-2.728786	-1.725628
78	1	0	-6.583410	-2.196195	-0.055340
79	6	0	-4.340608	1.363785	-4.254102
80	1	0	-4.507421	2.394531	-3.929060
81	1	0	-3.398532	1.334549	-4.804464
82	1	0	-5.147521	1.085487	-4.933834
83	6	0	6.518306	3.382711	0.964990
84	1	0	7.142289	3.073438	1.807696
85	1	0	6.827532	2.812142	0.088477
86	1	0	6.718379	4.438702	0.771686
87	6	0	2.341776	4.601862	3.579291
88	1	0	1.268144	4.641336	3.389555
89	1	0	2.491626	4.181069	4.577974
90	1	0	2.732644	5.621009	3.584186
91	6	0	2.978891	0.749692	-5.169150
92	1	0	3.804183	0.654777	-5.876054
93	1	0	2.142431	0.152412	-5.542180
94	1	0	2.660994	1.793835	-5.150815
95	6	0	6.178412	-1.764650	-2.132203
96	1	0	6.317245	-2.484907	-2.941116
97	1	0	7.048121	-1.101579	-2.128286
98	1	0	6.167559	-2.306477	-1.185704
99	29	0	-0.222351	1.374775	-0.357429
100	1	0	-0.676862	2.603938	-1.283279
101	6	0	-1.227924	3.415039	0.283904
102	6	0	-0.403772	4.666961	-0.005074
103	1	0	-0.731982	5.450241	0.693637
104	1	0	0.650122	4.455311	0.177400
105	1	0	-0.519924	5.038021	-1.024604
106	8	0	-0.901911	2.727733	1.312362
107	6	0	-2.694802	3.449342	-0.099568

108	6	0	-3.179158	4.196477	-1.184928
109	6	0	-3.614621	2.756502	0.700727
110	6	0	-4.545861	4.251708	-1.460901
111	1	0	-2.485205	4.723995	-1.831577
112	6	0	-4.981310	2.798647	0.417709
113	1	0	-3.241827	2.194686	1.549148
114	6	0	-5.454273	3.547454	-0.662415
115	1	0	-4.902504	4.841241	-2.302032
116	1	0	-5.676858	2.244937	1.042845
117	1	0	-6.517964	3.582128	-0.882451

Zero-point correction= 0.966720 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.861266
Sum of electronic and zero-point Energies= −4629.555761 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4640.9870591 (a.u.)

L_3-CuH-**TS1**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.091591	1.803043	-3.608944
2	6	0	1.367011	2.932809	-3.229433
3	6	0	0.936916	3.061397	-1.908032
4	6	0	1.196161	2.050966	-0.957179
5	6	0	1.901364	0.896894	-1.358675
6	6	0	2.356521	0.791332	-2.690248
7	6	0	0.792747	2.370676	0.452379
8	6	0	1.620119	3.290819	1.129132
9	6	0	1.289419	3.750002	2.403345
10	6	0	0.118604	3.299857	3.015092
11	6	0	-0.714103	2.391923	2.365376
12	6	0	-0.383210	1.918262	1.079158
13	15	0	1.916998	-0.620830	-0.309067
14	15	0	-1.419175	0.639568	0.243400
15	1	0	2.442659	1.709199	-4.627289
16	1	0	2.897774	-0.088054	-3.002716
17	1	0	-0.142284	3.658667	4.001033
18	1	0	-1.611979	2.042338	2.850751
19	29	0	-0.268945	-1.245076	-0.329143
20	6	0	-2.723786	0.269239	1.488548
21	6	0	-4.076813	0.599353	1.300145
22	6	0	-2.348596	-0.509449	2.597820
23	6	0	-5.046608	0.153993	2.208360
24	6	0	-3.308479	-0.957190	3.514521
25	1	0	-1.318683	-0.817867	2.714181
26	6	0	-4.652266	-0.622037	3.308935
27	6	0	-2.880808	-1.840844	4.676620
28	1	0	-5.401641	-0.975519	4.006935
29	6	0	-2.308915	1.553879	-1.072792
30	6	0	-2.629548	0.858019	-2.246317
31	6	0	-2.713814	2.892008	-0.917043
32	6	0	-3.367323	1.483326	-3.263331
33	1	0	-2.298490	-0.167303	-2.363536
34	6	0	-3.454459	3.523342	-1.920545
35	1	0	-2.445755	3.434521	-0.020358
36	6	0	-3.773981	2.808828	-3.087196
37	6	0	-3.699571	0.719060	-4.536328
38	6	0	-3.940898	4.955218	-1.741893
39	1	0	-4.346593	3.296387	-3.866949
40	6	0	3.139773	-1.721105	-1.140585
41	6	0	4.505187	-1.734293	-0.807844
42	6	0	2.660334	-2.589577	-2.134942
43	6	0	5.386873	-2.596167	-1.469120
44	1	0	4.876389	-1.083300	-0.028364
45	6	0	3.535677	-3.451080	-2.811930
46	1	0	1.602039	-2.594970	-2.367974

47	6	0	4.892327	-3.443735	-2.471843
48	6	0	6.865904	-2.621008	-1.110806
49	6	0	3.000026	-4.405467	-3.869944
50	1	0	5.572960	-4.110200	-2.987531
51	6	0	2.728018	-0.250483	1.289204
52	6	0	2.376163	-1.093184	2.356015
53	6	0	3.701052	0.747740	1.471366
54	6	0	3.012918	-0.965469	3.599328
55	1	0	1.602917	-1.840663	2.215016
56	6	0	4.339350	0.881774	2.708973
57	1	0	3.922052	1.443389	0.673016
58	6	0	3.995526	0.015938	3.758438
59	6	0	2.613405	-1.871572	4.754622
60	6	0	5.393363	1.957993	2.929872
61	1	0	4.496175	0.115960	4.713835
62	8	0	2.764973	3.683223	0.443826
63	8	0	0.238453	4.163041	-1.434871
64	6	0	3.543115	4.797406	0.984856
65	6	0	-0.106198	5.219305	-2.385569
66	1	0	1.928875	4.447567	2.920985
67	1	0	1.154120	3.700070	-3.956534
68	1	0	-0.642089	5.960352	-1.798536
69	1	0	-0.754706	4.840546	-3.178368
70	1	0	0.788570	5.670094	-2.822574
71	1	0	2.920787	5.684975	1.122041
72	1	0	4.016091	4.535875	1.934084
73	1	0	4.308540	4.994460	0.238236
74	1	0	7.481668	-2.373354	-1.978787
75	1	0	7.163803	-3.612547	-0.761698
76	1	0	2.552254	-5.285343	-3.398981
77	1	0	3.796898	-4.747306	-4.531966
78	1	0	5.022343	2.730133	3.610026
79	1	0	5.667998	2.434822	1.988275
80	1	0	2.553913	-2.912255	4.430673
81	1	0	1.631073	-1.587435	5.141411
82	1	0	3.331363	-1.806095	5.573298
83	1	0	-3.824449	5.530131	-2.662925
84	1	0	-5.000718	4.972018	-1.473186
85	1	0	-4.203517	-0.221196	-4.302334
86	1	0	-2.787868	0.478788	-5.089102
87	1	0	-3.741899	-2.172187	5.258422
88	1	0	-2.201238	-1.306492	5.345551
89	1	0	-2.357342	-2.722813	4.299605
90	1	0	7.087667	-1.903121	-0.320628
91	1	0	2.230376	-3.924870	-4.476467
92	1	0	-4.349657	1.303407	-5.188785
93	1	0	-3.387270	5.459297	-0.948532
94	1	0	6.297871	1.535335	3.372904
95	1	0	-0.788671	-2.414932	-1.324197
96	6	0	-0.990322	-3.474100	0.101489
97	6	0	0.061920	-4.489278	-0.339333
98	1	0	1.053043	-4.085990	-0.130630
99	1	0	-0.072867	-5.403069	0.257101
100	1	0	-0.000528	-4.746168	-1.398970
101	8	0	-0.753757	-2.825067	1.178773
102	6	0	-2.437854	-3.782337	-0.240152
103	6	0	-3.456317	-2.979391	0.296262
104	6	0	-2.797676	-4.875063	-1.043056
105	6	0	-4.794672	-3.261510	0.027461
106	1	0	-3.187171	-2.142834	0.923557
107	6	0	-4.140589	-5.158819	-1.311068
108	1	0	-2.033512	-5.515824	-1.469541
109	6	0	-5.146825	-4.350130	-0.778684
110	1	0	-5.567807	-2.625474	0.449843
111	1	0	-4.396529	-6.012817	-1.933153
112	1	0	-6.191777	-4.566613	-0.985149
113	1	0	-4.378006	1.180811	0.439947
114	6	0	-6.518293	0.480078	1.991613
115	1	0	-6.640103	1.249009	1.228036

116	1	0	-7.067061	-0.408064	1.664706
117	1	0	-6.982063	0.835919	2.914026

Zero-point correction= 0.967367 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.860728
Sum of electronic and zero-point Energies= −4629.553584 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4640.9826001 (a.u.)

L_3^*-CuH system

L_3^*-CuH-**TS1**-*si*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.547357	2.288213	-1.214986
2	6	0	0.855385	-2.935268	-3.116800
3	6	0	2.174343	-2.889604	-2.665694
4	6	0	2.457280	-2.335412	-1.416103
5	6	0	1.431490	-1.795479	-0.613027
6	6	0	0.102193	-1.840286	-1.082971
7	6	0	-0.177022	-2.418651	-2.337171
8	6	0	1.843289	-1.322496	0.752294
9	6	0	2.080509	-2.333229	1.706855
10	6	0	2.540056	-2.018507	2.986582
11	6	0	2.789750	-0.687959	3.321129
12	6	0	2.570412	0.327624	2.393487
13	6	0	2.092534	0.020049	1.103900
14	15	0	-1.217411	-0.931983	-0.169575
15	15	0	1.575091	1.377272	-0.032993
16	1	0	0.634106	-3.374175	-4.079772
17	1	0	-1.193467	-2.452978	-2.698088
18	1	0	3.153309	-0.443519	4.309502
19	1	0	2.755432	1.354777	2.667261
20	29	0	-0.674501	1.289244	-0.309990
21	6	0	2.204985	2.899907	0.788674
22	6	0	3.437483	3.497071	0.475187
23	6	0	1.373020	3.498193	1.758082
24	6	0	3.838809	4.665731	1.131439
25	1	0	4.073112	3.061777	-0.282515
26	6	0	1.788815	4.658633	2.417730
27	1	0	0.398606	3.072075	1.966438
28	6	0	3.020680	5.243691	2.105970
29	1	0	4.785959	5.122030	0.878675
30	1	0	1.145603	5.108321	3.161682
31	1	0	3.335429	6.146275	2.610902
32	6	0	2.642906	1.206711	-1.511852
33	6	0	2.115008	1.609409	-2.751150
34	6	0	3.967530	0.740962	-1.440021
35	6	0	2.907616	1.562032	-3.901502
36	1	0	1.088069	1.948046	-2.804231
37	6	0	4.756258	0.701807	-2.593814
38	1	0	4.364784	0.394570	-0.497127
39	6	0	4.228953	1.113321	-3.822829
40	1	0	2.495007	1.872132	-4.851436
41	1	0	5.778885	0.354975	-2.532914
42	1	0	4.843270	1.082075	-4.712018
43	6	0	-2.772948	-1.424975	-1.028032
44	6	0	-3.591158	-2.491922	-0.620577
45	6	0	-3.159403	-0.648939	-2.138604
46	6	0	-4.759333	-2.793896	-1.329165
47	1	0	-3.331329	-3.070626	0.253798
48	6	0	-4.320392	-0.963115	-2.849736
49	1	0	-2.562219	0.209285	-2.419871
50	6	0	-5.120336	-2.038560	-2.448993

51	1	0	-5.384138	-3.614648	-1.004545
52	1	0	-4.606174	-0.360889	-3.700938
53	1	0	-6.021646	-2.277330	-2.996295
54	6	0	-1.330280	-1.747238	1.468424
55	6	0	-1.568939	-0.926742	2.586244
56	6	0	-1.225534	-3.139423	1.636274
57	6	0	-1.727847	-1.499094	3.852976
58	1	0	-1.620745	0.147369	2.455122
59	6	0	-1.396007	-3.703819	2.904108
60	1	0	-0.993872	-3.768341	0.788567
61	6	0	-1.651006	-2.885959	4.010820
62	1	0	-1.908128	-0.863546	4.708953
63	1	0	-1.331553	-4.776522	3.027569
64	1	0	-1.783296	-3.327397	4.988978
65	8	0	3.734557	-2.270428	-0.877872
66	8	0	1.817557	-3.628349	1.283644
67	6	0	2.078491	-4.723460	2.216605
68	1	0	2.962909	-3.287971	-3.284022
69	1	0	2.705250	-2.792503	3.718796
70	1	0	1.835542	-5.627124	1.663264
71	1	0	1.441882	-4.648832	3.100905
72	1	0	3.128115	-4.747484	2.519949
73	6	0	4.834381	-2.854744	-1.643164
74	1	0	4.979992	-2.330463	-2.590325
75	1	0	5.712220	-2.728228	-1.014359
76	1	0	4.667173	-3.917798	-1.833086
77	6	0	-2.282854	2.847616	0.382878
78	6	0	-1.973268	4.311694	0.082488
79	1	0	-2.505027	4.921356	0.827201
80	1	0	-0.902396	4.487315	0.188862
81	1	0	-2.287852	4.626183	-0.913967
82	8	0	-1.686010	2.320660	1.386492
83	6	0	-3.682728	2.360569	0.061555
84	6	0	-4.417220	2.835197	-1.036677
85	6	0	-4.290394	1.440585	0.927612
86	6	0	-5.723393	2.401557	-1.262769
87	1	0	-3.957800	3.528303	-1.734448
88	6	0	-5.594896	0.997215	0.697345
89	1	0	-3.729839	1.087688	1.785319
90	6	0	-6.317193	1.474713	-0.398151
91	1	0	-6.275754	2.778177	-2.119976
92	1	0	-6.044962	0.276097	1.374611
93	1	0	-7.330739	1.127795	-0.580441

Zero-point correction= 0.747014 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.662991
Sum of electronic and zero-point Energies= −4316.890990 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = −4326.4231515(a.u.)

L_3^*-CuH-**TS1**-*re*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.009228	1.742246	-1.111043
2	6	0	-2.871707	-0.212030	-3.432257
3	6	0	-2.923639	-1.556608	-3.065320
4	6	0	-2.570412	-1.930485	-1.767658
5	6	0	-2.131567	-0.971331	-0.830574
6	6	0	-2.064856	0.383090	-1.217605
7	6	0	-2.447162	0.753973	-2.523120
8	6	0	-1.884592	-1.484279	0.558577
9	6	0	-3.036276	-1.744959	1.329561
10	6	0	-2.936007	-2.326937	2.593477
11	6	0	-1.681328	-2.674313	3.093814
12	6	0	-0.529934	-2.428589	2.349567

13	6	0	-0.620420	-1.824430	1.079423
14	15	0	-1.200045	1.607975	-0.144648
15	15	0	0.900127	-1.320057	0.161196
16	1	0	-3.159415	0.081121	-4.432342
17	1	0	-2.398122	1.788996	-2.823725
18	1	0	-1.602709	-3.135887	4.068245
19	1	0	0.435203	-2.692317	2.752215
20	29	0	0.976578	0.928853	-0.163647
21	6	0	2.269399	-1.955260	1.217989
22	6	0	3.088527	-3.031941	0.843088
23	6	0	2.559018	-1.251861	2.407038
24	6	0	4.168943	-3.409570	1.650456
25	1	0	2.893718	-3.564403	-0.076330
26	6	0	3.627588	-1.644307	3.216421
27	1	0	1.977387	-0.379113	2.669674
28	6	0	4.436829	-2.722950	2.838382
29	1	0	4.796250	-4.237582	1.350142
30	1	0	3.840508	-1.095082	4.123234
31	1	0	5.269906	-3.020615	3.459985
32	6	0	0.941061	-2.407706	-1.314429
33	6	0	1.483605	-1.885846	-2.501440
34	6	0	0.488435	-3.738649	-1.283290
35	6	0	1.588422	-2.691812	-3.639060
36	1	0	1.812088	-0.854269	-2.525285
37	6	0	0.598790	-4.539582	-2.423540
38	1	0	0.048119	-4.136185	-0.379913
39	6	0	1.149755	-4.018131	-3.599962
40	1	0	2.008115	-2.284723	-4.548401
41	1	0	0.261366	-5.566666	-2.392885
42	1	0	1.235325	-4.642226	-4.478792
43	6	0	-1.555378	3.230513	-0.944781
44	6	0	-2.593904	4.082766	-0.534758
45	6	0	-0.706346	3.638520	-1.993342
46	6	0	-2.787829	5.313740	-1.170779
47	1	0	-3.237555	3.793183	0.283202
48	6	0	-0.914529	4.862420	-2.634609
49	1	0	0.122157	3.003578	-2.281660
50	6	0	-1.955143	5.702642	-2.223489
51	1	0	-3.585630	5.965236	-0.841956
52	1	0	-0.259890	5.162930	-3.441067
53	1	0	-2.108659	6.654193	-2.712842
54	6	0	-2.123807	1.707830	1.433199
55	6	0	-1.378951	2.034054	2.581869
56	6	0	-3.514654	1.529543	1.530925
57	6	0	-2.025320	2.198922	3.810735
58	1	0	-0.303738	2.147237	2.506837
59	6	0	-4.151708	1.695394	2.764436
60	1	0	-4.081444	1.224524	0.663300
61	6	0	-3.410525	2.034908	3.901622
62	1	0	-1.448900	2.450184	4.690168
63	1	0	-5.222955	1.563880	2.837282
64	1	0	-3.909212	2.164857	4.852090
65	8	0	-4.242317	-1.381093	0.745384
66	8	0	-2.617446	-3.237830	-1.306869
67	6	0	-5.477163	-1.698377	1.461183
68	6	0	-3.065372	-4.278967	-2.230933
69	1	0	-3.816659	-2.514903	3.186760
70	1	0	-3.243212	-2.293925	-3.784467
71	1	0	-3.052319	-5.195748	-1.647044
72	1	0	-2.383945	-4.373069	-3.079160
73	1	0	-4.079278	-4.084219	-2.589098
74	1	0	-5.566051	-2.771711	1.645916
75	1	0	-5.537351	-1.159659	2.409796
76	1	0	-6.276538	-1.371420	0.800954
77	6	0	2.706250	2.410610	0.400848
78	6	0	2.291241	3.854205	0.128749
79	1	0	1.233278	3.972396	0.363184
80	1	0	2.868292	4.506700	0.799378
81	1	0	2.460150	4.169271	-0.902791

82	8	0	2.181334	1.842962	1.425210
83	6	0	4.115088	2.007104	0.005643
84	6	0	4.623727	0.774686	0.443246
85	6	0	4.951830	2.852145	-0.739012
86	6	0	5.928969	0.395131	0.132885
87	1	0	3.991304	0.127317	1.033839
88	6	0	6.261079	2.472100	-1.049384
89	1	0	4.590013	3.813423	-1.087396
90	6	0	6.756210	1.240267	-0.615618
91	1	0	6.302167	-0.564834	0.479600
92	1	0	6.893331	3.142882	-1.625594
93	1	0	7.773670	0.942710	-0.855308

Zero-point correction= 0.747395 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.660998
Sum of electronic and zero-point Energies= − 4316.888138 (a.u.)
SCF- Energy:B3LYP (PCM, toluene)/6-31+G(d, p) = − 4326.419839(a.u.)

S7. Reference 18 details

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