Supporting Information

Computational Investigations on the Phosphine-ligated CuH-Catalyzed Conjugate Reduction of α-β Unsaturated Ketones: Regionselectivity and Stereoselectivlity

Hangyu Liu, Wei Zhang, Ling He, Mingliang Luo, Song Qin*

Key Laboratory of Green Chemistry and Technology, Ministry of Education, College of Chemistry, Sichuan University, Chengdu, Sichuan, 610064, China.

Email of corresponding author: qinsong@mail.sc.cninfo.net, qinsong@scu.edu.cn

CONTENTS:

Part I: Results and brief discussion on diatomic CuH($^1\sum$) model reaction system

The energy profiles in the gas-phase system are given in Figure 1. The optimized structures of key stationary points along the reaction pathway are collected in Figure 2.

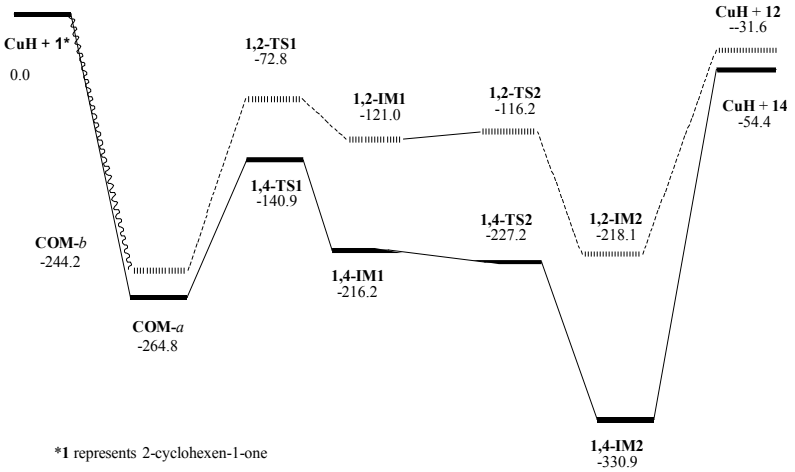

Figure 1. The potential energy curves of the gas-phase CuH/**1** system. Relative energies (in kJ/mol) are listed in the order of M06 /6-31G(d, p)/(BHLYP/6-31G(d, p))

As shown in Figure 2, the addition reaction begins with the coordination of the copper-hydride catalyst to the substrate **1**. In principle, CuH can coordinate to either carbon-carbon double bond or the carbon-oxygen double bond of **1**, and therefore two complexes (**CuH**-*a* and **CuH**-*b*) result in the first step of the reaction. Coordination of the CuH to the carbon-carbon (C=C) double bond in **1** leads to the formation of complex **CuH**-*a*, in which the metal center attaches to the C=C bond with the distances between Cu and two carbon atoms of 1.967 and 1.957Å, respectively. On the other hand, the catalyst can alternatively coordinate to C=O bond, which leads to the formation of the other complex **CuH**-*b*, an isomer of **CuH**-*a*. In this complex, the metal center of the catalyst interacts with the O-end of carbon-oxygen double bond with the Cu-O distance of 1.855 Å. DFT calculations predict that the coordination of CuH to the C=C double bond in **CuH**-*a* is energetically favored by ca. 20.6 kJ/mol than that to the C=O bond in **CuH**-*b*.

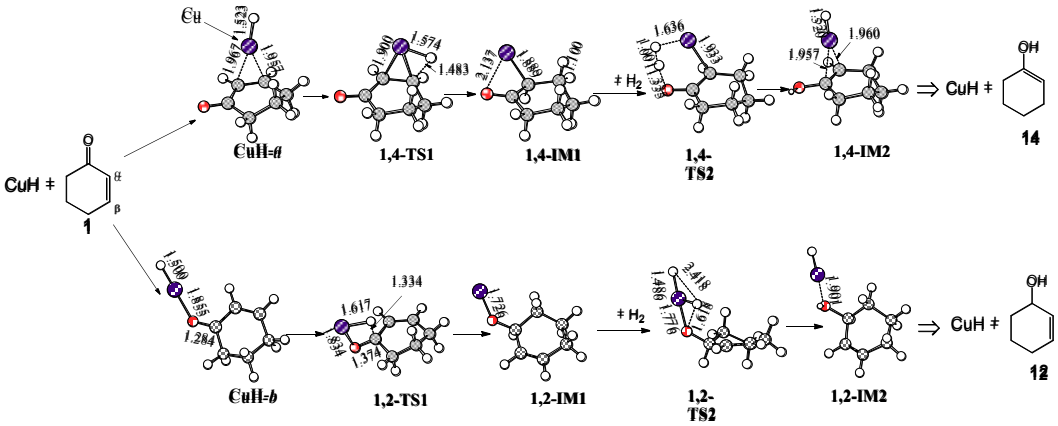

Figure 2. The reaction mechanism and the optimized structures calculated at the M06 /6-31G(d,p) level. The bond lengths are in Å.

From these two CuH-substrate complexes, the addition reaction could complete along two distinct paths and arise to the different final products. According to the structures of the final products, these reaction channels are labeled as the 1,4- and 1,2- path (see in Figure 2).

1,4-paths. From **CuH**-*a*, the conversion of this complex involves the 1,4-path. In the 1,4-path, the cleavage of Cu-H bond takes place via 1,4-**TS1**. For this transition state, the Cu-H bond is enlarged to 1.574 Å from 1.523 Å in **CuH**-*a* complex, and the distance of C_β-H shortens to 1.483 Å, respectively. This step involves the breakage of Cu-H bond of the catalyst and the formation of two new bonds, as suggested by the bond lengths of Cu-C_α (1.889 Å) and C_β-H (1.100 Å) in 1,4-**IM1**, respectively.

Next, from 1,4-**IM1,** an external H_2 molecule might coordinate to the bare Cu center followed by the cleavage of H-H bond via four-centered **TS2**. As a result, one H atom is delivered to the substrate with the recovery of CuH catalyst. As compared to the addition of CuH step, this process in carbocations is very easy, for the step bears a relatively smaller energy barrier than its corresponding CuH addition step.

1,2-path. In contrast, from the complex **CuH**-*b*, the addition of CuH to the C=O double bond can take place via 1,2-**TS1**. In this transition state, the H atom connecting with metal center transfers to C-end of the C=O double bond, accompanying by the migration of Cu center to O atom. As a result, the following step breaks the Cu-H bond and generates the intermediate 1,2-**IM1** with the bond length of Cu-O of 1.726 Å. From 1,2-**IM1**, an external H_2 molecule might coordinate to the bare Cu center and donate one H atom to recover CuH catalyst via 1,2-**TS2**.

In summary, the entire reaction can be generally divided into two subsequent stages: (1) the addition of CuH to the unsaturated bonds of the substrate; (2) the recovery of CuH catalyst. calculations indicate that the 1,4-path via intermediate 1,4-**IM1** might be predominant for its major part in potential energy surface is the lowest in all paths. The rate-determining step can be identified as the CuH addition step of the overall reactions. It should be emphasized that after the formation of **IM1**, the structures of the final products are also determined. This means that the addition step of CuH to the unsaturated bond in the gas-phase system is responsible for the region-selectivity of the reaction, while hydrogen molecule for regenerating CuH catalyst.

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

Species	M06 /6-31G(d,p)	
	E_{zpe}	E_r
CuH	-1640.683582	
1	-308.321814	
H_2	-1.159205	
CuH + 1 + H_2	-1950.164601	0.0
CuH-*a*	-1949.106266	
CuH−a + H_2	-1950.265471	−264.8
1,4-TS1	-1949.059065	
1,4-TS1 + H_2	-1950.21827	−140.9
1,4-IM1	-1949.087745	
1,4-IM1 + H_2	-1950.24695	−216.2
1,4-TS2	-1950.251142	−227.2
1,4-IM2	-1950.290652	−330.9
14−PRO	-309.501739	
CuH + 14	-1950.185321	−54.4
CuH-b	-1949.098401	
CuH-b + H_2	-1950.257606	−244.2
1,2-TS1	-1949.033126	
1,2-TS1 + H_2	-1950.192331	−72.8
1,2-IM1	-1949.051475	
1,2-IM1 + H_2	-1950.21068	-121.0
1,2-TS2	-1950.208876	−116.2
1,2-IM2	-1950.247657	−218.1
14−PRO	-309.493067	
CuH + 12	-1950.176649	−31.6

S2. Cartesian coordinates and energies of all optimized stationary points of model reaction system at the M06 /6-31G(d, p) level.

1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.324395	-1.227955	0.278335
2	6	0	-1.059767	-1.154270	-0.352372
3	6	0	-1.806793	0.082205	0.132685
4	6	0	-0.964008	1.313559	0.028108
5	6	0	0.373475	1.283594	-0.056211
6	6	0	1.136929	0.023330	0.017284
7	8	0	2.349934	0.001514	-0.080538
8	1	0	0.905463	-2.090345	-0.064306
9	1	0	0.227535	-1.323367	1.372316
10	1	0	-1.634415	-2.062152	-0.134701
11	1	0	-0.956742	-1.099776	-1.445578
12	1	0	-2.113214	-0.047829	1.184760
13	1	0	-2.741081	0.221649	-0.426530
14	1	0	-1.478034	2.275383	0.023629
15	1	0	0.965625	2.191549	-0.152261

Zero-point correction= 0.127051 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.097155
Sum of electronic and zero-point Energies= -308.321814

CuH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	0.047536
2	1	0	0.000000	0.000000	-1.378542

Zero-point correction= 0.004829 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= -0.01408
Sum of electronic and zero-point Energies= -1640.683582

H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.370365
2	1	0	0.000000	0.000000	-0.370365

Zero-point correction= 0.010096 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= -0.001386
Sum of electronic and zero-point Energies=-1.159205

CuH-*a*:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.893155	0.429136	-0.318699
2	6	0	-0.878682	1.479607	-0.762052
3	6	0	0.039019	1.888611	0.384594
4	6	0	0.594831	0.701343	1.116134
5	6	0	-0.053806	-0.523657	1.138479
6	6	0	-1.200724	-0.790429	0.242032

7	8	0	-1.533200	-1.930693	-0.025881
8	1	0	-2.548309	0.109535	-1.134994
9	1	0	-2.528173	0.840416	0.482035
10	1	0	-1.386888	2.356896	-1.176464
11	1	0	-0.261231	1.067190	-1.574889
12	1	0	-0.512582	2.507564	1.111155
13	1	0	0.862052	2.512820	0.013310
14	1	0	1.370680	0.897554	1.857402
15	1	0	0.221919	-1.317413	1.832204
16	29	0	1.217150	-0.424053	-0.359051
17	1	0	2.105874	-0.339142	-1.593148

Zero-point correction= 0.134367 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.100793
Sum of electronic and zero-point Energies= -1949.106266

1,4-TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.801243	0.495606	-0.641088
2	6	0	-0.776401	1.622212	-0.670659
3	6	0	-0.148779	1.787954	0.703390
4	6	0	0.647138	0.549191	1.028348
5	6	0	-0.063024	-0.761557	0.744912
6	6	0	-1.374853	-0.758383	0.124281
7	8	0	-2.155895	-1.699402	0.186903
8	1	0	-2.105056	0.184748	-1.648398
9	1	0	-2.722369	0.841579	-0.150865
10	1	0	-1.233750	2.555282	-1.020700
11	1	0	0.040069	1.402082	-1.384350
12	1	0	-0.943553	1.880919	1.460687
13	1	0	0.475721	2.687995	0.761997
14	1	0	1.860819	0.911776	0.256306
15	1	0	0.072250	-1.549913	1.485407
16	1	0	1.143534	0.572811	2.000815
17	29	0	1.440085	-0.465593	-0.379008

Zero-point correction= 0.134603 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.101778
Sum of electronic and zero-point Energies= -1949.059065

1,4-IM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.041606	1.479785	-0.138441
2	6	0	2.106446	0.594904	-0.770715
3	6	0	2.443678	-0.559252	0.162068
4	6	0	1.238782	-1.482184	0.308666
5	6	0	-0.033913	-0.726878	0.645729
6	6	0	-0.112367	0.719777	0.465893
7	8	0	-1.145302	1.371077	0.818373
8	1	0	0.643167	2.230492	-0.832669
9	1	0	1.474495	2.048724	0.699537
10	1	0	2.995968	1.190267	-1.011447
11	1	0	1.734186	0.186967	-1.724697
12	1	0	2.725855	-0.151955	1.146226
13	1	0	3.309349	-1.123695	-0.207535
14	1	0	1.125996	-2.043095	-0.630477
15	1	0	-0.501932	-1.031946	1.590026
16	1	0	1.434627	-2.237470	1.081125
17	29	0	-1.582231	-0.351511	-0.368837

Zero-point correction= 0.13936 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.106172
Sum of electronic and zero-point Energies= -1949.087745

1,4-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.027806	1.459316	-0.282253
2	6	0	2.072103	0.530359	-0.883188
3	6	0	2.493749	-0.503338	0.151670
4	6	0	1.323431	-1.413393	0.504288
5	6	0	0.038376	-0.644293	0.754111
6	6	0	-0.052496	0.748305	0.485033
7	8	0	-1.035377	1.492712	0.911049
8	1	0	0.551508	2.102102	-1.034562
9	1	0	1.496208	2.149746	0.436600
10	1	0	2.931029	1.109504	-1.242906
11	1	0	1.652525	0.013953	-1.762031
12	1	0	2.834291	0.024551	1.056296
13	1	0	3.342817	-1.099282	-0.204763
14	1	0	1.194777	-2.154853	-0.297851
15	1	0	-0.523962	-0.952674	1.643430
16	1	0	1.566307	-1.997469	1.401972
17	29	0	-1.489810	-0.465164	-0.415656
18	1	0	-2.137695	0.905001	0.441570
19	1	0	-2.838099	0.385746	-0.050087

Zero-point correction= 0.152219 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.118402
Sum of electronic and zero-point Energies= -1950.251142

1,4-IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.483410	1.358232	-0.774757
2	6	0	1.549587	0.325498	-1.121853
3	6	0	2.272838	-0.112488	0.144263
4	6	0	1.327845	-0.829233	1.104513
5	6	0	-0.016457	-0.143862	1.203483
6	6	0	-0.382937	0.883579	0.354321
7	1	0	-0.144813	1.579425	-1.653181
8	1	0	0.949756	2.308780	-0.471014
9	1	0	2.248748	0.740466	-1.856072
10	1	0	1.064940	-0.542521	-1.595938
11	1	0	2.683841	0.779372	0.641145
12	1	0	3.124813	-0.758746	-0.097039
13	1	0	1.205368	-1.879009	0.790044
14	1	0	-0.587254	-0.239922	2.127511
15	1	0	1.777342	-0.876246	2.104930
16	8	0	-1.398342	1.708565	0.740798
17	1	0	-1.727712	2.187573	-0.029246
18	29	0	-1.008134	-0.835741	-0.339246
19	1	0	-1.578104	-1.621557	-1.509205

Zero-point correction= 0.158207 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.124909
Sum of electronic and zero-point Energies= -1950.290652

14:

Standard orientation:

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

1	6	0	-0.416535	1.241750	0.069623
2	6	0	1.059554	1.233575	-0.312281
3	6	0	1.774892	0.073155	0.365866
4	6	0	1.200556	-1.257248	-0.108982
5	6	0	-0.298953	-1.250676	-0.102273
6	6	0	-1.016385	-0.128941	-0.000282
7	1	0	-0.978509	1.916161	-0.597624
8	1	0	-0.548471	1.643828	1.088182
9	1	0	1.522252	2.193509	-0.052423
10	1	0	1.149394	1.121968	-1.403284
11	1	0	1.642484	0.159169	1.455378
12	1	0	2.853988	0.116801	0.172325
13	1	0	1.577706	-1.479061	-1.122007
14	1	0	-0.835155	-2.196057	-0.167370
15	1	0	1.573934	-2.073479	0.525493
16	8	0	-2.379396	-0.195827	0.075767
17	1	0	-2.741231	0.694089	0.025169

Zero-point correction= 0.150266 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.119711
Sum of electronic and zero-point Energies= -309.501739

CuH-b:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.604525	-0.169482	-0.441058
2	1	0	1.635900	-0.891818	-1.755634
3	6	0	-0.642635	-0.901394	1.026719
4	6	0	-1.593868	-1.308867	-0.089916
5	6	0	-2.598095	-0.197912	-0.379137
6	6	0	-1.951353	1.148025	-0.449279
7	6	0	-0.713813	1.396279	0.007700
8	6	0	0.091833	0.357785	0.648932
9	8	0	1.224502	0.647897	1.180558
10	1	0	0.084360	-1.686537	1.263220
11	1	0	-1.200253	-0.690234	1.953966
12	1	0	-2.110966	-2.242361	0.157431
13	1	0	-0.989539	-1.498396	-0.988910
14	1	0	-3.376017	-0.169226	0.403074
15	1	0	-3.138468	-0.395717	-1.314413
16	1	0	-2.528675	1.962102	-0.886955
17	1	0	-0.256001	2.380503	-0.075665

Zero-point correction= 0.13447 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.100853
Sum of electronic and zero-point Energies= -1949.098401

1,2-TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.956284	-0.076451	-0.335676
2	1	0	0.473770	-0.221471	-0.964849
3	6	0	-0.765749	-1.114796	0.597797
4	6	0	-1.969001	-1.243008	-0.321915
5	6	0	-2.874807	-0.021960	-0.190708
6	6	0	-2.090040	1.255343	-0.184571
7	6	0	-0.767032	1.302781	-0.014056
8	6	0	0.078818	0.103729	0.267438
9	8	0	1.054696	0.357752	1.201119
10	1	0	-0.129131	-2.009090	0.582240
11	1	0	-1.084917	-0.971074	1.641640
12	1	0	-2.528955	-2.162264	-0.111233
13	1	0	-1.618240	-1.321477	-1.363209

14	1	0	-3.462002	-0.087163	0.740467
15	1	0	-3.616752	-0.001566	-1.001230
16	1	0	-2.646363	2.184715	-0.311043
17	1	0	-0.230337	2.251908	-0.011048

Zero-point correction= 0.134525 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.10182
Sum of electronic and zero-point Energies= -1949.033126

1,2-IM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-2.158521	-0.199847	-0.110863
2	6	0	0.432537	-0.896666	-0.013178
3	6	0	1.823673	-1.390370	0.340325
4	6	0	2.878444	-0.516201	-0.334990
5	6	0	2.539405	0.943202	-0.247553
6	6	0	1.345504	1.400325	0.133503
7	6	0	0.187817	0.519640	0.509200
8	8	0	-0.995330	1.068923	0.016167
9	1	0	-0.366160	-1.543032	0.394200
10	1	0	0.302900	-0.867093	-1.107439
11	1	0	1.958805	-2.442335	0.059869
12	1	0	1.952818	-1.335887	1.432041
13	1	0	2.976151	-0.801451	-1.395867
14	1	0	3.867670	-0.701847	0.107057
15	1	0	3.321538	1.650948	-0.524605
16	1	0	1.146059	2.470648	0.175855
17	1	0	0.155695	0.454646	1.620732

Zero-point correction= 0.139407 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.105747
Sum of electronic and zero-point Energies= -1949.051475

1,2-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-2.056211	-0.177428	-0.276924
2	6	0	0.617381	-0.991486	0.433525
3	6	0	2.110312	-1.271135	0.375021
4	6	0	2.775158	-0.376749	-0.667860
5	6	0	2.266663	1.031887	-0.606858
6	6	0	1.199480	1.400479	0.106162
7	6	0	0.354549	0.437575	0.887345
8	8	0	-1.010393	0.787741	0.785660
9	1	0	0.091120	-1.696020	1.092748
10	1	0	0.181953	-1.093347	-0.575249
11	1	0	2.304631	-2.327569	0.156445
12	1	0	2.549668	-1.069223	1.363651
13	1	0	2.595703	-0.779139	-1.678379
14	1	0	3.866757	-0.384436	-0.543340
15	1	0	2.808333	1.782910	-1.182241
16	1	0	0.876695	2.441054	0.138788
17	1	0	0.598551	0.527501	1.962572
18	1	0	-1.193338	0.842292	-0.821222
19	1	0	-2.908080	-0.783967	-1.332248

Zero-point correction= 0.152485 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.11836
Sum of electronic and zero-point Energies= -1950.208876

1,2-IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-2.140499	-0.179228	-0.016618
2	6	0	0.423973	-0.859115	-0.173856
3	6	0	1.753307	-1.459153	0.251635
4	6	0	2.914895	-0.619360	-0.271080
5	6	0	2.683114	0.846562	-0.065079
6	6	0	1.496491	1.364981	0.259503
7	6	0	0.265372	0.538510	0.402847
8	8	0	-0.861902	1.210709	-0.229420
9	1	0	-0.448537	-1.452459	0.139973
10	1	0	0.381935	-0.789806	-1.273221
11	1	0	1.835301	-2.494201	-0.097485
12	1	0	1.798214	-1.495124	1.350214
13	1	0	3.068832	-0.809285	-1.346080
14	1	0	3.855534	-0.915805	0.212013
15	1	0	3.539060	1.511764	-0.177126
16	1	0	1.385447	2.435515	0.432159
17	1	0	-0.044900	0.480877	1.457203
18	1	0	-0.596674	1.472171	-1.122590
19	1	0	-3.027445	-1.306254	0.318396

Zero-point correction=0.158791 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.124799
Sum of electronic and zero-point Energies= -1950.247657

12:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.228832	-1.215920	-0.211467
2	6	0	1.214615	-1.135475	0.265521
3	6	0	1.873187	0.147993	-0.233714
4	6	0	0.971025	1.335749	-0.074636
5	6	0	-0.326869	1.235446	0.218746
6	6	0	-1.048538	-0.073736	0.372531
7	8	0	-2.346521	-0.010171	-0.190172
8	1	0	-0.695809	-2.174447	0.043899
9	1	0	-0.255142	-1.128187	-1.310935
10	1	0	1.786455	-2.012950	-0.059868
11	1	0	1.228394	-1.143216	1.366137
12	1	0	2.146726	0.042215	-1.296825
13	1	0	2.821219	0.327575	0.292321
14	1	0	1.416299	2.322791	-0.205169
15	1	0	-0.941157	2.127601	0.345180
16	1	0	-1.223517	-0.269684	1.443459
17	1	0	-2.238823	0.225333	-1.118706

Zero-point correction= 0.150599 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.120465
Sum of electronic and zero-point Energies= -309.493067

Part II: Ph_3P-CuH system

S3: The summarize energies of species in the Ph_3P-CuH/1/H_2 system at the M06/6-31G(d, p) level.

spices	M06(PCM)/6−31G(d,p)			
	SCF_{PCM}	*Gc*	G_{solv}	$\square G_{solv}$
H_2	-1.1693618	-0.001386	-1.1707478	
1	-308.4568858	0.097155	-308.3634875	
Ph_3P-CuH	-2676.515427	0.231149	-2676.284278	
Ph_3P-CuH + H_2 +**1**			-2985.814756	0.0
1,4-COM1	-2985.039832	0.355266	-2984.684566	
1,4-COM1 + H_2			-2985.855314	-106.5
1,4-TS1	-2985.018102	0.352548	-2984.665554	
1,4- TS1 + H_2			-2985.836301	-56.6
1,4-IM1	-2985.045593	0.356358	-2984.689235	
1,4-IM1 + H_2			-2985.859983	-118.7
14−COM2- H_2	-2986.222689	0.373133	-2985.849556	-91.4
1,4-TS2- H_2	-2986.206638	0.371449	-2985.835189	-53.6
14−COM3- H_2	-2986.228344	0.376346	-2985.851998	-97.8
14pro	-309.6599427	0.11972	-309.5402227	
14pro+Ph3P-CuH			-2985.8245	-25.6
1,2-COM1	-2985.013468	0.350478	-2984.66299	
1,2-COM1 + H_2			-2985.833738	-49.8
1,2-TS1	-2985.002988	0.351273	-2984.651715	
1,2-TS1 + H_2			-2985.822462	-20.2
1,2-IM1	-2985.032298	0.357667	-2984.674631	
1,2-IM1 + H_2			-2985.845379	-80.4
12−COM2- H_2	-2986.205298	0.372793	-2985.832505	-46.6
1,2-TS2- H_2	-2986.170322	0.373084	-2985.797238	46.0
12−COM3- H_2	-2986.203597	0.37412	-2985.829477	-38.6
12pro	-309.6529324	0.120464	-309.5324684	
12pro+Ph3P-CuH			-2985.816746	-5.2

S4. Cartesian coordinates and energies of all optimized structures along 1,4−path over the Ph_3P-CuH system at the M06/6-31G(d, p) level.

Ph_3P-CuH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000172	-0.791447	2.413193
2	15	0	-0.000007	-0.019321	0.437002
3	1	0	0.000261	-1.587226	3.704562
4	6	0	0.000109	1.762635	0.075923
5	6	0	-1.206500	2.463803	0.005663
6	6	0	1.206813	2.463597	0.005290
7	6	0	-1.204164	3.844941	-0.150916
8	1	0	-2.150950	1.924952	0.071188
9	6	0	1.204660	3.844737	-0.151282
10	1	0	2.151197	1.924594	0.070515
11	6	0	0.000295	4.537502	-0.231172
12	1	0	-2.147486	4.383055	-0.210007
13	1	0	2.148053	4.382694	-0.210669
14	1	0	0.000370	5.617969	-0.353698
15	6	0	1.470254	-0.690994	-0.399126
16	6	0	1.806752	-0.504317	-1.742370
17	6	0	2.297578	-1.460480	0.422292
18	6	0	2.953695	-1.097604	-2.254743
19	1	0	1.180792	0.115317	-2.383625
20	6	0	3.446169	-2.051682	-0.090506
21	1	0	2.001488	-1.572130	1.467666
22	6	0	3.769656	-1.872365	-1.430784
23	1	0	3.217010	-0.955142	-3.300330
24	1	0	4.084334	-2.650386	0.554581
25	1	0	4.666191	-2.333408	-1.839179
26	6	0	-1.470483	-0.690755	-0.398920
27	6	0	-2.297322	-1.460880	0.422388
28	6	0	-1.807586	-0.503331	-1.741909
29	6	0	-3.445985	-2.052038	-0.090292
30	1	0	-2.000824	-1.573002	1.467595
31	6	0	-2.954615	-1.096557	-2.254162
32	1	0	-1.182064	0.116907	-2.383010
33	6	0	-3.770060	-1.871997	-1.430332
34	1	0	-4.083783	-2.651225	0.554711
35	1	0	-3.218408	-0.953501	-3.299548
36	1	0	-4.666670	-2.332980	-1.838632

Zero-point correction= 0.280278 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.231149
Sum of electronic and zero-point Energies= -2676.224158
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2676.515427 (a.u.)

1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.324395	-1.227955	0.278335
2	6	0	-1.059767	-1.154270	-0.352372
3	6	0	-1.806793	0.082205	0.132685
4	6	0	-0.964008	1.313559	0.028108
5	6	0	0.373475	1.283594	-0.056211
6	6	0	1.136929	0.023330	0.017284
7	8	0	2.349934	0.001514	-0.080538
8	1	0	0.905463	-2.090345	-0.064306
9	1	0	0.227535	-1.323367	1.372316
10	1	0	-1.634415	-2.062152	-0.134701
11	1	0	-0.956742	-1.099776	-1.445578
12	1	0	-2.113214	-0.047829	1.184760

13	1	0	-2.741081	0.221649	-0.426530
14	1	0	-1.478034	2.275383	0.023629
15	1	0	0.965625	2.191549	-0.152261

Zero-point correction= 0.127051 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.097155
Sum of electronic and zero-point Energies= -308.321814
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -308.4568858 (a.u.)

H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.370365
2	1	0	0.000000	0.000000	-0.370365

Zero-point correction= 0.010096 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= -0.001386
Sum of electronic and zero-point Energies= -1.159205
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -1.1693618 (a.u.)

SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.000001	-0.000031	-0.000020
2	1	0	1.246582	-0.454195	-0.663438
3	1	0	0.096533	-0.251268	1.458638
4	1	0	-1.155911	-0.745908	-0.554777
5	1	0	-0.187184	1.451810	-0.240137

Zero-point correction= 0.031841 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.010285
Sum of electronic and zero-point Energies= -291.816037
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -291.8480121 (a.u.)

1,4-COM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.630564	-0.220060	0.416485
2	6	0	-3.487446	-1.432454	-0.493722
3	6	0	-3.679072	-1.049736	-1.955461
4	6	0	-2.737884	0.054273	-2.353166
5	6	0	-2.341353	1.024074	-1.396856
6	6	0	-2.827976	0.990933	-0.015171
7	8	0	-2.630507	1.911667	0.769447
8	1	0	-3.354779	-0.442186	1.455680
9	1	0	-4.680873	0.111177	0.439883
10	1	0	-4.202471	-2.210512	-0.200033
11	1	0	-2.487480	-1.878807	-0.365146
12	1	0	-4.715910	-0.702561	-2.107477
13	1	0	-3.537022	-1.919588	-2.607121
14	1	0	-0.588738	-1.525731	-2.605152
15	1	0	-1.994965	2.004027	-1.731297
16	1	0	-2.735412	0.337182	-3.405787
17	29	0	-0.933601	-0.311501	-1.734463
18	15	0	0.621026	-0.037284	-0.164600
19	6	0	1.338701	1.633414	0.000067
20	6	0	2.069264	-1.134221	-0.306524
21	6	0	-0.097220	-0.497002	1.448952
22	6	0	-0.355560	0.408742	2.476942
23	6	0	-0.991809	-0.018926	3.639294

24	6	0	-1.372980	-1.348241	3.783416
25	6	0	-1.117105	-2.258712	2.759789
26	6	0	-0.485332	-1.836236	1.597800
27	6	0	0.475926	2.722521	0.190844
28	6	0	2.710765	1.862592	-0.140254
29	6	0	3.215139	3.157854	-0.079749
30	6	0	2.358681	4.233168	0.127252
31	6	0	0.991431	4.011183	0.265473
32	6	0	2.867628	-1.448719	0.798421
33	6	0	4.008278	-2.224786	0.635946
34	6	0	4.363988	-2.683021	-0.631190
35	6	0	3.575540	-2.370765	-1.733276
36	6	0	2.427700	-1.600520	-1.571776
37	1	0	-0.064521	1.451571	2.373721
38	1	0	-1.190453	0.695751	4.434164
39	1	0	-1.870554	-1.676965	4.692894
40	1	0	-1.409695	-3.300593	2.867857
41	1	0	-0.279075	-2.551085	0.799709
42	1	0	-0.600375	2.570059	0.294583
43	1	0	3.390760	1.028362	-0.301515
44	1	0	4.283932	3.323855	-0.194475
45	1	0	2.755587	5.244615	0.177376
46	1	0	0.314892	4.847503	0.425374
47	1	0	2.589267	-1.083440	1.786746
48	1	0	4.622810	-2.472856	1.498363
49	1	0	5.257473	-3.290603	-0.756334
50	1	0	3.848333	-2.734548	-2.721063
51	1	0	1.779918	-1.377295	-2.419325

Zero-point correction= 0.410209 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.355266
Sum of electronic and zero-point Energies= -2984.614848
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2985.039832 (a.u.)

1,4-TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.052415	0.068246	0.625096
2	6	0	-3.733745	-1.372052	0.247758
3	6	0	-3.892857	-1.580742	-1.250694
4	6	0	-2.944129	-0.677749	-2.005734
5	6	0	-2.831153	0.698194	-1.517484
6	6	0	-3.432617	1.129901	-0.276436
7	8	0	-3.475707	2.308100	0.079829
8	1	0	-3.759080	0.301473	1.656211
9	1	0	-5.139342	0.235760	0.579640
10	1	0	-4.373113	-2.065158	0.808802
11	1	0	-2.696928	-1.623997	0.531694
12	1	0	-4.920365	-1.315657	-1.547998
13	1	0	-3.732433	-2.631118	-1.524485
14	1	0	-1.658303	-1.646083	-1.908345
15	1	0	-2.647576	1.496598	-2.237506
16	1	0	-2.992320	-0.771602	-3.091750
17	29	0	-1.172464	-0.327692	-1.233590
18	15	0	0.654300	-0.012034	-0.139113
19	6	0	0.870853	1.633591	0.608140
20	6	0	2.216053	-0.291744	-1.041401
21	6	0	0.685830	-1.198480	1.247408
22	6	0	1.342469	-0.958558	2.456294
23	6	0	1.363435	-1.940154	3.440906
24	6	0	0.735917	-3.164291	3.223873
25	6	0	0.078113	-3.408226	2.022089
26	6	0	0.050881	-2.426816	1.038538
27	6	0	-0.267989	2.428257	0.753326
28	6	0	2.109641	2.103934	1.059568
29	6	0	2.198372	3.350457	1.666974

30	6	0	1.055216	4.133664	1.822657
31	6	0	-0.174475	3.674759	1.364229
32	6	0	3.072608	-1.357396	-0.765484
33	6	0	4.225904	-1.538061	-1.524809
34	6	0	4.528240	-0.659449	-2.558606
35	6	0	3.675644	0.406623	-2.837541
36	6	0	2.523975	0.589286	-2.084375
37	1	0	1.824849	0.001822	2.631704
38	1	0	1.869921	-1.748307	4.384015
39	1	0	0.755256	-3.928002	3.997945
40	1	0	-0.418613	-4.360586	1.852621
41	1	0	-0.470649	-2.582692	0.092342
42	1	0	-1.227687	2.088614	0.366434
43	1	0	3.005787	1.498469	0.922255
44	1	0	3.161627	3.716650	2.015178
45	1	0	1.130589	5.110771	2.294987
46	1	0	-1.071866	4.280334	1.464633
47	1	0	2.840622	-2.047998	0.043656
48	1	0	4.890812	-2.369876	-1.304013
49	1	0	5.429584	-0.803707	-3.149625
50	1	0	3.909787	1.096593	-3.644805
51	1	0	1.859421	1.427322	-2.297176

Zero-point correction= 0.409651 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.352548
Sum of electronic and zero-point Energies= -2984.593091
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2985.018102 (a.u.)

1,4-IM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.141484	-1.025138	1.280517
2	6	0	4.798535	0.342108	1.408921
3	6	0	5.320534	0.797461	0.053595
4	6	0	4.166590	1.012029	-0.920092
5	6	0	3.173266	-0.130425	-0.895595
6	6	0	3.205401	-1.137935	0.101473
7	8	0	2.370478	-2.120492	0.092243
8	1	0	3.588053	-1.310421	2.184754
9	1	0	4.908509	-1.802649	1.138771
10	1	0	5.602988	0.307747	2.154549
11	1	0	4.062824	1.076046	1.777679
12	1	0	5.996124	0.022472	-0.342354
13	1	0	5.913777	1.716285	0.147985
14	1	0	3.676202	1.968541	-0.674668
15	1	0	2.808960	-0.476331	-1.869573
16	1	0	4.563761	1.139440	-1.936963
17	29	0	1.349955	-0.324486	-0.036344
18	15	0	-0.729028	0.051918	0.030301
19	6	0	-1.184329	1.744003	-0.476967
20	6	0	-2.456985	2.298329	-0.309786
21	6	0	-0.182416	2.492751	-1.097455
22	6	0	-2.723203	3.579850	-0.777758
23	1	0	-3.234429	1.735017	0.206266
24	6	0	-0.451502	3.772288	-1.569856
25	1	0	0.808811	2.041658	-1.178397
26	6	0	-1.723087	4.313713	-1.412340
27	1	0	-3.712690	4.011266	-0.643872
28	1	0	0.333849	4.349112	-2.052384
29	1	0	-1.935499	5.316787	-1.775417
30	6	0	-1.656940	-0.222303	1.575824
31	6	0	-2.359206	-1.406289	1.806979
32	6	0	-1.574936	0.738942	2.588708
33	6	0	-2.983835	-1.618201	3.032217
34	1	0	-2.418526	-2.164215	1.027624
35	6	0	-2.203460	0.525239	3.808588

36	1	0	-1.020911	1.661195	2.413650
37	6	0	-2.909832	-0.654379	4.031637
38	1	0	-3.531093	-2.541991	3.205109
39	1	0	-2.139434	1.279502	4.589471
40	1	0	-3.399646	-0.822211	4.988033
41	6	0	-1.482429	-1.077043	-1.187526
42	6	0	-0.704357	-2.177658	-1.559082
43	6	0	-2.766523	-0.920088	-1.714520
44	6	0	-1.214984	-3.119919	-2.445971
45	1	0	0.300993	-2.277863	-1.143430
46	6	0	-3.268869	-1.860592	-2.604709
47	1	0	-3.371184	-0.058012	-1.435666
48	6	0	-2.494149	-2.961375	-2.967591
49	1	0	-0.608373	-3.975889	-2.731481
50	1	0	-4.267006	-1.736708	-3.018745
51	1	0	-2.891746	-3.695745	-3.664684

Zero-point correction= 0.41442 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=0.356358
Sum of electronic and zero-point Energies= -2984.618988
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) =-2985.045593 (a.u.)

1,4-COM2−H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.057270	-0.623322	0.870425
2	6	0	4.846034	0.675629	0.970676
3	6	0	5.344424	1.097695	-0.404207
4	6	0	4.165024	1.422457	-1.313637
5	6	0	3.119854	0.324191	-1.302432
6	6	0	3.122592	-0.700628	-0.314379
7	8	0	2.297762	-1.678754	-0.354306
8	1	0	3.477432	-0.829032	1.781802
9	1	0	4.741433	-1.478280	0.755414
10	1	0	5.676863	0.557424	1.677918
11	1	0	4.203129	1.472827	1.376622
12	1	0	5.931634	0.274145	-0.841168
13	1	0	6.016789	1.962044	-0.327689
14	1	0	3.738911	2.387162	-0.996619
15	1	0	2.769336	-0.018426	-2.282862
16	1	0	4.521806	1.582741	-2.340140
17	29	0	1.303456	0.262789	-0.473145
18	15	0	-0.781961	0.119430	-0.043813
19	6	0	-1.554056	-1.052523	-1.205076
20	6	0	-2.935394	-1.216655	-1.342467
21	6	0	-0.677775	-1.881567	-1.910443
22	6	0	-3.433748	-2.188144	-2.201151
23	1	0	-3.621893	-0.582951	-0.781606
24	6	0	-1.183458	-2.859422	-2.760988
25	1	0	0.397370	-1.766566	-1.757748
26	6	0	-2.557672	-3.007627	-2.911112
27	1	0	-4.508393	-2.312098	-2.314026
28	1	0	-0.499926	-3.505269	-3.306663
29	1	0	-2.952406	-3.768099	-3.581262
30	6	0	-1.752188	1.657056	-0.106215
31	6	0	-1.709503	2.534888	0.982763
32	6	0	-2.397336	2.055180	-1.279673
33	6	0	-2.329600	3.775805	0.907159
34	1	0	-1.188146	2.239799	1.892781
35	6	0	-3.013555	3.299851	-1.352605
36	1	0	-2.415980	1.389945	-2.141316
37	6	0	-2.985533	4.159371	-0.259328
38	1	0	-2.297810	4.447907	1.761551
39	1	0	-3.517217	3.598897	-2.268925
40	1	0	-3.469099	5.131656	-0.317871
41	6	0	-1.099709	-0.622685	1.595122

42	6	0	-0.136591	-1.519214	2.070933
43	6	0	-2.267650	-0.406169	2.330545
44	6	0	-0.341412	-2.181762	3.276079
45	1	0	0.769737	-1.705270	1.487402
46	6	0	-2.461636	-1.064633	3.539806
47	1	0	-3.023663	0.286398	1.962672
48	6	0	-1.498619	-1.951132	4.013375
49	1	0	0.409066	-2.878738	3.641601
50	1	0	-3.369088	-0.886579	4.112475
51	1	0	-1.652383	-2.464098	4.960202
52	1	0	1.690263	1.199293	1.483528
53	1	0	1.800751	1.323023	2.217764

Zero-point correction= 0.431359 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.373133
Sum of electronic and zero-point Energies=-2985.780216
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2986.222689 (a.u.)

1,4-COM2−SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.249123	0.429088	-0.918498
2	6	0	-4.998226	0.382627	0.406634
3	6	0	-5.205932	-1.063161	0.834775
4	6	0	-3.864681	-1.732247	1.113688
5	6	0	-2.851835	-1.475529	0.017028
6	6	0	-3.056876	-0.498958	-0.985438
7	8	0	-2.212347	-0.314602	-1.943294
8	1	0	-3.918743	1.445454	-1.180621
9	1	0	-4.915735	0.121138	-1.739179
10	1	0	-5.954473	0.914611	0.320380
11	1	0	-4.417788	0.907639	1.183405
12	1	0	-5.724888	-1.600011	0.024637
13	1	0	-5.853108	-1.121151	1.719665
14	1	0	-3.494189	-1.376923	2.088343
15	1	0	-2.246693	-2.333247	-0.289530
16	1	0	-4.012371	-2.814396	1.235642
17	29	0	-1.271068	-0.157499	-0.059855
18	15	0	0.869783	-0.145957	0.073476
19	6	0	1.620351	-1.249424	-1.165637
20	6	0	3.005046	-1.417458	-1.280081
21	6	0	0.764791	-1.873620	-2.076060
22	6	0	3.525606	-2.233414	-2.275407
23	1	0	3.674058	-0.900933	-0.591398
24	6	0	1.293579	-2.684045	-3.077342
25	1	0	-0.309302	-1.686206	-2.013351
26	6	0	2.667719	-2.870026	-3.171642
27	1	0	4.601586	-2.366819	-2.361377
28	1	0	0.626042	-3.164481	-3.788557
29	1	0	3.077756	-3.505643	-3.953463
30	6	0	1.548946	-0.615625	1.698908
31	6	0	1.213192	0.196528	2.790191
32	6	0	2.276535	-1.785085	1.921549
33	6	0	1.622944	-0.140405	4.072648
34	1	0	0.625853	1.101424	2.627186
35	6	0	2.676568	-2.126814	3.210959
36	1	0	2.526944	-2.435674	1.086086
37	6	0	2.356650	-1.305696	4.285312
38	1	0	1.361547	0.501257	4.910846
39	1	0	3.240474	-3.042431	3.373776
40	1	0	2.671119	-1.575029	5.290835
41	6	0	1.646845	1.463684	-0.324448
42	6	0	1.226762	2.066213	-1.516705
43	6	0	2.597580	2.104986	0.469376
44	6	0	1.741369	3.298212	-1.899272
45	1	0	0.481785	1.567564	-2.140715

46	6	0	3.107216	3.342706	0.085107
47	1	0	2.939467	1.640995	1.393184
48	6	0	2.678724	3.941595	-1.094036
49	1	0	1.406585	3.759447	-2.825489
50	1	0	3.844390	3.839579	0.711901
51	1	0	3.076026	4.910116	-1.388858
52	1	0	-1.740904	1.417243	0.735288
53	14	0	-1.769204	2.868947	0.314707
54	1	0	-0.556668	3.517649	0.872491
55	1	0	-2.992987	3.470025	0.901543
56	1	0	-1.796427	2.992387	-1.158218

Zero-point correction= 0.448070 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.386091
Sum of electronic and zero-point Energies= -3276.451325
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -3276.911608 (a.u.)

1,4-TS2−H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.247243	-1.613217	-0.241601
2	6	0	3.500128	-0.701685	0.951422
3	6	0	4.247728	0.549432	0.511947
4	6	0	3.381711	1.355752	-0.447546
5	6	0	2.842201	0.507029	-1.584270
6	6	0	2.863596	-0.889873	-1.504425
7	8	0	2.539776	-1.659026	-2.508981
8	1	0	2.470990	-2.362410	-0.028289
9	1	0	4.152160	-2.189153	-0.490901
10	1	0	4.047169	-1.245505	1.732348
11	1	0	2.539747	-0.400979	1.398726
12	1	0	5.181750	0.257991	0.005760
13	1	0	4.530083	1.160508	1.379067
14	1	0	2.566739	1.821046	0.134805
15	1	0	2.948132	0.917848	-2.589646
16	1	0	3.957901	2.192428	-0.865011
17	29	0	0.844517	-0.030382	-1.660024
18	15	0	-0.699337	-0.018397	-0.160581
19	6	0	-1.176661	1.730109	0.057428
20	6	0	-2.334319	2.159465	0.709215
21	6	0	-0.284286	2.671865	-0.460809
22	6	0	-2.585036	3.519488	0.849146
23	1	0	-3.042577	1.429861	1.100757
24	6	0	-0.533386	4.031778	-0.316794
25	1	0	0.601720	2.300359	-0.979380
26	6	0	-1.684543	4.453681	0.340278
27	1	0	-3.487372	3.854732	1.355399
28	1	0	0.166216	4.758728	-0.722009
29	1	0	-1.886420	5.516500	0.452882
30	6	0	-0.197286	-0.565338	1.508683
31	6	0	0.030675	-1.931508	1.712758
32	6	0	0.081011	0.335450	2.538028
33	6	0	0.520911	-2.386934	2.929522
34	1	0	-0.175401	-2.639825	0.909257
35	6	0	0.573401	-0.124623	3.756550
36	1	0	-0.081183	1.401399	2.384626
37	6	0	0.793972	-1.483013	3.954354
38	1	0	0.693247	-3.450290	3.079257
39	1	0	0.785553	0.584334	4.553593
40	1	0	1.180534	-1.840269	4.905973
41	6	0	-2.255278	-0.922538	-0.462804
42	6	0	-2.566994	-1.223360	-1.790572
43	6	0	-3.144922	-1.288069	0.552761
44	6	0	-3.759466	-1.866753	-2.103473
45	1	0	-1.849635	-0.963769	-2.569864

46	6	0	-4.333654	-1.936275	0.238787
47	1	0	-2.896197	-1.080075	1.593186
48	6	0	-4.642769	-2.221746	-1.088981
49	1	0	-3.993164	-2.100739	-3.139328
50	1	0	-5.020121	-2.223429	1.032086
51	1	0	-5.572109	-2.732226	-1.331468
52	1	0	0.778521	-0.462391	-3.280994
53	1	0	1.580688	-1.030127	-3.057186

Zero-point correction= 0.428437 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.371449
Sum of electronic and zero-point Energies=-2985.766534
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2986.206638 (a.u.)

1,4-TS2−SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.340884	3.094334	-0.290165
2	1	0	-1.159713	4.005815	0.066856
3	1	0	-3.416085	4.101238	-0.075092
4	1	0	-1.880054	2.787789	-1.684394
5	6	0	-4.021273	-0.105364	0.972331
6	6	0	-3.546147	-1.541487	1.139741
7	6	0	-3.673274	-2.275861	-0.187511
8	6	0	-2.754239	-1.664226	-1.240024
9	6	0	-2.760513	-0.146499	-1.206305
10	6	0	-3.506531	0.568167	-0.273273
11	8	0	-3.798095	1.832801	-0.382444
12	1	0	-3.746812	0.528789	1.828103
13	1	0	-5.120028	-0.061016	0.916766
14	1	0	-4.120602	-2.044128	1.927744
15	1	0	-2.493172	-1.554745	1.471519
16	1	0	-4.717461	-2.195898	-0.528078
17	1	0	-3.460461	-3.346376	-0.074032
18	1	0	-1.733409	-2.061610	-1.115441
19	1	0	-2.630128	0.362994	-2.166328
20	1	0	-3.070276	-1.996649	-2.239160
21	1	0	-1.736379	2.032927	0.731404
22	29	0	-1.215775	0.666094	-0.163926
23	15	0	0.837592	-0.007581	-0.010652
24	6	0	2.067560	1.328788	-0.132115
25	6	0	1.590106	2.636436	-0.026886
26	6	0	3.436121	1.101208	-0.305483
27	6	0	2.472053	3.710588	-0.088909
28	1	0	0.521081	2.815418	0.098731
29	6	0	4.313874	2.175624	-0.369184
30	1	0	3.813147	0.083384	-0.399839
31	6	0	3.831976	3.479695	-0.260384
32	1	0	2.084975	4.723769	-0.010141
33	1	0	5.377995	1.998338	-0.507680
34	1	0	4.523466	4.317496	-0.315117
35	6	0	1.372880	-1.247467	-1.237088
36	6	0	2.360167	-2.204579	-0.984918
37	6	0	0.785665	-1.187639	-2.504028
38	6	0	2.755752	-3.082549	-1.988028
39	1	0	2.810479	-2.272833	0.005011
40	6	0	1.185838	-2.062385	-3.507608
41	1	0	-0.003854	-0.458265	-2.690794
42	6	0	2.171593	-3.009858	-3.249663
43	1	0	3.521441	-3.827530	-1.784213
44	1	0	0.722028	-2.008743	-4.489558
45	1	0	2.481095	-3.699095	-4.031849
46	6	0	1.130409	-0.802853	1.603978
47	6	0	0.551726	-2.054451	1.849640
48	6	0	1.805012	-0.145785	2.634006
49	6	0	0.664993	-2.644275	3.101666

50	1	0	0.018827	-2.571960	1.050838
51	6	0	1.910363	-0.737944	3.889319
52	1	0	2.249961	0.831868	2.455462
53	6	0	1.343884	-1.985749	4.124281
54	1	0	0.219290	-3.619866	3.281527
55	1	0	2.438871	-0.220051	4.686227
56	1	0	1.428540	-2.446377	5.105702

Zero-point correction= 0.449181 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.389221
Sum of electronic and zero-point Energies= -3276.437405
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -3276.899351 (a.u.)

1,4-COM3−H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.949508	-0.637001	0.829495
2	6	0	3.400531	0.812567	0.739906
3	6	0	4.453624	0.953338	-0.351289
4	6	0	3.897046	0.601274	-1.729255
5	6	0	3.002153	-0.626281	-1.704172
6	6	0	2.518278	-1.153385	-0.507128
7	8	0	2.066825	-2.460603	-0.430047
8	1	0	2.155306	-0.775135	1.572259
9	1	0	3.793119	-1.264789	1.163472
10	1	0	3.792806	1.143245	1.709432
11	1	0	2.535223	1.462435	0.516823
12	1	0	5.284924	0.272718	-0.109914
13	1	0	4.874027	1.966609	-0.367161
14	1	0	3.358895	1.466771	-2.145241
15	1	0	3.051981	-1.282246	-2.575823
16	1	0	4.727137	0.416567	-2.424150
17	29	0	1.115422	-0.081409	-1.487634
18	15	0	-0.596974	0.069005	-0.096532
19	6	0	-1.245328	1.773998	-0.008467
20	6	0	-2.365527	2.128022	0.749611
21	6	0	-0.580365	2.752095	-0.750028
22	6	0	-2.805651	3.445222	0.770852
23	1	0	-2.889889	1.370165	1.330769
24	6	0	-1.020099	4.071909	-0.726019
25	1	0	0.266123	2.452088	-1.369753
26	6	0	-2.131407	4.417763	0.034336
27	1	0	-3.677875	3.716370	1.361504
28	1	0	-0.496970	4.827532	-1.307183
29	1	0	-2.479156	5.448294	0.051770
30	6	0	-0.399742	-0.436034	1.643880
31	6	0	-0.295701	-1.803896	1.925284
32	6	0	-0.151170	0.487633	2.662676
33	6	0	0.023227	-2.236718	3.205578
34	1	0	-0.446721	-2.529807	1.127693
35	6	0	0.174325	0.050446	3.943547
36	1	0	-0.209149	1.554819	2.453566
37	6	0	0.258495	-1.310196	4.218922
38	1	0	0.098315	-3.301889	3.411871
39	1	0	0.361483	0.779021	4.729364
40	1	0	0.512790	-1.649349	5.220472
41	6	0	-1.974571	-0.971167	-0.697816
42	6	0	-1.972999	-1.295012	-2.057593
43	6	0	-3.021120	-1.416126	0.116086
44	6	0	-3.006732	-2.053233	-2.597230
45	1	0	-1.144268	-0.938582	-2.672145
46	6	0	-4.051286	-2.174346	-0.426567
47	1	0	-3.018337	-1.186339	1.180857
48	6	0	-4.046112	-2.491009	-1.783282
49	1	0	-2.997550	-2.303689	-3.655485
50	1	0	-4.861988	-2.520822	0.210634

51	1	0	-4.854446	-3.085049	-2.204137
52	1	0	0.625011	0.467834	-2.868697
53	1	0	2.055739	-2.835343	-1.319013

Zero-point correction= 0.433436 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.376346
Sum of electronic and zero-point Energies=-2985.77909
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2986.228344 (a.u.)

1,4-COM3−SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.479697	2.764208	-0.216909
2	1	0	3.911151	2.630201	-1.626799
3	1	0	4.395622	3.679592	0.505291
4	1	0	2.100167	3.312717	-0.151243
5	6	0	4.065607	-0.546570	-0.836731
6	6	0	3.596913	-1.947969	-1.204014
7	6	0	3.256204	-2.730386	0.056744
8	6	0	2.077859	-2.098606	0.791756
9	6	0	2.235218	-0.594847	0.931919
10	6	0	3.134006	0.119264	0.136064
11	8	0	3.596277	1.330004	0.625857
12	1	0	4.192608	0.078125	-1.729972
13	1	0	5.050623	-0.603429	-0.342675
14	1	0	4.374124	-2.458303	-1.785877
15	1	0	2.709199	-1.887772	-1.856703
16	1	0	4.137495	-2.732855	0.716904
17	1	0	3.034037	-3.779083	-0.178176
18	1	0	1.145531	-2.365569	0.263086
19	1	0	1.970941	-0.139972	1.887949
20	1	0	1.971532	-2.540056	1.792639
21	1	0	1.472507	1.055013	-1.904542
22	29	0	1.278310	0.334253	-0.541842
23	15	0	-0.875208	0.063201	-0.050495
24	6	0	-1.705007	1.655884	0.267984
25	6	0	-1.163877	2.774655	-0.373510
26	6	0	-2.842816	1.801435	1.066940
27	6	0	-1.759127	4.022306	-0.223590
28	1	0	-0.268715	2.647366	-0.984781
29	6	0	-3.433457	3.050891	1.215845
30	1	0	-3.257055	0.938907	1.587982
31	6	0	-2.893840	4.160239	0.569277
32	1	0	-1.331195	4.888445	-0.722794
33	1	0	-4.317263	3.160332	1.840286
34	1	0	-3.357588	5.136793	0.689907
35	6	0	-1.243804	-0.965226	1.409085
36	6	0	-1.643839	-2.298766	1.295905
37	6	0	-0.930829	-0.455713	2.676079
38	6	0	-1.739979	-3.103048	2.428273
39	1	0	-1.878063	-2.713550	0.316766
40	6	0	-1.034343	-1.257944	3.804695
41	1	0	-0.601130	0.579017	2.774292
42	6	0	-1.437721	-2.586016	3.682757
43	1	0	-2.053385	-4.139698	2.327100
44	1	0	-0.794963	-0.847530	4.783075
45	1	0	-1.512671	-3.216002	4.565956
46	6	0	-1.804844	-0.713927	-1.415586
47	6	0	-1.082449	-1.074106	-2.554783
48	6	0	-3.183673	-0.943394	-1.371462
49	6	0	-1.726730	-1.674854	-3.632476
50	1	0	-0.016683	-0.842503	-2.590933
51	6	0	-3.825726	-1.538921	-2.449077
52	1	0	-3.754660	-0.658965	-0.487985
53	6	0	-3.095913	-1.907654	-3.578495
54	1	0	-1.157907	-1.952232	-4.516741

55	1	0	-4.898307	-1.715340	-2.411990
56	1	0	-3.601809	-2.374296	-4.420879

Zero-point correction= 0.448577 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.387074
Sum of electronic and zero-point Energies= -3276.465951
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -3276.925719 (a.u.)

14–Pro–H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.416420	1.241752	0.069806
2	6	0	1.059483	1.233468	-0.312449
3	6	0	1.774870	0.073135	0.365815
4	6	0	1.200394	-1.257226	-0.109062
5	6	0	-0.298968	-1.250627	-0.102079
6	6	0	-1.016420	-0.128886	0.000102
7	1	0	-0.978454	1.916475	-0.597014
8	1	0	-0.548373	1.644131	1.088252
9	1	0	1.521925	2.193466	-0.052843
10	1	0	1.149312	1.122128	-1.403467
11	1	0	1.642980	0.159288	1.455366
12	1	0	2.853860	0.116516	0.172255
13	1	0	1.577591	-1.479392	-1.122009
14	1	0	-0.835430	-2.195752	-0.167197
15	1	0	1.574038	-2.073490	0.525130
16	8	0	-2.379252	-0.195887	0.075502
17	1	0	-2.741064	0.694038	0.024713

Zero-point correction= 0.150272 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.11972
Sum of electronic and zero-point Energies= -309.501732
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -309.6599427 (a.u.)

1,4-Pro–SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.784105	0.195742	0.071694
2	1	0	2.953538	1.077263	-1.110611
3	1	0	3.911040	-0.754554	0.159451
4	1	0	2.703871	1.036770	1.291335
5	6	0	-0.855861	-1.398039	0.065676
6	6	0	-2.272553	-0.934650	-0.251038
7	6	0	-2.554509	0.403375	0.418373
8	6	0	-1.618694	1.476488	-0.125973
9	6	0	-0.195517	1.002234	-0.180131
10	6	0	0.138917	-0.288602	-0.069868
11	8	0	1.422589	-0.756595	-0.065593
12	1	0	-0.544313	-2.219315	-0.593862
13	1	0	-0.796110	-1.800845	1.089345
14	1	0	-2.997458	-1.695520	0.062518
15	1	0	-2.384208	-0.821482	-1.340086
16	1	0	-2.398595	0.300771	1.503207
17	1	0	-3.600413	0.701214	0.274184
18	1	0	-1.952631	1.782932	-1.131584
19	1	0	0.580362	1.757493	-0.317411
20	1	0	-1.683963	2.382810	0.492316

Zero-point correction= 0.16664 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.132457
Sum of electronic and zero-point Energies= -600.184762
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -600.3544537 (a.u.)

S5. Cartesian coordinates and energies of all optimized structures along 1,2−path over the Ph_3P-CuH system at the M06/6-31G(d, p) level.

1,2 –COM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.460706	0.211161	0.203815
2	6	0	3.969814	-1.158918	0.664755
3	6	0	4.902436	-0.193863	1.381786
4	6	0	5.867713	0.464880	0.399886
5	6	0	5.170015	0.950051	-0.833814
6	6	0	3.944414	0.541773	-1.190017
7	6	0	3.193376	-0.460084	-0.423347
8	8	0	2.182112	-1.055291	-0.979441
9	1	0	3.275308	-1.653259	1.356017
10	1	0	4.554390	-1.959771	0.180071
11	1	0	5.456669	-0.708794	2.175617
12	1	0	4.291007	0.582160	1.863143
13	1	0	6.660406	-0.244616	0.106280
14	1	0	6.392882	1.300732	0.882466
15	1	0	5.701169	1.659722	-1.467971
16	1	0	3.459766	0.911676	-2.093471
17	15	0	-0.763556	0.031519	0.012575
18	1	0	1.797020	1.263062	1.250218
19	6	0	-1.439512	-1.141524	-1.206785
20	6	0	-0.680037	-1.382114	-2.355757
21	6	0	-2.684050	-1.763187	-1.059114
22	6	0	-1.168766	-2.222984	-3.349949
23	1	0	0.309822	-0.936842	-2.445446
24	6	0	-3.166674	-2.605226	-2.054480
25	1	0	-3.273463	-1.589501	-0.158847
26	6	0	-2.410707	-2.831824	-3.201712
27	1	0	-0.571091	-2.412577	-4.238366
28	1	0	-4.134586	-3.086805	-1.934061
29	1	0	-2.788334	-3.493726	-3.977938
30	6	0	-1.525249	1.632580	-0.410047
31	6	0	-0.838485	2.787519	-0.022383
32	6	0	-2.766049	1.744859	-1.042952
33	6	0	-1.392209	4.041039	-0.260098
34	1	0	0.135732	2.678766	0.456219
35	6	0	-3.313747	2.999868	-1.281961
36	1	0	-3.301175	0.848413	-1.353702
37	6	0	-2.628896	4.147132	-0.888422
38	1	0	-0.852893	4.935855	0.041641
39	1	0	-4.278503	3.084281	-1.777184
40	1	0	-3.060941	5.127617	-1.076479
41	6	0	-1.546630	-0.466888	1.580352
42	6	0	-1.161639	-1.698774	2.122664
43	6	0	-2.465807	0.328517	2.263955
44	6	0	-1.701125	-2.132919	3.325797
45	1	0	-0.438593	-2.319763	1.590988
46	6	0	-2.999666	-0.107619	3.473939
47	1	0	-2.765698	1.290048	1.849594
48	6	0	-2.621349	-1.335845	4.003672
49	1	0	-1.400101	-3.092512	3.739599
50	1	0	-3.715869	0.516763	4.003197
51	1	0	-3.039967	-1.673735	4.948891

Zero-point correction= 0.409445 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.350478
Sum of electronic and zero-point Energies= -2984.591484
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2985.013468 (a.u.)

1,2-TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.231139	0.108822	0.498002
2	6	0	-3.958547	-0.518204	-0.710537
3	6	0	-4.925062	0.622862	-0.980696
4	6	0	-5.947129	0.744887	0.146582
5	6	0	-5.302616	0.657546	1.498249
6	6	0	-4.059564	0.210373	1.691179
7	6	0	-3.206196	-0.332252	0.596115
8	8	0	-2.404066	-1.327566	0.950329
9	1	0	-3.242251	-0.661724	-1.530363
10	1	0	-4.507882	-1.467155	-0.599047
11	1	0	-5.430426	0.486243	-1.944644
12	1	0	-4.355138	1.561429	-1.053694
13	1	0	-6.706469	-0.050121	0.056789
14	1	0	-6.503662	1.688599	0.059263
15	1	0	-5.897789	0.966652	2.358041
16	1	0	-3.623341	0.152468	2.688465
17	15	0	0.843328	0.097241	0.072925
18	1	0	-2.486750	1.015904	0.207509
19	6	0	1.004312	-1.071493	-1.319721
20	6	0	-0.015129	-2.021053	-1.441431
21	6	0	2.087716	-1.094553	-2.200303
22	6	0	0.058851	-2.994500	-2.431794
23	1	0	-0.859720	-1.981330	-0.749376
24	6	0	2.152580	-2.065578	-3.192725
25	1	0	2.876635	-0.348739	-2.112977
26	6	0	1.140975	-3.016953	-3.305614
27	1	0	-0.733373	-3.733766	-2.522482
28	1	0	2.995081	-2.081587	-3.880360
29	1	0	1.197529	-3.776576	-4.082129
30	6	0	1.608731	1.657165	-0.482594
31	6	0	2.992627	1.852114	-0.542085
32	6	0	0.751338	2.683467	-0.882283
33	6	0	3.506715	3.054327	-1.013919
34	1	0	3.666787	1.066746	-0.199832
35	6	0	1.267378	3.884837	-1.356012
36	1	0	-0.324143	2.523862	-0.790470
37	6	0	2.644556	4.068520	-1.424303
38	1	0	4.583188	3.203841	-1.056322
39	1	0	0.593367	4.681339	-1.662248
40	1	0	3.049911	5.009655	-1.789220
41	6	0	1.997149	-0.517006	1.346883
42	6	0	2.236637	0.298172	2.458737
43	6	0	2.583556	-1.781201	1.282341
44	6	0	3.061194	-0.141523	3.485241
45	1	0	1.777662	1.285777	2.513876
46	6	0	3.407658	-2.219653	2.315443
47	1	0	2.395243	-2.424993	0.424993
48	6	0	3.648816	-1.402832	3.413872
49	1	0	3.245848	0.499117	4.344373
50	1	0	3.863099	-3.205640	2.258615
51	1	0	4.292960	-1.748762	4.218914

Zero-point correction= 0.409131 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.351273
Sum of electronic and zero-point Energies= -2984.573856
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2985.002988 (a.u.)

1,2-IM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.706680	-0.073954	-1.708572
2	6	0	-3.453565	-1.288485	-1.081687
3	6	0	-4.415584	-1.022228	0.065859

4	6	0	-3.798459	-0.034634	1.053023
5	6	0	-3.151735	1.118211	0.345479
6	6	0	-2.916846	1.127015	-0.972397
7	6	0	-3.193374	-0.028274	-1.909787
8	8	0	-2.124476	-0.185152	-2.790946
9	1	0	-3.793614	-2.098361	-1.738345
10	1	0	-2.470445	-1.593996	-0.678166
11	1	0	-4.689908	-1.952865	0.578974
12	1	0	-5.349193	-0.598839	-0.336576
13	1	0	-3.048201	-0.548113	1.679393
14	1	0	-4.556703	0.340872	1.755572
15	1	0	-2.865520	1.982680	0.949087
16	1	0	-2.513011	2.020673	-1.454541
17	15	0	0.738978	-0.012148	-0.198852
18	1	0	-4.117108	0.197359	-2.483482
19	6	0	1.269840	1.688601	0.179473
20	6	0	0.549456	2.707259	-0.446919
21	6	0	2.314422	2.014554	1.048170
22	6	0	0.855160	4.040841	-0.200006
23	1	0	-0.249474	2.415812	-1.129314
24	6	0	2.622317	3.346996	1.292271
25	1	0	2.888205	1.225605	1.533355
26	6	0	1.891906	4.358798	0.670522
27	1	0	0.288895	4.828327	-0.691103
28	1	0	3.436686	3.600541	1.967005
29	1	0	2.137586	5.400358	0.865035
30	6	0	0.075247	-0.649353	1.375353
31	6	0	-0.168829	-2.024015	1.473581
32	6	0	-0.300529	0.190762	2.423464
33	6	0	-0.762490	-2.551264	2.612653
34	1	0	0.108683	-2.681479	0.649224
35	6	0	-0.896619	-0.341151	3.564177
36	1	0	-0.128647	1.263371	2.350115
37	6	0	-1.125930	-1.709287	3.661579
38	1	0	-0.944953	-3.620966	2.682332
39	1	0	-1.183874	0.318544	4.379665
40	1	0	-1.591814	-2.121344	4.553641
41	6	0	2.255793	-0.981107	-0.466603
42	6	0	2.607754	-1.251617	-1.790809
43	6	0	3.083757	-1.424605	0.569055
44	6	0	3.778925	-1.942190	-2.081183
45	1	0	1.935284	-0.931730	-2.587220
46	6	0	4.253459	-2.116525	0.278319
47	1	0	2.796993	-1.248935	1.605674
48	6	0	4.603111	-2.370933	-1.045821
49	1	0	4.042045	-2.153568	-3.114700
50	1	0	4.892672	-2.463998	1.086687
51	1	0	5.517145	-2.916072	-1.269982

Zero-point correction= 0.414631 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.357667
Sum of electronic and zero-point Energies= -2984.601517
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2985.032298 (a.u.)

1,2-COM2−H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.721517	0.282254	-1.612972
2	6	0	-3.512411	-1.053265	-1.328766
3	6	0	-4.453130	-1.105579	-0.134701
4	6	0	-3.796728	-0.455975	1.081083
5	6	0	-3.148221	0.847561	0.720909
6	6	0	-2.922960	1.224816	-0.543542
7	6	0	-3.225132	0.383807	-1.764035
8	8	0	-2.159253	0.461062	-2.662253
9	1	0	-3.884618	-1.630849	-2.183500

10	1	0	-2.535938	-1.490014	-1.049700
11	1	0	-4.747009	-2.137694	0.095034
12	1	0	-5.378882	-0.561887	-0.379639
13	1	0	-3.041391	-1.138063	1.510610
14	1	0	-4.532929	-0.293886	1.881717
15	1	0	-2.853171	1.507295	1.540009
16	1	0	-2.520971	2.218001	-0.759001
17	15	0	0.766792	0.011401	-0.169557
18	1	0	-4.142517	0.783312	-2.245951
19	6	0	1.285254	1.595131	0.564588
20	6	0	0.539767	2.713626	0.187934
21	6	0	2.343690	1.740526	1.464716
22	6	0	0.836585	3.966865	0.711596
23	1	0	-0.268960	2.563323	-0.527727
24	6	0	2.643557	2.993659	1.983911
25	1	0	2.935609	0.874047	1.757654
26	6	0	1.888936	4.104685	1.610182
27	1	0	0.250676	4.832812	0.413628
28	1	0	3.469011	3.107536	2.682740
29	1	0	2.128208	5.083350	2.019929
30	6	0	0.147729	-0.973021	1.233175
31	6	0	-0.044621	-2.346094	1.043051
32	6	0	-0.263153	-0.381883	2.428116
33	6	0	-0.622427	-3.118190	2.042128
34	1	0	0.256643	-2.809441	0.103418
35	6	0	-0.846146	-1.157908	3.426527
36	1	0	-0.131089	0.688420	2.578828
37	6	0	-1.024450	-2.524035	3.236569
38	1	0	-0.765390	-4.185006	1.887456
39	1	0	-1.163660	-0.690855	4.355976
40	1	0	-1.481350	-3.127085	4.017644
41	6	0	2.286054	-0.846108	-0.685093
42	6	0	2.598706	-0.817734	-2.046001
43	6	0	3.151684	-1.489252	0.205180
44	6	0	3.765753	-1.411708	-2.513064
45	1	0	1.899519	-0.342757	-2.734683
46	6	0	4.316555	-2.085292	-0.262593
47	1	0	2.898353	-1.544700	1.263534
48	6	0	4.625617	-2.042996	-1.620195
49	1	0	3.998443	-1.389606	-3.574821
50	1	0	4.984274	-2.588967	0.432547
51	1	0	5.536496	-2.513023	-1.983786
52	1	0	-1.767032	3.425111	-3.516845
53	1	0	-1.869226	2.745915	-3.217548

Zero-point correction= 0.431030 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.372793
Sum of electronic and zero-point Energies= -2985.759040
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2986.205298 (a.u.)

1,2-COM2−SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.833346	0.699417	-0.755505
2	6	0	-2.949837	-1.148973	-1.376377
3	6	0	-3.906089	-2.240369	-0.926019
4	6	0	-3.987310	-2.278161	0.598042
5	6	0	-4.070685	-0.900010	1.187740
6	6	0	-3.845229	0.216296	0.488174
7	6	0	-3.438231	0.239906	-0.965382
8	8	0	-2.476678	1.217686	-1.209597
9	1	0	-2.766932	-1.166416	-2.458776
10	1	0	-1.965972	-1.281520	-0.885350
11	1	0	-3.606980	-3.220074	-1.319208
12	1	0	-4.904438	-2.028538	-1.338509
13	1	0	-3.098381	-2.793832	1.004836

14	1	0	-4.847338	-2.879775	0.925271
15	1	0	-4.328560	-0.827196	2.246225
16	1	0	-3.930687	1.193996	0.965435
17	15	0	1.019217	0.002329	-0.069208
18	1	0	-4.342449	0.477507	-1.565858
19	6	0	1.976494	1.298354	0.776830
20	6	0	1.418459	2.578115	0.780219
21	6	0	3.197981	1.076539	1.419909
22	6	0	2.071441	3.630367	1.412866
23	1	0	0.458308	2.722756	0.283671
24	6	0	3.850699	2.127656	2.050142
25	1	0	3.638951	0.080426	1.425917
26	6	0	3.288209	3.403649	2.045719
27	1	0	1.628094	4.622847	1.410973
28	1	0	4.801335	1.954447	2.549209
29	1	0	3.802799	4.222895	2.542606
30	6	0	0.740222	-1.305483	1.167148
31	6	0	-0.537062	-1.351963	1.729704
32	6	0	1.722605	-2.198291	1.604467
33	6	0	-0.826086	-2.263792	2.738646
34	1	0	-1.305477	-0.680261	1.340924
35	6	0	1.429567	-3.113056	2.608423
36	1	0	2.710190	-2.192016	1.143658
37	6	0	0.158635	-3.140967	3.180638
38	1	0	-1.824191	-2.290905	3.171652
39	1	0	2.193106	-3.809892	2.946414
40	1	0	-0.064419	-3.858110	3.967247
41	6	0	2.146205	-0.743478	-1.288159
42	6	0	3.261371	-0.064753	-1.781503
43	6	0	1.804564	-1.989654	-1.825747
44	6	0	4.038222	-0.635577	-2.785235
45	1	0	3.525736	0.911351	-1.378214
46	6	0	2.583754	-2.556445	-2.825573
47	1	0	0.925515	-2.517363	-1.454711
48	6	0	3.703315	-1.880744	-3.305220
49	1	0	4.908514	-0.103211	-3.161801
50	1	0	2.315860	-3.527627	-3.234890
51	1	0	4.311836	-2.325162	-4.089191
52	14	0	-2.917229	3.799815	-0.708738
53	1	0	-2.580562	3.262654	0.635682
54	1	0	-1.772336	3.702933	-1.647380
55	1	0	-4.195722	3.269462	-1.236876
56	1	0	-3.139659	5.268690	-0.498791

Zero-point correction= 0.448953 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.383793
Sum of electronic and zero-point Energies= -3276.426236
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -3276.888559 (a.u.)

1,2-TS2–H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.470804	0.338727	-1.809550
2	6	0	2.832704	-0.760268	-1.012254
3	6	0	3.682505	-1.536530	-0.020654
4	6	0	5.141924	-1.096999	-0.117403
5	6	0	5.274188	0.393328	-0.240996
6	6	0	4.240698	1.203150	-0.476715
7	6	0	2.827992	0.730758	-0.670359
8	8	0	2.150123	1.512063	-1.611409
9	1	0	1.793717	-1.136630	-1.020563
10	1	0	3.231807	-0.886963	-2.031094
11	1	0	3.593407	-2.617900	-0.187267
12	1	0	3.307046	-1.345952	0.997641
13	1	0	5.620987	-1.575461	-0.988092

14	1	0	5.706403	-1.454708	0.755765
15	1	0	6.275790	0.813014	-0.139342
16	1	0	4.385635	2.280165	-0.561520
17	15	0	-0.911952	0.003929	-0.264364
18	1	0	2.298807	0.826740	0.311040
19	6	0	-1.319226	1.602890	0.509897
20	6	0	-0.377575	2.629235	0.371220
21	6	0	-2.472947	1.813785	1.269106
22	6	0	-0.587882	3.849843	1.004857
23	1	0	0.514278	2.470360	-0.241423
24	6	0	-2.680296	3.038913	1.891445
25	1	0	-3.213751	1.021065	1.367295
26	6	0	-1.736141	4.054752	1.763082
27	1	0	0.145792	4.644981	0.896267
28	1	0	-3.581449	3.203086	2.477839
29	1	0	-1.900681	5.012564	2.251820
30	6	0	-2.514492	-0.783599	-0.622576
31	6	0	-3.256844	-1.474863	0.339833
32	6	0	-3.029789	-0.640117	-1.912669
33	6	0	-4.497680	-2.010463	0.013304
34	1	0	-2.854360	-1.604238	1.344284
35	6	0	-4.273175	-1.171198	-2.236463
36	1	0	-2.432140	-0.126503	-2.666381
37	6	0	-5.007251	-1.856277	-1.273208
38	1	0	-5.067935	-2.551846	0.764680
39	1	0	-4.665525	-1.057897	-3.244210
40	1	0	-5.976674	-2.278828	-1.527168
41	6	0	-0.205413	-1.001014	1.086385
42	6	0	0.041823	-2.355664	0.834758
43	6	0	0.203032	-0.442258	2.298039
44	6	0	0.677519	-3.141167	1.787059
45	1	0	-0.265407	-2.793117	-0.116056
46	6	0	0.846951	-1.231342	3.247689
47	1	0	0.025800	0.613458	2.497923
48	6	0	1.085493	-2.577460	2.994399
49	1	0	0.864531	-4.193220	1.584564
50	1	0	1.165043	-0.789202	4.188950
51	1	0	1.591312	-3.189939	3.737021
52	1	0	1.139303	0.422167	-3.349563
53	1	0	1.746531	0.891686	-2.735401

Zero-point correction= 0.428195 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.373084
Sum of electronic and zero-point Energies= -2985.728714
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2986.170322 (a.u.)

1,2-COM3^{-}H$_2$:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.344131	-0.055836	-2.001622
2	6	0	2.799566	-0.836301	-0.947028
3	6	0	3.680734	-1.507588	0.092576
4	6	0	5.123146	-1.027757	-0.052024
5	6	0	5.204294	0.455147	-0.261611
6	6	0	4.144932	1.217189	-0.541519
7	6	0	2.766357	0.660940	-0.705502
8	8	0	2.047951	1.338620	-1.741707
9	1	0	1.766295	-1.216874	-0.939810
10	1	0	3.198173	-1.022637	-1.957481
11	1	0	3.622714	-2.598986	0.006045
12	1	0	3.309472	-1.253914	1.097999
13	1	0	5.609240	-1.535769	-0.901234
14	1	0	5.714166	-1.309752	0.830315
15	1	0	6.186564	0.919707	-0.172913
16	1	0	4.248221	2.295701	-0.661709
17	15	0	-0.835965	0.018766	-0.232961

18	1	0	2.165920	0.867707	0.198443
19	6	0	-1.399621	1.678515	0.290791
20	6	0	-0.557414	2.759413	0.007163
21	6	0	-2.589475	1.905605	0.987783
22	6	0	-0.896274	4.042747	0.424909
23	1	0	0.361440	2.593472	-0.556937
24	6	0	-2.928683	3.189427	1.398430
25	1	0	-3.262577	1.075463	1.195671
26	6	0	-2.080981	4.258382	1.120844
27	1	0	-0.237144	4.877179	0.196634
28	1	0	-3.860178	3.357021	1.934556
29	1	0	-2.349443	5.262627	1.441170
30	6	0	-2.366491	-0.950931	-0.452650
31	6	0	-3.139636	-1.440426	0.605226
32	6	0	-2.775495	-1.180180	-1.768306
33	6	0	-4.316111	-2.133943	0.345993
34	1	0	-2.808455	-1.292574	1.633394
35	6	0	-3.955429	-1.870069	-2.025266
36	1	0	-2.124719	-0.834417	-2.573302
37	6	0	-4.726475	-2.343732	-0.969037
38	1	0	-4.913074	-2.516880	1.170817
39	1	0	-4.264747	-2.048127	-3.052494
40	1	0	-5.646127	-2.889511	-1.168852
41	6	0	-0.107588	-0.700798	1.282560
42	6	0	0.161049	-2.075683	1.282699
43	6	0	0.312906	0.075145	2.364485
44	6	0	0.828117	-2.662206	2.349912
45	1	0	-0.159429	-2.685599	0.436982
46	6	0	0.987329	-0.515008	3.430724
47	1	0	0.110869	1.145782	2.372816
48	6	0	1.245443	-1.881534	3.426783
49	1	0	1.027028	-3.731653	2.342135
50	1	0	1.306706	0.096927	4.271513
51	1	0	1.769646	-2.340774	4.261720
52	1	0	0.401530	-0.501938	-3.480072
53	1	0	2.518776	1.218478	-2.577904

Zero-point correction= 0.432658 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.37412
Sum of electronic and zero-point Energies= -2985.750929
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -2986.203597 (a.u.)

1,2−Pro−H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.228924	-1.215840	-0.211562
2	6	0	1.214518	-1.135552	0.265481
3	6	0	1.873265	0.147906	-0.233539
4	6	0	0.971146	1.335708	-0.074671
5	6	0	-0.326788	1.235506	0.218576
6	6	0	-1.048532	-0.073631	0.372501
7	8	0	-2.346607	-0.010007	-0.189948
8	1	0	-0.695967	-2.174352	0.043755
9	1	0	-0.255162	-1.128038	-1.311037
10	1	0	1.786297	-2.013031	-0.060019
11	1	0	1.228245	-1.143477	1.366097
12	1	0	2.147108	0.042182	-1.296581
13	1	0	2.821164	0.327389	0.292775
14	1	0	1.416470	2.322707	-0.205387
15	1	0	-0.941098	2.127691	0.344681
16	1	0	-1.223270	-0.269594	1.443472
17	1	0	-2.239037	0.223995	-1.118878

Zero-point correction= 0.150598 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.120464
Sum of electronic and zero-point Energies= -309.493069

SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -309.6529324 (a.u.)

1,2-TS2–SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.613434	-2.726262	-1.004906
2	1	0	-2.954935	-2.690427	-2.453101
3	1	0	-3.842914	-2.615219	-0.145359
4	1	0	-2.360178	-4.199509	-0.747876
5	6	0	-4.396292	0.200858	-1.471565
6	6	0	-5.449827	1.203152	-1.018340
7	6	0	-6.133850	0.732982	0.263646
8	6	0	-5.155280	0.176498	1.254699
9	6	0	-3.891628	-0.118023	0.946141
10	6	0	-3.300553	0.096862	-0.422269
11	8	0	-2.340067	-0.888177	-0.744114
12	1	0	-3.954120	0.479453	-2.436400
13	1	0	-4.853726	-0.791432	-1.598199
14	1	0	-6.193476	1.371876	-1.806795
15	1	0	-4.965414	2.174976	-0.834366
16	1	0	-6.878987	-0.044707	0.027690
17	1	0	-6.705552	1.554604	0.718060
18	1	0	-5.519289	-0.012948	2.264884
19	1	0	-3.222801	-0.544127	1.697593
20	1	0	-2.745514	1.057460	-0.410724
21	29	0	-0.431201	-1.031305	-0.722064
22	15	0	1.303429	-0.024952	-0.090258
23	6	0	2.775453	-1.081636	0.099562
24	6	0	4.069638	-0.597460	0.314155
25	6	0	2.554102	-2.458988	0.053547
26	6	0	5.121754	-1.486574	0.498153
27	1	0	4.258719	0.475849	0.313530
28	6	0	3.606326	-3.347988	0.242193
29	1	0	1.541090	-2.805952	-0.155503
30	6	0	4.889223	-2.860165	0.467664
31	1	0	6.128426	-1.108203	0.660613
32	1	0	3.425430	-4.419299	0.202884
33	1	0	5.715773	-3.552609	0.609845
34	6	0	0.931010	0.621476	1.576170
35	6	0	1.866553	1.144368	2.471142
36	6	0	-0.420870	0.604289	1.923063
37	6	0	1.442053	1.647095	3.695354
38	1	0	2.925518	1.154385	2.216601
39	6	0	-0.847315	1.113892	3.143026
40	1	0	-1.112292	0.167357	1.203907
41	6	0	0.088039	1.636625	4.029481
42	1	0	2.169582	2.051243	4.395626
43	1	0	-1.905862	1.097892	3.394174
44	1	0	-0.234970	2.035093	4.988541
45	6	0	1.892702	1.415019	-1.039959
46	6	0	1.534367	2.718595	-0.691513
47	6	0	2.628225	1.192258	-2.208815
48	6	0	1.922572	3.786841	-1.493937
49	1	0	0.951331	2.899413	0.210338
50	6	0	3.016094	2.261636	-3.005569
51	1	0	2.901908	0.175004	-2.488385
52	6	0	2.665216	3.561145	-2.648010
53	1	0	1.644357	4.800358	-1.214328
54	1	0	3.592806	2.080894	-3.909682
55	1	0	2.968665	4.398275	-3.272267
56	1	0	-0.957827	-2.611023	-0.984080

Zero-point correction= 0.448323 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.386079
Sum of electronic and zero-point Energies= -3276.407849
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -3276.86933 (a.u)

1,2-COM3−SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.050344	-2.631440	-1.356634
2	1	0	-3.579349	-1.934321	-2.549193
3	1	0	-4.190682	-3.188885	-0.580670
4	1	0	-2.113558	-3.712985	-1.708079
5	6	0	-2.604432	0.717621	-0.959476
6	6	0	-3.251713	2.000208	-0.465392
7	6	0	-4.731893	1.762946	-0.178318
8	6	0	-4.958283	0.485505	0.573498
9	6	0	-4.022624	-0.455021	0.723419
10	6	0	-2.653966	-0.340483	0.129382
11	8	0	-2.169474	-1.595504	-0.358397
12	1	0	-1.552615	0.865380	-1.254735
13	1	0	-3.134097	0.346807	-1.849910
14	1	0	-3.122704	2.805591	-1.198319
15	1	0	-2.744894	2.331470	0.455053
16	1	0	-5.300413	1.729893	-1.122143
17	1	0	-5.155816	2.604284	0.386895
18	1	0	-5.938986	0.336589	1.025577
19	1	0	-4.225197	-1.348429	1.314240
20	1	0	-1.934828	-0.061281	0.922940
21	29	0	-0.419116	-0.882985	-1.520408
22	15	0	0.989233	-0.061920	-0.133762
23	6	0	2.567824	0.279469	-0.985036
24	6	0	3.504092	1.223704	-0.553127
25	6	0	2.847722	-0.507232	-2.104858
26	6	0	4.711516	1.366015	-1.228147
27	1	0	3.280650	1.856412	0.305950
28	6	0	4.059450	-0.369534	-2.772098
29	1	0	2.077923	-1.196353	-2.455936
30	6	0	4.991881	0.564842	-2.332494
31	1	0	5.435989	2.104725	-0.892215
32	1	0	4.270069	-0.983919	-3.644229
33	1	0	5.937642	0.679017	-2.857777
34	6	0	1.460067	-1.136846	1.268858
35	6	0	2.702697	-1.065176	1.905075
36	6	0	0.502119	-2.040391	1.740791
37	6	0	2.981617	-1.881981	2.994220
38	1	0	3.460077	-0.375096	1.536200
39	6	0	0.782275	-2.853968	2.834338
40	1	0	-0.461930	-2.116068	1.235862
41	6	0	2.021196	-2.775683	3.461238
42	1	0	3.953419	-1.822744	3.479254
43	1	0	0.033074	-3.556783	3.191590
44	1	0	2.243183	-3.416121	4.311923
45	6	0	0.575771	1.539203	0.645426
46	6	0	0.358792	1.691171	2.016030
47	6	0	0.356658	2.630795	-0.205472
48	6	0	-0.065581	2.915649	2.527648
49	1	0	0.522732	0.848992	2.687432
50	6	0	-0.061303	3.851335	0.307920
51	1	0	0.521599	2.519149	-1.278331
52	6	0	-0.276046	3.995806	1.677704
53	1	0	-0.228598	3.024462	3.597654
54	1	0	-0.223244	4.692971	-0.361894
55	1	0	-0.607552	4.950325	2.079897
56	1	0	-0.632432	-1.431237	-2.945469

Zero-point correction= 0.448803 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.388595
Sum of electronic and zero-point Energies= -3276.43437
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -3276.898428 (a.u)

1,2-Pro−SiH_4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.411396	0.201761	-0.500580
2	1	0	-1.798949	0.081451	-1.851792
3	1	0	-2.615901	1.646446	-0.216285
4	1	0	-3.721464	-0.484815	-0.485300
5	6	0	0.647394	-1.279056	-0.178591
6	6	0	2.135759	-0.964803	-0.140394
7	6	0	2.387048	0.475987	-0.576400
8	6	0	1.425344	1.426154	0.071546
9	6	0	0.322607	1.030924	0.711921
10	6	0	-0.103824	-0.405930	0.816891
11	8	0	-1.508276	-0.552157	0.665224
12	1	0	0.443000	-2.334531	0.036437
13	1	0	0.256357	-1.074233	-1.187298
14	1	0	2.698468	-1.661815	-0.772572
15	1	0	2.508969	-1.101269	0.886232
16	1	0	2.296913	0.561029	-1.671857
17	1	0	3.418091	0.777286	-0.345364
18	1	0	1.660038	2.489671	0.022082
19	1	0	-0.321091	1.760155	1.205388
20	1	0	0.115355	-0.766416	1.836831

Zero-point correction= 0.16672 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.134061
Sum of electronic and zero-point Energies= -600.175557
SCF- Energy: M06 (PCM, toluene)/6-31G(d,p) = -600.3479058 (a.u)

Part III: (R)-SEGPHOS-CuH system

S6: The summarize energies of species along all reaction paths in the (*R*)−SEGPHOS-CuH system .

Speices	M06/6−31G(d,p)					M06(PCM)/6-31G**		
	ZPE	ZPG	Ezpe	E_{ZPG}	G_{RT}	PCM	PCM_{ZPG}	G_{sol}
2	0.210174	0.17545	-426.099915	-426.13464		-426.3167695	-426.1413195	
CAT	0.566456	0.496123	-4087.413591	-4087.483925		-4088.003977	-4087.507854	
H_2	0.010096	-0.001386	-1.159205	-1.170687		-1.1693618	-1.1707478	
H_{2+} CAT+**2**	0.786726	0.670187	-4514.672711	-4514.789252	0.0	-4515.490108	-4514.819922	0.0
Pro	0.234852	0.200588	-427.272208	-427.306473		-427.5143545	-427.3137665	
Pro+CAT	0.801308	0.696711	-4514.685799	-4514.790398	-3.0	-4515.518332	-4514.821621	-4.5
S-out−COM1	0.796673	0.715501	-4514.713863	-4514.795035	-15.2	-4515.534704	-4514.819203	1.9
S-out−TS1	0.796007	0.715117	-4514.709088	-4514.789978	-1.9	-4515.530101	-4514.814984	13.0
S-out−COM2	0.802115	0.721165	-4514.726804	-4514.807753	-48.6	-4515.55391	-4514.832745	-33.7
S-out−TS2	0.798817	0.718748	-4514.717787	-4514.797855	-22.6	-4515.539952	-4514.821204	-3.4
S-out−COM3	0.803356	0.72223	-4514.718215	-4514.799341	-26.5	-4515.545863	-4514.823633	-9.7
R-out−COM1	0.795678	0.714736	-4514.721998	-4514.802940	-35.9	-4515.54048	-4514.825744	-15.3
R-out−TS1	0.796826	0.716579	-4514.714205	-4514.794452	-13.7	-4515.535035	-4514.818456	3.8
R-out−COM2	0.802014	0.72083	-4514.732756	-4514.81394	-64.8	-4515.560408	-4514.839578	-51.6
R-out−TS2	0.798826	0.718763	-4514.718754	-4514.798817	-25.1	-4515.541149	-4514.822386	-6.5
R-out−COM3	0.803976	0.723722	-4514.721758	-4514.802012	-33.5	-4515.548217	-4514.824495	-12.0

CAT=(*R*)−SEGPHOS-CuH

S7. Cartesian coordinates and energies of species along all reaction paths over the SEGPHOS-CuH system at the M06/6-31G(d,p) level.

(R)−SEGPHOS−CuH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011142	-0.034260	0.007693
2	6	0	-0.002936	-0.014903	1.380695
3	6	0	1.183621	0.006756	2.101643
4	6	0	2.427219	-0.022883	1.508556
5	6	0	2.438258	0.004310	0.084920
6	6	0	1.239917	-0.015428	-0.627188
7	6	0	3.642251	-0.064216	2.363930
8	6	0	4.002866	1.053030	3.085992
9	6	0	5.139303	1.108463	3.882952
10	6	0	5.977792	0.029867	4.019211
11	6	0	5.615405	-1.136168	3.329192
12	6	0	4.473177	-1.208838	2.532868
13	8	0	-1.059131	-0.017438	2.240892
14	6	0	-0.506662	-0.029956	3.548559
15	8	0	3.349166	2.248529	3.144010
16	6	0	4.174626	3.109850	3.911487
17	8	0	5.230041	2.338051	4.462329
18	8	0	0.906052	0.025515	3.435676
19	15	0	4.041677	-0.176804	-0.782535
20	15	0	4.142125	-2.702462	1.522538
21	1	0	-0.939039	-0.057000	-0.555106
22	1	0	1.270513	-0.016594	-1.714294
23	1	0	6.868345	0.076492	4.637989
24	1	0	6.249901	-2.014148	3.425383
25	1	0	-0.796739	-0.961078	4.059494
26	1	0	-0.864445	0.844355	4.109509
27	1	0	3.585042	3.558106	4.720985
28	1	0	4.594890	3.892331	3.258682
29	29	0	4.747947	-2.261204	-0.554653
30	6	0	5.182568	-3.978961	2.319725
31	6	0	4.944484	-4.514116	3.589419
32	6	0	6.294661	-4.407926	1.591839
33	6	0	5.815234	-5.454061	4.125922
34	1	0	4.073503	-4.198652	4.162047
35	6	0	7.171651	-5.342448	2.134848
36	1	0	6.437650	-4.009260	0.584928
37	6	0	6.932584	-5.864718	3.400869
38	1	0	5.623555	-5.869886	5.112762
39	1	0	8.035988	-5.668713	1.561050
40	1	0	7.613485	-6.600194	3.824023
41	6	0	2.420624	-3.142756	1.945305
42	6	0	1.603482	-3.641984	0.927111
43	6	0	1.891721	-2.995720	3.231278
44	6	0	0.282124	-3.988758	1.190455
45	1	0	2.006544	-3.744349	-0.081127
46	6	0	0.575408	-3.354334	3.497152
47	1	0	2.503819	-2.560975	4.021383
48	6	0	-0.232587	-3.848183	2.475299
49	1	0	-0.347740	-4.367263	0.388906
50	1	0	0.177688	-3.245240	4.504928
51	1	0	-1.265338	-4.120998	2.681166
52	6	0	3.648806	0.264696	-2.513101
53	6	0	3.235388	1.533010	-2.933115
54	6	0	3.785606	-0.758250	-3.453977
55	6	0	2.954286	1.768243	-4.272756
56	1	0	3.132051	2.340794	-2.209921
57	6	0	3.497133	-0.523004	-4.795328
58	1	0	4.146181	-1.730684	-3.111358
59	6	0	3.082499	0.738738	-5.204277

60	1	0	2.635979	2.757457	-4.594579
61	1	0	3.608302	-1.325438	-5.520853
62	1	0	2.863199	0.927222	-6.253112
63	6	0	5.045064	1.206671	-0.135545
64	6	0	6.405925	0.974238	0.082772
65	6	0	4.513725	2.466463	0.156873
66	6	0	7.222120	1.982244	0.585617
67	1	0	6.822039	-0.011324	-0.129714
68	6	0	5.333376	3.478979	0.642211
69	1	0	3.444562	2.644442	0.042444
70	6	0	6.687435	3.236433	0.862265
71	1	0	8.277120	1.786916	0.762495
72	1	0	4.912271	4.460986	0.852177
73	1	0	7.325857	4.026446	1.251813
74	1	0	5.506487	-3.154395	-1.567067

Zero-point correction= 0.566456 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.496123
Sum of electronic and zero-point Energies= -4087.413591
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4088.003977 (a.u.)

H_2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.370365
2	1	0	0.000000	0.000000	-0.370365

Zero-point correction= 0.010096 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= -0.001386
Sum of electronic and zero-point Energies= -1.159205
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -1.1693618 (a.u.)

2:
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.430884	1.593204	-0.127886
2	6	0	0.903845	1.016622	-0.550644
3	6	0	-1.532085	0.631771	0.019026
4	6	0	-1.356639	-0.696521	-0.094108
5	6	0	-0.003819	-1.287947	-0.367121
6	6	0	1.175380	-0.382808	0.008016
7	8	0	-0.592631	2.789754	0.037713
8	6	0	2.457336	-0.941660	-0.597516
9	6	0	1.331035	-0.320480	1.527936
10	1	0	1.691819	1.727397	-0.270060
11	1	0	0.894374	0.968368	-1.652865
12	1	0	0.048872	-1.532358	-1.443507
13	1	0	0.086838	-2.255891	0.152862
14	1	0	-2.513628	1.058687	0.223424
15	6	0	-2.486441	-1.662968	0.021273
16	1	0	-2.333922	-2.335579	0.876281
17	1	0	-3.450416	-1.159927	0.141754
18	1	0	-2.536827	-2.305420	-0.868661
19	1	0	3.319839	-0.316737	-0.332685
20	1	0	2.396780	-0.985529	-1.692867
21	1	0	2.654115	-1.957419	-0.228971
22	1	0	0.425432	0.051318	2.021159
23	1	0	2.158754	0.345335	1.802907
24	1	0	1.552647	-1.315551	1.935673

Zero-point correction= 0.210174 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.17545

Sum of electronic and zero-point Energies= -426.099915
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -426.3167695 (a.u.)

R-out-COM1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.112878	0.785457	-2.378739
2	6	0	1.881562	-2.520879	-3.102500
3	6	0	3.036262	-2.099965	-2.490590
4	6	0	3.015899	-1.506870	-1.235487
5	6	0	1.854625	-1.268585	-0.528872
6	6	0	0.648137	-1.698509	-1.149311
7	6	0	0.686236	-2.306696	-2.401923
8	6	0	1.962085	-0.691925	0.836316
9	6	0	2.473631	-1.487366	1.839788
10	6	0	2.630674	-1.056180	3.149749
11	6	0	2.320251	0.227884	3.522465
12	6	0	1.824403	1.070186	2.516720
13	6	0	1.632788	0.642283	1.204794
14	8	0	4.324864	-2.214981	-2.918929
15	6	0	5.100979	-1.484559	-1.981489
16	8	0	2.888494	-2.782009	1.735619
17	6	0	3.188395	-3.204384	3.054973
18	8	0	3.138158	-2.068619	3.905520
19	8	0	4.294528	-1.240503	-0.841415
20	15	0	-0.939888	-1.261717	-0.327622
21	15	0	0.887086	1.716867	-0.087659
22	1	0	1.894892	-3.001765	-4.075589
23	1	0	-0.240756	-2.635745	-2.862765
24	1	0	2.453139	0.575430	4.542347
25	1	0	1.579775	2.093470	2.786454
26	1	0	5.403444	-0.521236	-2.427084
27	1	0	5.977283	-2.075437	-1.691868
28	1	0	4.195169	-3.639468	3.081841
29	1	0	2.435201	-3.938387	3.384876
30	29	0	-1.160666	1.010825	-0.831495
31	6	0	0.864880	3.392523	0.649865
32	6	0	1.559823	4.465137	0.084493
33	6	0	0.028881	3.631651	1.752287
34	6	0	1.440731	5.744328	0.621173
35	1	0	2.200709	4.303132	-0.779671
36	6	0	-0.074515	4.908131	2.292077
37	1	0	-0.567296	2.824138	2.182229
38	6	0	0.630962	5.968068	1.728381
39	1	0	1.987030	6.568871	0.168286
40	1	0	-0.722052	5.073186	3.150066
41	1	0	0.541430	6.967855	2.147335
42	6	0	2.237487	1.800936	-1.322404
43	6	0	1.930925	1.690654	-2.679516
44	6	0	3.568458	1.969912	-0.925381
45	6	0	2.946284	1.749804	-3.630861
46	1	0	0.891061	1.530372	-2.970732
47	6	0	4.578402	2.040200	-1.876462
48	1	0	3.809769	2.041107	0.135243
49	6	0	4.266984	1.928663	-3.231415
50	1	0	2.703977	1.654342	-4.686835
51	1	0	5.611435	2.178010	-1.562643
52	1	0	5.058478	1.981144	-3.976729
53	6	0	-2.222618	-2.276719	-1.167571
54	6	0	-2.980772	-3.235848	-0.488585
55	6	0	-2.554438	-1.981737	-2.499120
56	6	0	-4.023740	-3.900570	-1.129578
57	1	0	-2.761190	-3.465893	0.551751
58	6	0	-3.585431	-2.657849	-3.140449
59	1	0	-2.015335	-1.187343	-3.017008
60	6	0	-4.322926	-3.622068	-2.457952

61	1	0	-4.602201	-4.642307	-0.583203
62	1	0	-3.822791	-2.419015	-4.174789
63	1	0	-5.134877	-4.145492	-2.957654
64	6	0	-0.760751	-2.084173	1.304684
65	6	0	-1.025386	-1.352653	2.464694
66	6	0	-0.322715	-3.409426	1.417699
67	6	0	-0.861335	-1.937497	3.717688
68	1	0	-1.342342	-0.311495	2.397695
69	6	0	-0.174902	-3.996788	2.668104
70	1	0	-0.088551	-3.979681	0.518503
71	6	0	-0.441724	-3.259096	3.821562
72	1	0	-1.061495	-1.349630	4.610822
73	1	0	0.154188	-5.031907	2.744919
74	1	0	-0.315681	-3.716221	4.801085
75	6	0	-3.016426	1.410793	1.367151
76	6	0	-4.066913	0.360629	1.074105
77	6	0	-2.485060	2.140972	0.223358
78	6	0	-2.963159	1.966490	-1.084481
79	6	0	-4.118375	1.018660	-1.342347
80	6	0	-4.978933	0.732844	-0.100534
81	8	0	-2.645358	1.631216	2.519145
82	6	0	-5.925988	-0.423918	-0.398659
83	6	0	-5.801304	1.971553	0.258999
84	1	0	-4.642003	0.198974	1.995943
85	1	0	-3.552876	-0.590831	0.855300
86	1	0	-3.761987	0.068632	-1.761782
87	1	0	-4.761542	1.457486	-2.122782
88	1	0	-1.954095	3.061566	0.466537
89	6	0	-2.825561	3.103512	-2.055768
90	1	0	-3.706938	3.760387	-1.963782
91	1	0	-1.929109	3.703890	-1.858830
92	1	0	-2.777127	2.747171	-3.089574
93	1	0	-6.580735	-0.624377	0.460063
94	1	0	-5.374750	-1.346926	-0.626626
95	1	0	-6.566279	-0.190647	-1.260259
96	1	0	-5.168050	2.848608	0.444498
97	1	0	-6.398111	1.794693	1.163443
98	1	0	-6.492989	2.224089	-0.555686
99	1	0	-0.568718	1.315938	4.774372
100	1	0	-1.089025	1.484540	4.264866

Zero-point correction= 0.795678 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.714736
Sum of electronic and zero-point Energies= -4514.721998
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.54048 (a.u.)

R−out−TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.709569	1.123423	-1.978118
2	6	0	1.995394	-2.477976	-3.091294
3	6	0	3.134195	-1.981024	-2.507474
4	6	0	3.102684	-1.380132	-1.255746
5	6	0	1.943901	-1.200399	-0.528442
6	6	0	0.751420	-1.697160	-1.126182
7	6	0	0.802088	-2.321224	-2.371002
8	6	0	2.063750	-0.604823	0.829703
9	6	0	2.631702	-1.373474	1.824193
10	6	0	2.862926	-0.908569	3.112297
11	6	0	2.562557	0.382174	3.471679
12	6	0	1.994918	1.192276	2.477574
13	6	0	1.735542	0.732080	1.188427
14	8	0	4.418519	-2.022484	-2.960191
15	6	0	5.170002	-1.244141	-2.040961
16	8	0	3.067040	-2.662035	1.723266
17	6	0	3.380762	-3.061273	3.047156

18	8	0	3.439640	-1.894592	3.854112
19	8	0	4.370743	-1.037762	-0.887687
20	15	0	-0.844311	-1.319258	-0.293601
21	15	0	0.848867	1.753158	-0.054829
22	1	0	2.019133	-2.971660	-4.057755
23	1	0	-0.113597	-2.709152	-2.808573
24	1	0	2.755423	0.757298	4.471884
25	1	0	1.747345	2.218017	2.736894
26	1	0	5.407631	-0.267803	-2.498026
27	1	0	6.082182	-1.783817	-1.763375
28	1	0	4.353882	-3.564462	3.058280
29	1	0	2.584996	-3.726943	3.423558
30	29	0	-1.174637	0.897582	-0.515951
31	6	0	0.808549	3.440170	0.651101
32	6	0	1.447213	4.524635	0.044959
33	6	0	0.005599	3.669485	1.779072
34	6	0	1.300322	5.808529	0.563249
35	1	0	2.062735	4.369607	-0.838598
36	6	0	-0.126836	4.950592	2.300311
37	1	0	-0.527701	2.842243	2.249285
38	6	0	0.518870	6.024029	1.692230
39	1	0	1.802373	6.643255	0.078888
40	1	0	-0.747752	5.109481	3.178672
41	1	0	0.406630	7.027717	2.095917
42	6	0	2.065585	1.858096	-1.419413
43	6	0	1.609597	1.711265	-2.730408
44	6	0	3.428625	2.063114	-1.182749
45	6	0	2.505674	1.756839	-3.794254
46	1	0	0.544833	1.542429	-2.901455
47	6	0	4.320291	2.126513	-2.247185
48	1	0	3.789683	2.161684	-0.158848
49	6	0	3.859643	1.965498	-3.553829
50	1	0	2.144939	1.629355	-4.812255
51	1	0	5.378870	2.297379	-2.058450
52	1	0	4.560833	2.004686	-4.385040
53	6	0	-2.094081	-2.356728	-1.147496
54	6	0	-2.801041	-3.370885	-0.496498
55	6	0	-2.445921	-2.029179	-2.464949
56	6	0	-3.821736	-4.053997	-1.153732
57	1	0	-2.559932	-3.625060	0.533576
58	6	0	-3.451903	-2.723963	-3.124642
59	1	0	-1.938776	-1.201388	-2.962886
60	6	0	-4.143229	-3.740401	-2.469062
61	1	0	-4.365605	-4.837796	-0.631300
62	1	0	-3.707528	-2.460605	-4.148483
63	1	0	-4.938734	-4.277458	-2.980440
64	6	0	-0.648305	-2.121772	1.338225
65	6	0	-1.026457	-1.419993	2.485040
66	6	0	-0.107992	-3.407157	1.461335
67	6	0	-0.860206	-1.996441	3.741741
68	1	0	-1.444213	-0.415496	2.406455
69	6	0	0.042359	-3.985275	2.715580
70	1	0	0.200989	-3.951375	0.568543
71	6	0	-0.326732	-3.275200	3.858340
72	1	0	-1.150579	-1.435319	4.627059
73	1	0	0.451374	-4.990488	2.804677
74	1	0	-0.200107	-3.725108	4.841173
75	6	0	-3.326084	1.110216	1.460405
76	6	0	-4.354515	0.115455	0.954146
77	6	0	-2.643180	1.900096	0.461588
78	6	0	-2.952807	1.851035	-0.942813
79	6	0	-4.105213	0.946798	-1.378198
80	6	0	-5.119083	0.631234	-0.269973
81	8	0	-3.128731	1.237685	2.671509
82	6	0	-6.073023	-0.448061	-0.771521
83	6	0	-5.926712	1.874874	0.101425
84	1	0	-5.034266	-0.107126	1.787757
85	1	0	-3.847290	-0.830557	0.696485
86	1	0	-3.724381	-0.007860	-1.759967

87	1	0	-4.625997	1.420606	-2.226241
88	1	0	-2.186633	2.815937	0.840570
89	6	0	-2.876814	3.176679	-1.661138
90	1	0	-3.758705	3.778936	-1.391712
91	1	0	-1.981475	3.740870	-1.371838
92	1	0	-2.865759	3.053122	-2.749952
93	1	0	-6.817706	-0.696854	-0.003803
94	1	0	-5.532998	-1.369692	-1.031440
95	1	0	-6.614140	-0.110406	-1.666320
96	1	0	-5.286846	2.687196	0.467263
97	1	0	-6.654784	1.644104	0.890301
98	1	0	-6.481667	2.248473	-0.770112
99	1	0	-1.211040	1.378781	4.029126
100	1	0	-0.481429	1.272323	4.164709

Zero-point correction= 0.796826 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.716579
Sum of electronic and zero-point Energies= -4514.714205
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.535035 (a.u.)

R−out−TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.281635	-1.678226	3.330544
2	6	0	-3.332354	-0.965588	2.807613
3	6	0	-3.305086	-0.486526	1.504942
4	6	0	-2.233965	-0.658816	0.652135
5	6	0	-1.129776	-1.383581	1.181926
6	6	0	-1.182976	-1.880706	2.484251
7	6	0	-2.378285	-0.132714	-0.734267
8	6	0	-3.196486	-0.811778	-1.611143
9	6	0	-3.507144	-0.343542	-2.883638
10	6	0	-3.044532	0.867373	-3.336103
11	6	0	-2.204095	1.579951	-2.468808
12	6	0	-1.860663	1.107888	-1.205152
13	8	0	-4.512948	-0.629886	3.394435
14	6	0	-5.217840	0.153593	2.442039
15	8	0	-3.860327	-1.985886	-1.391580
16	6	0	-4.311675	-2.383894	-2.675239
17	8	0	-4.348402	-1.226696	-3.494616
18	8	0	-4.478085	0.153658	1.233510
19	15	0	0.377120	-1.563693	0.150545
20	15	0	-0.502472	1.860361	-0.233992
21	1	0	-2.304371	-2.068156	4.343263
22	1	0	-0.339465	-2.446397	2.870255
23	1	0	-3.307815	1.246872	-4.318340
24	1	0	-1.792887	2.526923	-2.810194
25	1	0	-5.309834	1.185583	2.815109
26	1	0	-6.209464	-0.284046	2.268203
27	1	0	-5.316130	-2.810074	-2.595318
28	1	0	-3.598218	-3.113946	-3.097652
29	29	0	1.095505	0.365930	-0.636606
30	6	0	-0.169555	3.503792	-0.961119
31	6	0	-0.374287	4.699041	-0.267396
32	6	0	0.472437	3.546571	-2.208336
33	6	0	0.034779	5.911475	-0.815661
34	1	0	-0.849504	4.686591	0.711422
35	6	0	0.865734	4.759764	-2.758624
36	1	0	0.668232	2.614540	-2.740339
37	6	0	0.649504	5.946269	-2.062071
38	1	0	-0.128927	6.833699	-0.262405
39	1	0	1.355385	4.776752	-3.729571
40	1	0	0.969140	6.894892	-2.487346
41	6	0	-1.300594	2.237717	1.367491
42	6	0	-0.618603	1.955059	2.551815
43	6	0	-2.587172	2.782715	1.434536

44	6	0	-1.216527	2.197871	3.785121
45	1	0	0.380424	1.521222	2.502138
46	6	0	-3.179028	3.040495	2.665637
47	1	0	-3.128085	2.995246	0.512212
48	6	0	-2.497033	2.738686	3.842823
49	1	0	-0.682745	1.961688	4.702734
50	1	0	-4.175474	3.477315	2.708209
51	1	0	-2.964109	2.928451	4.806780
52	6	0	1.547982	-2.434524	1.254742
53	6	0	1.991716	-3.737887	1.026538
54	6	0	2.088837	-1.713349	2.327346
55	6	0	2.957448	-4.306814	1.854340
56	1	0	1.587282	-4.310459	0.193765
57	6	0	3.034363	-2.288785	3.165054
58	1	0	1.759098	-0.687498	2.502677
59	6	0	3.476699	-3.589188	2.925058
60	1	0	3.301267	-5.320262	1.660093
61	1	0	3.442871	-1.715490	3.994915
62	1	0	4.229431	-4.036521	3.569996
63	6	0	-0.070602	-2.831312	-1.083355
64	6	0	0.780604	-2.987233	-2.183273
65	6	0	-1.185228	-3.660366	-0.944553
66	6	0	0.510786	-3.964236	-3.135126
67	1	0	1.650434	-2.334840	-2.292740
68	6	0	-1.458889	-4.625895	-1.909375
69	1	0	-1.848793	-3.540119	-0.089305
70	6	0	-0.611916	-4.778019	-3.003837
71	1	0	1.174747	-4.081967	-3.988165
72	1	0	-2.331700	-5.267267	-1.799248
73	1	0	-0.824893	-5.535109	-3.755649
74	1	0	1.893059	-0.051797	-2.554138
75	1	0	0.932099	0.227806	-2.377289
76	1	0	2.754421	2.083813	1.126642
77	6	0	3.443632	0.030394	-1.355929
78	6	0	4.405035	-0.844977	-0.595849
79	6	0	2.993609	1.241013	-0.833626
80	6	0	3.576686	1.858137	0.422730
81	6	0	4.520811	0.900190	1.166009
82	6	0	5.359414	-0.039836	0.290638
83	8	0	3.064604	-0.412414	-2.523273
84	6	0	6.144584	-0.987400	1.192400
85	6	0	6.350375	0.723780	-0.588788
86	1	0	4.963258	-1.434630	-1.337113
87	1	0	3.843612	-1.572761	0.014708
88	1	0	3.922101	0.258780	1.832147
89	1	0	5.188572	1.481287	1.822819
90	1	0	2.677004	1.974511	-1.580707
91	6	0	4.197881	3.218530	0.103116
92	1	0	5.015396	3.143760	-0.622889
93	1	0	3.436872	3.883703	-0.329151
94	1	0	4.589736	3.700272	1.008478
95	1	0	6.729917	-1.699688	0.594985
96	1	0	5.475860	-1.565713	1.844796
97	1	0	6.845658	-0.430155	1.829191
98	1	0	5.844742	1.308605	-1.365222
99	1	0	7.027723	0.022471	-1.094700
100	1	0	6.964156	1.409233	0.011951

Zero-point correction= 0.798826 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.718763
Sum of electronic and zero-point Energies= -4514.718754
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.541149 (a.u.)

S-out-COM1:

Standard orientation:

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

1	1	0	1.602130	0.525639	-2.348934
2	6	0	-3.725222	0.006384	-2.746661
3	6	0	-4.011661	-1.102761	-1.989449
4	6	0	-3.342507	-1.365327	-0.800594
5	6	0	-2.339174	-0.561170	-0.304988
6	6	0	-2.031807	0.596448	-1.076963
7	6	0	-2.720588	0.854661	-2.259214
8	6	0	-1.740675	-0.854060	1.023181
9	6	0	-2.527853	-0.647158	2.137946
10	6	0	-2.054337	-0.755099	3.437975
11	6	0	-0.742009	-1.064768	3.698457
12	6	0	0.080554	-1.301422	2.588586
13	6	0	-0.398080	-1.255790	1.276944
14	8	0	-4.950055	-2.066887	-2.204926
15	6	0	-4.728504	-3.047766	-1.203726
16	8	0	-3.838058	-0.271897	2.161422
17	6	0	-4.131475	0.014571	3.519094
18	8	0	-3.060101	-0.472086	4.313113
19	8	0	-3.846520	-2.500692	-0.238694
20	15	0	-0.649928	1.660593	-0.494388
21	15	0	0.755710	-1.431665	-0.128820
22	1	0	-4.258341	0.220362	-3.667740
23	1	0	-2.480630	1.748920	-2.828457
24	1	0	-0.352379	-1.099985	4.710961
25	1	0	1.137512	-1.480985	2.769381
26	1	0	-4.263868	-3.937372	-1.660554
27	1	0	-5.680451	-3.307001	-0.726129
28	1	0	-5.060738	-0.489783	3.808246
29	1	0	-4.214333	1.106880	3.647619
30	29	0	1.426919	0.652027	-0.803292
31	6	0	-0.200699	-2.400238	-1.368271
32	6	0	-0.840022	-3.586854	-0.995585
33	6	0	-0.224080	-1.996168	-2.703135
34	6	0	-1.509800	-4.349406	-1.943914
35	1	0	-0.817596	-3.912285	0.044475
36	6	0	-0.901946	-2.758790	-3.651065
37	1	0	0.283300	-1.071307	-2.982669
38	6	0	-1.546988	-3.931720	-3.273787
39	1	0	-1.999071	-5.275660	-1.646959
40	1	0	-0.925090	-2.433285	-4.688712
41	1	0	-2.072683	-4.528006	-4.016878
42	6	0	2.004861	-2.716395	0.277924
43	6	0	2.016423	-3.577757	1.375496
44	6	0	3.012827	-2.840382	-0.688088
45	6	0	3.038325	-4.512999	1.524238
46	1	0	1.226039	-3.527136	2.120547
47	6	0	4.021532	-3.783843	-0.546618
48	1	0	2.995425	-2.186125	-1.562593
49	6	0	4.044770	-4.614508	0.571264
50	1	0	3.041143	-5.168992	2.391951
51	1	0	4.794478	-3.867695	-1.307909
52	1	0	4.841233	-5.344727	0.693636
53	6	0	-0.664490	3.144816	-1.569605
54	6	0	-0.822729	4.436421	-1.060329
55	6	0	-0.313086	2.989753	-2.919095
56	6	0	-0.650618	5.546650	-1.884373
57	1	0	-1.073727	4.581330	-0.011613
58	6	0	-0.162605	4.097704	-3.741696
59	1	0	-0.119983	1.991761	-3.312152
60	6	0	-0.327584	5.381119	-3.225663
61	1	0	-0.770744	6.545320	-1.470094
62	1	0	0.103894	3.959352	-4.787167
63	1	0	-0.194435	6.249220	-3.867188
64	6	0	-1.303409	2.276598	1.107944
65	6	0	-0.510377	2.245480	2.258926
66	6	0	-2.615577	2.760871	1.193917
67	6	0	-1.022473	2.707938	3.470258
68	1	0	0.498727	1.829376	2.243296
69	6	0	-3.118849	3.228191	2.401304

70	1	0	-3.246014	2.764088	0.304248
71	6	0	-2.318618	3.203505	3.543842
72	1	0	-0.396348	2.671273	4.359200
73	1	0	-4.137103	3.609555	2.453663
74	1	0	-2.711488	3.566449	4.491673
75	6	0	2.595683	1.658194	0.520000
76	6	0	3.175832	1.699875	-0.759895
77	6	0	4.384027	0.820412	-1.036873
78	6	0	3.098677	0.815072	1.601854
79	6	0	4.309055	-0.044323	1.301613
80	6	0	5.224243	0.536514	0.218137
81	8	0	2.585462	0.812806	2.717989
82	1	0	1.997153	2.509006	0.851913
83	1	0	5.015914	1.313092	-1.792995
84	1	0	4.083336	-0.136701	-1.483537
85	1	0	3.954396	-1.040507	0.989301
86	1	0	4.848346	-0.190691	2.247549
87	6	0	3.092847	2.965871	-1.564984
88	1	0	3.961865	3.601340	-1.325997
89	1	0	3.113731	2.758728	-2.640291
90	1	0	2.182035	3.539494	-1.350890
91	6	0	6.311441	-0.475123	-0.124783
92	1	0	6.975496	-0.089636	-0.910288
93	1	0	6.928908	-0.700660	0.754902
94	1	0	5.875742	-1.419306	-0.478772
95	6	0	5.882858	1.821762	0.720983
96	1	0	6.487868	1.622776	1.615246
97	1	0	6.546262	2.243364	-0.046343
98	1	0	5.144575	2.589334	0.983833
99	1	0	1.609352	0.897137	4.874299
100	1	0	0.956285	0.821516	5.228109

Zero-point correction= 0.796673 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.715501
Sum of electronic and zero-point Energies= -4514.713863
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.534704 (a.u.)

S−out−TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.128237	0.811137	-2.010455
2	6	0	-3.799418	0.476279	-2.652658
3	6	0	-4.157552	-0.657788	-1.965631
4	6	0	-3.499088	-1.042026	-0.805699
5	6	0	-2.427615	-0.353722	-0.282083
6	6	0	-2.035123	0.820528	-0.986422
7	6	0	-2.722635	1.211267	-2.133409
8	6	0	-1.820566	-0.780139	1.004189
9	6	0	-2.548475	-0.575550	2.160145
10	6	0	-2.034745	-0.780154	3.432623
11	6	0	-0.739869	-1.198389	3.625625
12	6	0	0.013029	-1.449872	2.472160
13	6	0	-0.510106	-1.300911	1.185457
14	8	0	-5.161603	-1.539220	-2.230946
15	6	0	-5.035451	-2.575655	-1.268099
16	8	0	-3.824613	-0.104189	2.255458
17	6	0	-4.040751	0.142360	3.635673
18	8	0	-2.979665	-0.460962	4.360949
19	8	0	-4.077363	-2.170388	-0.305414
20	15	0	-0.536794	1.698135	-0.385854
21	15	0	0.620469	-1.512411	-0.236521
22	1	0	-4.327806	0.790233	-3.547422
23	1	0	-2.423266	2.119459	-2.650921
24	1	0	-0.314444	-1.307433	4.618066
25	1	0	1.054563	-1.740704	2.592455
26	1	0	-4.688761	-3.496163	-1.766151

27	1	0	-6.002837	-2.740935	-0.778112
28	1	0	-4.994123	-0.302327	3.943579
29	1	0	-4.035291	1.230954	3.816350
30	29	0	1.407356	0.536367	-0.640940
31	6	0	-0.418238	-2.251095	-1.560699
32	6	0	-1.230268	-3.364092	-1.324952
33	6	0	-0.358705	-1.706547	-2.844247
34	6	0	-1.986454	-3.910026	-2.354391
35	1	0	-1.283605	-3.797992	-0.326904
36	6	0	-1.125191	-2.247489	-3.873030
37	1	0	0.284455	-0.842938	-3.023631
38	6	0	-1.943380	-3.345142	-3.628346
39	1	0	-2.608840	-4.782886	-2.163839
40	1	0	-1.082670	-1.809262	-4.867567
41	1	0	-2.541788	-3.769054	-4.431971
42	6	0	1.677813	-2.956727	0.170561
43	6	0	1.359302	-3.960221	1.089849
44	6	0	2.845854	-3.084331	-0.587509
45	6	0	2.210213	-5.045508	1.269986
46	1	0	0.450899	-3.886626	1.684607
47	6	0	3.693703	-4.172530	-0.412358
48	1	0	3.087154	-2.318027	-1.326625
49	6	0	3.381169	-5.151363	0.525413
50	1	0	1.956088	-5.813107	1.997571
51	1	0	4.601153	-4.252583	-1.006724
52	1	0	4.047368	-5.997991	0.673584
53	6	0	-0.439414	3.234249	-1.377434
54	6	0	-0.481482	4.506471	-0.802766
55	6	0	-0.131006	3.118868	-2.740900
56	6	0	-0.234182	5.638574	-1.576185
57	1	0	-0.698006	4.616846	0.257711
58	6	0	0.095104	4.249605	-3.513509
59	1	0	-0.042323	2.128917	-3.189212
60	6	0	0.048569	5.514565	-2.930819
61	1	0	-0.262538	6.621991	-1.112218
62	1	0	0.327749	4.143142	-4.570682
63	1	0	0.242996	6.399751	-3.531977
64	6	0	-1.054439	2.267166	1.279042
65	6	0	-0.216773	2.069635	2.380522
66	6	0	-2.301420	2.878402	1.463140
67	6	0	-0.617544	2.500649	3.643971
68	1	0	0.733552	1.541471	2.280934
69	6	0	-2.693451	3.311667	2.723294
70	1	0	-2.968713	3.009628	0.611085
71	6	0	-1.846613	3.126066	3.816551
72	1	0	0.039092	2.329992	4.493939
73	1	0	-3.660374	3.794159	2.855159
74	1	0	-2.153678	3.462918	4.804780
75	6	0	2.764776	1.445418	0.553498
76	6	0	3.221074	1.497298	-0.811422
77	6	0	4.418417	0.616197	-1.166898
78	6	0	3.317092	0.564746	1.560207
79	6	0	4.490551	-0.303475	1.138105
80	6	0	5.339703	0.311799	0.021379
81	8	0	2.898621	0.524595	2.721318
82	1	0	2.251138	2.326409	0.945298
83	1	0	4.994248	1.103913	-1.969837
84	1	0	4.083043	-0.341865	-1.584290
85	1	0	4.103093	-1.282572	0.809008
86	1	0	5.091722	-0.498033	2.037308
87	6	0	3.240477	2.869611	-1.441060
88	1	0	4.115194	3.421574	-1.064463
89	1	0	3.314065	2.817055	-2.533571
90	1	0	2.343227	3.448946	-1.190266
91	6	0	6.402810	-0.687810	-0.422684
92	1	0	7.026503	-0.271752	-1.225720
93	1	0	7.063880	-0.951822	0.413302
94	1	0	5.949268	-1.616316	-0.795728
95	6	0	6.039596	1.575335	0.522647

96	1	0	6.725088	1.332478	1.345294
97	1	0	6.629653	2.038745	-0.280201
98	1	0	5.327265	2.321193	0.894239
99	1	0	3.239639	-1.966433	3.219328
100	1	0	3.311483	-2.640454	2.901920

Zero-point correction= 0.796007 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.715117
Sum of electronic and zero-point Energies= -4514.709088
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.530101 (a.u.)

S−out−TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.554120	0.832426	3.746956
2	6	0	1.315146	-0.311145	3.752258
3	6	0	1.868254	-0.821045	2.585099
4	6	0	1.691576	-0.238963	1.348436
5	6	0	0.970280	0.988755	1.333937
6	6	0	0.393820	1.472134	2.509152
7	6	0	2.228703	-0.907108	0.135306
8	6	0	3.586960	-0.893079	-0.096729
9	6	0	4.168841	-1.412578	-1.244996
10	6	0	3.414760	-2.005885	-2.227179
11	6	0	2.033350	-2.077310	-1.997911
12	6	0	1.435748	-1.572597	-0.843586
13	8	0	1.648884	-1.112874	4.801524
14	6	0	2.320371	-2.231097	4.240690
15	8	0	4.553975	-0.362077	0.703526
16	6	0	5.761093	-0.442355	-0.038362
17	8	0	5.517024	-1.228273	-1.195086
18	8	0	2.554917	-1.962428	2.867374
19	15	0	0.581367	1.734269	-0.290162
20	15	0	-0.396115	-1.563892	-0.694423
21	1	0	0.100774	1.218975	4.654388
22	1	0	-0.213140	2.373627	2.471398
23	1	0	3.866149	-2.397761	-3.133284
24	1	0	1.406958	-2.544792	-2.753734
25	1	0	1.681488	-3.124753	4.333619
26	1	0	3.278613	-2.379962	4.753567
27	1	0	6.536496	-0.919360	0.573184
28	1	0	6.068029	0.571274	-0.344740
29	6	0	-0.951107	-2.929541	-1.789044
30	6	0	-0.383237	-4.211051	-1.788420
31	6	0	-2.041614	-2.674687	-2.625232
32	6	0	-0.892170	-5.210395	-2.606538
33	1	0	0.480070	-4.428947	-1.162766
34	6	0	-2.553073	-3.681356	-3.441709
35	1	0	-2.497518	-1.684280	-2.649683
36	6	0	-1.981513	-4.946922	-3.434523
37	1	0	-0.437032	-6.198447	-2.599323
38	1	0	-3.401063	-3.464530	-4.086880
39	1	0	-2.379264	-5.730610	-4.075681
40	6	0	-0.670688	-2.232377	0.996565
41	6	0	-1.550080	-1.536225	1.825509
42	6	0	-0.068320	-3.397158	1.482496
43	6	0	-1.841146	-1.992251	3.107493
44	1	0	-1.993355	-0.612301	1.456659
45	6	0	-0.365352	-3.863878	2.757887
46	1	0	0.653106	-3.937828	0.872806
47	6	0	-1.253406	-3.163080	3.573365
48	1	0	-2.523546	-1.426772	3.739670
49	1	0	0.097545	-4.780949	3.118731
50	1	0	-1.480288	-3.529020	4.572433
51	6	0	0.247371	3.519296	-0.031847
52	6	0	-0.423362	4.138378	-1.093358

53	6	0	0.686371	4.306538	1.036336
54	6	0	-0.672436	5.505720	-1.077457
55	1	0	-0.743862	3.536077	-1.944875
56	6	0	0.420661	5.672172	1.060248
57	1	0	1.240367	3.856906	1.858108
58	6	0	-0.262082	6.273652	0.008029
59	1	0	-1.193966	5.970043	-1.911119
60	1	0	0.756962	6.270466	1.904295
61	1	0	-0.467567	7.341358	0.030678
62	6	0	2.200082	1.858993	-1.145799
63	6	0	2.265813	1.493569	-2.490944
64	6	0	3.337940	2.371989	-0.516392
65	6	0	3.459603	1.623157	-3.196140
66	1	0	1.374335	1.099685	-2.981042
67	6	0	4.524894	2.513655	-1.224938
68	1	0	3.296022	2.653662	0.535573
69	6	0	4.588825	2.133518	-2.565601
70	1	0	3.504216	1.326645	-4.241568
71	1	0	5.403220	2.929654	-0.733553
72	1	0	5.520709	2.239457	-3.116852
73	29	0	-1.062545	0.523084	-1.172265
74	1	0	-1.241105	0.677909	-2.870895
75	1	0	-2.241062	0.571156	-2.864101
76	6	0	-3.201046	1.918516	0.720761
77	6	0	-4.469920	-0.408167	-0.647888
78	6	0	-2.889025	1.550723	-0.723541
79	6	0	-3.558414	0.531495	-1.392306
80	8	0	-3.447931	0.334730	-2.675383
81	1	0	-5.157122	-0.853884	-1.381059
82	1	0	-3.884446	-1.242538	-0.225826
83	1	0	-2.622829	2.406966	-1.349161
84	6	0	-4.225516	0.981611	1.393620
85	1	0	-4.768256	1.541582	2.172398
86	1	0	-3.696044	0.180864	1.930961
87	6	0	-5.239944	0.297331	0.470884
88	6	0	-6.224986	1.297785	-0.132998
89	6	0	-6.016229	-0.735977	1.280833
90	1	0	-5.729734	2.004948	-0.808486
91	1	0	-6.729324	1.874231	0.654626
92	1	0	-6.996417	0.774380	-0.713651
93	1	0	-5.338292	-1.479429	1.723747
94	1	0	-6.574315	-0.258511	2.097827
95	1	0	-6.737252	-1.272137	0.649595
96	1	0	-2.277450	1.847837	1.325076
97	6	0	-3.627035	3.385147	0.805378
98	1	0	-3.815837	3.682438	1.845040
99	1	0	-4.540936	3.576088	0.228830
100	1	0	-2.841234	4.040891	0.407073

Zero-point correction= 0.798817 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.718748
Sum of electronic and zero-point Energies= -4514.717787
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.539952 (a.u.)

S−out−COM3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.269285	1.006480	3.640649
2	6	0	1.102062	-0.080346	3.749865
3	6	0	1.782521	-0.587027	2.651616
4	6	0	1.660473	-0.066323	1.380505
5	6	0	0.869052	1.110470	1.263389
6	6	0	0.174923	1.597658	2.372666
7	6	0	2.326999	-0.756891	0.246227
8	6	0	3.700209	-0.711319	0.141432
9	6	0	4.405758	-1.309911	-0.893950

10	6	0	3.766695	-1.995962	-1.897513
11	6	0	2.370386	-2.086288	-1.802543
12	6	0	1.650594	-1.514497	-0.753890
13	8	0	1.386050	-0.832040	4.849474
14	6	0	2.290588	-1.837627	4.421020
15	8	0	4.571264	-0.090044	0.986526
16	6	0	5.849067	-0.205635	0.381697
17	8	0	5.739380	-1.093304	-0.720090
18	8	0	2.516249	-1.670578	3.030337
19	15	0	0.545881	1.768003	-0.410515
20	15	0	-0.184861	-1.586531	-0.745569
21	1	0	-0.282245	1.388830	4.493685
22	1	0	-0.473019	2.463884	2.255335
23	1	0	4.315636	-2.448851	-2.717061
24	1	0	1.831355	-2.626618	-2.577081
25	1	0	1.848160	-2.827964	4.602772
26	1	0	3.242495	-1.735025	4.961765
27	1	0	6.564541	-0.609243	1.108895
28	1	0	6.175086	0.783378	0.021819
29	6	0	-0.605713	-3.012304	-1.824070
30	6	0	-0.046283	-4.287523	-1.675697
31	6	0	-1.601072	-2.816981	-2.782999
32	6	0	-0.461735	-5.337778	-2.482850
33	1	0	0.726935	-4.461719	-0.929263
34	6	0	-2.024384	-3.873601	-3.585879
35	1	0	-2.043045	-1.828529	-2.900031
36	6	0	-1.453530	-5.131320	-3.440285
37	1	0	-0.014660	-6.322310	-2.362634
38	1	0	-2.801408	-3.706156	-4.327958
39	1	0	-1.780067	-5.956146	-4.070043
40	6	0	-0.555976	-2.264090	0.919847
41	6	0	-1.730696	-1.826745	1.531782
42	6	0	0.234518	-3.214166	1.572630
43	6	0	-2.109506	-2.313321	2.778858
44	1	0	-2.341935	-1.089238	1.013120
45	6	0	-0.147423	-3.710112	2.814191
46	1	0	1.174547	-3.541446	1.129447
47	6	0	-1.315429	-3.256100	3.423542
48	1	0	-3.024684	-1.952956	3.246066
49	1	0	0.472108	-4.455699	3.310728
50	1	0	-1.606546	-3.640641	4.398559
51	6	0	0.069316	3.528995	-0.218130
52	6	0	-0.684191	4.058922	-1.271750
53	6	0	0.468861	4.376737	0.819528
54	6	0	-1.058832	5.398097	-1.271924
55	1	0	-0.972744	3.408862	-2.099987
56	6	0	0.081187	5.712322	0.825513
57	1	0	1.079160	3.993145	1.635059
58	6	0	-0.687335	6.223981	-0.216253
59	1	0	-1.647928	5.793682	-2.095902
60	1	0	0.386237	6.358000	1.646176
61	1	0	-0.990572	7.268409	-0.207312
62	6	0	2.198296	1.964434	-1.177013
63	6	0	2.331921	1.639060	-2.527868
64	6	0	3.287922	2.500247	-0.484642
65	6	0	3.551384	1.825279	-3.173812
66	1	0	1.475917	1.221708	-3.060606
67	6	0	4.501386	2.693017	-1.133635
68	1	0	3.190801	2.751431	0.571417
69	6	0	4.635206	2.350326	-2.478680
70	1	0	3.652550	1.560250	-4.223719
71	1	0	5.343828	3.121234	-0.592560
72	1	0	5.586759	2.499530	-2.984663
73	29	0	-0.862715	0.423766	-1.457981
74	1	0	-1.181444	0.591719	-3.012452
75	1	0	-2.744183	0.348677	-2.895091
76	6	0	-3.291077	1.383724	0.868357
77	6	0	-4.996000	-0.459137	-0.763285
78	6	0	-3.040167	1.083129	-0.588006

79	6	0	-3.830606	0.280567	-1.338225
80	8	0	-3.667558	0.058946	-2.650578
81	1	0	-5.747577	-0.585718	-1.556054
82	1	0	-4.670291	-1.478276	-0.489405
83	1	0	-2.337653	1.743800	-1.111083
84	6	0	-4.471699	0.576226	1.435457
85	1	0	-4.890895	1.104462	2.306592
86	1	0	-4.100621	-0.386517	1.821733
87	6	0	-5.602536	0.248449	0.451283
88	6	0	-6.350608	1.502119	-0.004733
89	6	0	-6.594138	-0.686120	1.137168
90	1	0	-5.722352	2.154483	-0.621504
91	1	0	-6.703818	2.083418	0.857872
92	1	0	-7.228532	1.225717	-0.603927
93	1	0	-6.099635	-1.600294	1.492618
94	1	0	-7.062057	-0.196994	2.002132
95	1	0	-7.395367	-0.983944	0.447623
96	1	0	-2.396735	1.084542	1.447613
97	6	0	-3.442172	2.889175	1.100376
98	1	0	-3.535688	3.110484	2.171913
99	1	0	-4.325997	3.294407	0.594663
100	1	0	-2.569064	3.435364	0.718286

Zero-point correction= 0.803356 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.722230
Sum of electronic and zero-point Energies= -4514.718215
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.545863 (a.u.)

R-out-COM3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.925968	-1.245827	3.602639
2	6	0	-2.795181	-0.224004	3.312918
3	6	0	-2.888670	0.303181	2.032699
4	6	0	-2.109803	-0.122195	0.976215
5	6	0	-1.181150	-1.161332	1.263992
6	6	0	-1.125250	-1.705022	2.546691
7	6	0	-2.382053	0.461067	-0.365181
8	6	0	-3.537749	0.081191	-1.015838
9	6	0	-3.922624	0.591412	-2.249857
10	6	0	-3.184322	1.559193	-2.886750
11	6	0	-2.009957	1.976024	-2.244405
12	6	0	-1.599806	1.452762	-1.020506
13	8	0	-3.688346	0.398307	4.130893
14	6	0	-4.281287	1.426057	3.350490
15	8	0	-4.477271	-0.809528	-0.584520
16	6	0	-5.293856	-1.055168	-1.716511
17	8	0	-5.099402	0.016077	-2.629089
18	8	0	-3.857044	1.263383	2.008104
19	15	0	-0.062003	-1.692626	-0.102771
20	15	0	0.079261	1.772217	-0.363351
21	1	0	-1.868619	-1.682728	4.594748
22	1	0	-0.446334	-2.528254	2.748046
23	1	0	-3.492319	1.974173	-3.841350
24	1	0	-1.392200	2.725563	-2.732930
25	1	0	-3.946463	2.407203	3.725343
26	1	0	-5.373978	1.344184	3.403514
27	1	0	-6.344509	-1.088938	-1.411228
28	1	0	-4.979680	-2.003844	-2.188211
29	29	0	1.146729	-0.070794	-1.011636
30	6	0	0.693684	3.287035	-1.186879
31	6	0	0.917288	4.490564	-0.512299
32	6	0	1.098287	3.177279	-2.525928
33	6	0	1.509860	5.566937	-1.166933
34	1	0	0.634175	4.590770	0.533380
35	6	0	1.675429	4.259036	-3.179761

36	1	0	0.971560	2.221877	-3.039552
37	6	0	1.883929	5.457642	-2.501346
38	1	0	1.679944	6.496196	-0.627387
39	1	0	1.976843	4.160641	-4.220280
40	1	0	2.346725	6.300319	-3.010128
41	6	0	-0.254670	2.313451	1.354476
42	6	0	0.516199	1.785133	2.392163
43	6	0	-1.282674	3.211777	1.660514
44	6	0	0.269843	2.149112	3.712522
45	1	0	1.293942	1.056318	2.159783
46	6	0	-1.520358	3.588062	2.977416
47	1	0	-1.909625	3.602580	0.858731
48	6	0	-0.747425	3.051720	4.005878
49	1	0	0.866525	1.720135	4.514144
50	1	0	-2.313751	4.298687	3.203478
51	1	0	-0.941395	3.336562	5.037772
52	6	0	0.892784	-3.099377	0.572501
53	6	0	1.005995	-4.294611	-0.143842
54	6	0	1.678043	-2.929994	1.721676
55	6	0	1.856282	-5.305112	0.294913
56	1	0	0.426633	-4.435453	-1.054171
57	6	0	2.498823	-3.954941	2.177783
58	1	0	1.654851	-1.980658	2.258342
59	6	0	2.592973	-5.146023	1.463062
60	1	0	1.935928	-6.225633	-0.278867
61	1	0	3.081283	-3.816316	3.086583
62	1	0	3.245916	-5.942364	1.812218
63	6	0	-1.274194	-2.499194	-1.224831
64	6	0	-1.253778	-2.208091	-2.588900
65	6	0	-2.232096	-3.386654	-0.721446
66	6	0	-2.178648	-2.804327	-3.443337
67	1	0	-0.515673	-1.493054	-2.959040
68	6	0	-3.146339	-3.988541	-1.576467
69	1	0	-2.260021	-3.601395	0.346968
70	6	0	-3.117398	-3.699276	-2.941168
71	1	0	-2.161414	-2.569244	-4.505196
72	1	0	-3.883933	-4.683703	-1.180366
73	1	0	-3.833346	-4.171625	-3.611513
74	1	0	2.420286	-0.859666	-2.881369
75	1	0	0.989089	-0.098877	-2.655414
76	1	0	2.853992	1.829059	0.639362
77	6	0	3.481096	-0.708067	-1.335826
78	6	0	4.205080	-1.605320	-0.380795
79	6	0	3.210253	0.612012	-1.084523
80	6	0	3.706631	1.317545	0.156421
81	6	0	4.258609	0.326032	1.185684
82	6	0	5.078689	-0.840652	0.618978
83	8	0	3.235457	-1.298992	-2.520473
84	6	0	5.470085	-1.767196	1.765974
85	6	0	6.360027	-0.376516	-0.076205
86	1	0	4.820767	-2.288783	-0.984348
87	1	0	3.483882	-2.246189	0.148045
88	1	0	3.408256	-0.121882	1.729506
89	1	0	4.854619	0.866405	1.938341
90	1	0	3.016963	1.256879	-1.943070
91	6	0	4.673539	2.442264	-0.220814
92	1	0	5.543232	2.081658	-0.780254
93	1	0	4.163005	3.182933	-0.850619
94	1	0	5.037506	2.962684	0.674268
95	1	0	5.944330	-2.682901	1.387032
96	1	0	4.592014	-2.065571	2.352930
97	1	0	6.180297	-1.274497	2.443621
98	1	0	6.158071	0.122993	-1.030116
99	1	0	7.002869	-1.240495	-0.291916
100	1	0	6.929552	0.315134	0.559575

Zero-point correction= 0.803976 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.723722
Sum of electronic and zero-point Energies= -4514.721758

SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.548217 (a.u.)

S−out−COM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.709327	0.991212	3.664526
2	6	0	1.456449	-0.161550	3.684381
3	6	0	1.953236	-0.727221	2.517753
4	6	0	1.730304	-0.194545	1.266023
5	6	0	1.013808	1.034987	1.231424
6	6	0	0.498343	1.577663	2.408592
7	6	0	2.233274	-0.907331	0.065263
8	6	0	3.588952	-0.940935	-0.183616
9	6	0	4.141879	-1.527355	-1.313662
10	6	0	3.356106	-2.118555	-2.272175
11	6	0	1.975398	-2.135625	-2.026810
12	6	0	1.408304	-1.580672	-0.879418
13	8	0	1.825623	-0.921416	4.751395
14	6	0	2.491381	-2.056095	4.216826
15	8	0	4.580187	-0.408562	0.585034
16	6	0	5.789953	-0.624288	-0.124708
17	8	0	5.496363	-1.391106	-1.282185
18	8	0	2.637407	-1.865374	2.818697
19	15	0	0.578479	1.775023	-0.387891
20	15	0	-0.418088	-1.561581	-0.657508
21	1	0	0.304533	1.422895	4.574525
22	1	0	-0.082540	2.495725	2.357793
23	1	0	3.783571	-2.556454	-3.168684
24	1	0	1.327785	-2.612548	-2.758125
25	1	0	1.884192	-2.956321	4.402482
26	1	0	3.481953	-2.153329	4.679735
27	1	0	6.495554	-1.173924	0.512022
28	1	0	6.214566	0.344888	-0.428063
29	6	0	-1.006084	-2.957598	-1.696029
30	6	0	-0.381858	-4.213920	-1.710233
31	6	0	-2.174313	-2.775168	-2.441388
32	6	0	-0.908230	-5.258267	-2.456861
33	1	0	0.540601	-4.373890	-1.155506
34	6	0	-2.700348	-3.828685	-3.187897
35	1	0	-2.695686	-1.815655	-2.455324
36	6	0	-2.072875	-5.066783	-3.197968
37	1	0	-0.408516	-6.224563	-2.461810
38	1	0	-3.608529	-3.665724	-3.763224
39	1	0	-2.485539	-5.885384	-3.783783
40	6	0	-0.622819	-2.191170	1.057556
41	6	0	-1.458235	-1.477768	1.917057
42	6	0	0.006154	-3.345677	1.534017
43	6	0	-1.670349	-1.902511	3.225234
44	1	0	-1.933105	-0.568126	1.550326
45	6	0	-0.216480	-3.782925	2.834483
46	1	0	0.688156	-3.903779	0.895586
47	6	0	-1.053552	-3.060822	3.684411
48	1	0	-2.315820	-1.321920	3.881609
49	1	0	0.267702	-4.691492	3.188455
50	1	0	-1.220853	-3.402178	4.703773
51	6	0	0.266443	3.549986	-0.035552
52	6	0	-0.709952	4.181092	-0.809027
53	6	0	1.023182	4.321290	0.854625
54	6	0	-0.935615	5.549874	-0.691525
55	1	0	-1.307278	3.586359	-1.499417
56	6	0	0.792319	5.685164	0.979415
57	1	0	1.790377	3.851480	1.467184
58	6	0	-0.187455	6.302518	0.205213
59	1	0	-1.703148	6.023636	-1.299665
60	1	0	1.382838	6.270698	1.680632
61	1	0	-0.365566	7.370942	0.303463

62	6	0	2.186898	1.899452	-1.269116
63	6	0	2.210536	1.662330	-2.644046
64	6	0	3.367571	2.287020	-0.627224
65	6	0	3.394346	1.790943	-3.365445
66	1	0	1.295149	1.358273	-3.152261
67	6	0	4.546983	2.427076	-1.348107
68	1	0	3.373097	2.458954	0.448505
69	6	0	4.563746	2.173481	-2.718348
70	1	0	3.400556	1.593134	-4.434709
71	1	0	5.457566	2.739120	-0.838905
72	1	0	5.489198	2.277521	-3.280364
73	29	0	-1.169942	0.538596	-1.051779
74	1	0	-0.841979	0.480050	-3.017193
75	1	0	-1.595970	0.356489	-2.922594
76	6	0	-3.411128	2.154385	0.343518
77	6	0	-4.414915	-0.572274	-0.401082
78	6	0	-2.977528	1.454878	-0.946910
79	6	0	-3.700557	0.305217	-1.421335
80	8	0	-3.732921	-0.039079	-2.621449
81	1	0	-5.105276	-1.222352	-0.956895
82	1	0	-3.680132	-1.235739	0.084989
83	1	0	-2.881785	2.170830	-1.777147
84	6	0	-4.171909	1.225953	1.301271
85	1	0	-4.707450	1.834503	2.048650
86	1	0	-3.440451	0.635687	1.877439
87	6	0	-5.155878	0.233006	0.668286
88	6	0	-6.356659	0.932408	0.027241
89	6	0	-5.673636	-0.706066	1.753820
90	1	0	-6.083537	1.473080	-0.885776
91	1	0	-6.819928	1.645426	0.723257
92	1	0	-7.117113	0.191450	-0.253584
93	1	0	-4.849766	-1.237445	2.249698
94	1	0	-6.230576	-0.152489	2.522601
95	1	0	-6.348287	-1.461013	1.328453
96	1	0	-2.516422	2.486219	0.900253
97	6	0	-4.184270	3.438849	0.033273
98	1	0	-4.534240	3.930697	0.951245
99	1	0	-5.054141	3.258633	-0.608972
100	1	0	-3.536087	4.151150	-0.494411

Zero-point correction= 0.802115 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.721165
Sum of electronic and zero-point Energies= -4514.726804
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.55391 (a.u.)

R−out−COM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.446525	-1.801450	3.228334
2	6	0	-3.483779	-1.126249	2.634067
3	6	0	-3.385765	-0.637948	1.336962
4	6	0	-2.251793	-0.767427	0.562116
5	6	0	-1.162341	-1.451352	1.168299
6	6	0	-1.282438	-1.955711	2.462163
7	6	0	-2.305244	-0.249039	-0.833626
8	6	0	-2.993331	-0.976215	-1.779324
9	6	0	-3.220430	-0.523203	-3.076023
10	6	0	-2.821095	0.726631	-3.479757
11	6	0	-2.112167	1.490215	-2.540451
12	6	0	-1.832462	1.027180	-1.256985
13	8	0	-4.718618	-0.848838	3.133508
14	6	0	-5.365920	-0.049718	2.154366
15	8	0	-3.587754	-2.195168	-1.621161
16	6	0	-3.861454	-2.624523	-2.944691
17	8	0	-3.925340	-1.465480	-3.762305
18	8	0	-4.563490	-0.047289	0.985977

19	15	0	0.424338	-1.518749	0.254942
20	15	0	-0.610008	1.852780	-0.177060
21	1	0	-2.527338	-2.198159	4.235457
22	1	0	-0.442676	-2.484349	2.905152
23	1	0	-3.027866	1.096586	-4.478890
24	1	0	-1.748190	2.469274	-2.841834
25	1	0	-5.464801	0.980666	2.532626
26	1	0	-6.350244	-0.475421	1.925074
27	1	0	-4.822009	-3.146214	-2.971414
28	1	0	-3.036405	-3.274854	-3.288410
29	29	0	1.160018	0.497207	-0.272116
30	6	0	-0.311973	3.509796	-0.879926
31	6	0	-0.587908	4.685688	-0.177819
32	6	0	0.367826	3.597177	-2.104471
33	6	0	-0.213638	5.921838	-0.696251
34	1	0	-1.094514	4.638913	0.783960
35	6	0	0.725650	4.833827	-2.626031
36	1	0	0.625365	2.690629	-2.651648
37	6	0	0.437507	5.999956	-1.921816
38	1	0	-0.434359	6.827950	-0.136414
39	1	0	1.245201	4.884416	-3.579964
40	1	0	0.729360	6.966755	-2.325295
41	6	0	-1.510229	2.171821	1.377206
42	6	0	-0.868340	1.905370	2.588179
43	6	0	-2.818126	2.666695	1.388542
44	6	0	-1.525847	2.120181	3.795536
45	1	0	0.150087	1.513499	2.579928
46	6	0	-3.469831	2.894878	2.594908
47	1	0	-3.323896	2.869236	0.444365
48	6	0	-2.826412	2.613538	3.799104
49	1	0	-1.022598	1.902446	4.734558
50	1	0	-4.481367	3.297433	2.597713
51	1	0	-3.339761	2.784321	4.742735
52	6	0	1.561182	-2.364320	1.411686
53	6	0	2.079553	-3.636400	1.167332
54	6	0	2.010141	-1.650457	2.530933
55	6	0	3.030841	-4.183189	2.025625
56	1	0	1.748695	-4.197751	0.295116
57	6	0	2.944486	-2.203963	3.395296
58	1	0	1.620757	-0.648941	2.724250
59	6	0	3.461960	-3.473137	3.139616
60	1	0	3.435509	-5.171477	1.819899
61	1	0	3.283849	-1.638069	4.260211
62	1	0	4.206459	-3.901460	3.806549
63	6	0	0.154924	-2.740220	-1.068944
64	6	0	1.053093	-2.747322	-2.142708
65	6	0	-0.857529	-3.701828	-0.999034
66	6	0	0.923765	-3.709719	-3.139464
67	1	0	1.850967	-1.999455	-2.214823
68	6	0	-0.980921	-4.657093	-2.002569
69	1	0	-1.559960	-3.695927	-0.166703
70	6	0	-0.090214	-4.660624	-3.074020
71	1	0	1.619730	-3.708149	-3.974809
72	1	0	-1.769044	-5.405698	-1.941884
73	1	0	-0.186784	-5.409451	-3.857580
74	1	0	0.922848	0.049876	-3.187156
75	1	0	0.182571	0.146825	-3.290541
76	1	0	2.784458	2.449081	1.012683
77	6	0	3.387794	0.116943	-1.391952
78	6	0	4.332157	-0.723545	-0.539241
79	6	0	2.858877	1.333335	-0.836633
80	6	0	3.550435	2.063856	0.310314
81	6	0	4.425383	1.114924	1.139192
82	6	0	5.264819	0.100480	0.351174
83	8	0	3.078417	-0.318067	-2.520858
84	6	0	5.976460	-0.818817	1.340922
85	6	0	6.325585	0.773396	-0.522608
86	1	0	4.907814	-1.355683	-1.230174
87	1	0	3.737151	-1.411325	0.084552

88	1	0	3.769715	0.530305	1.808859
89	1	0	5.087182	1.702614	1.797174
90	1	0	2.541431	2.012701	-1.639452
91	6	0	4.278645	3.315173	-0.184268
92	1	0	5.022208	3.089046	-0.956442
93	1	0	3.553272	4.012451	-0.625854
94	1	0	4.788456	3.838545	0.636774
95	1	0	6.537904	-1.601861	0.812942
96	1	0	5.260490	-1.314797	2.011289
97	1	0	6.689017	-0.255165	1.959865
98	1	0	5.886341	1.284220	-1.386768
99	1	0	7.023431	0.020653	-0.913585
100	1	0	6.908154	1.508447	0.050158

Zero-point correction= 0.802014 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.720830
Sum of electronic and zero-point Energies= -4514.732756
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.560408 (a.u.)

Product:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.974843	-1.680012	0.223250
2	1	0	1.042509	1.849618	-1.550180
3	6	0	1.230333	-0.977795	-0.070878
4	6	0	-0.189442	-1.431226	-0.172487
5	6	0	1.624493	0.287650	-0.249626
6	6	0	0.691064	1.411517	-0.599995
7	6	0	-0.732376	0.895320	-0.860025
8	6	0	-1.188718	-0.284044	0.009421
9	8	0	2.069620	-2.012291	0.211798
10	6	0	-2.566957	-0.736979	-0.463016
11	6	0	-1.284031	0.086027	1.490195
12	1	0	-0.361911	-2.215462	0.580069
13	1	0	-0.341370	-1.914241	-1.151855
14	1	0	-0.793061	0.561206	-1.907872
15	1	0	-1.452207	1.722980	-0.759521
16	1	0	2.684615	0.536579	-0.146913
17	6	0	0.759534	2.542645	0.428423
18	1	0	0.425776	2.219275	1.420247
19	1	0	1.788918	2.907777	0.533094
20	1	0	0.135202	3.391247	0.121292
21	1	0	-2.896659	-1.627637	0.088562
22	1	0	-2.561922	-0.985432	-1.532521
23	1	0	-3.315161	0.050864	-0.303900
24	1	0	-0.297571	0.254730	1.935587
25	1	0	-1.765576	-0.725067	2.052756
26	1	0	-1.886784	0.993208	1.631445

Zero-point correction= 0.234852 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.200588
Sum of electronic and zero-point Energies= -427.272208
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -427.5143545 (a.u.)

R−in−TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.976670	0.794923	-2.017279
2	6	0	2.189289	-2.468323	-2.954682
3	6	0	3.287692	-1.919090	-2.340515
4	6	0	3.186474	-1.295186	-1.105624
5	6	0	1.995008	-1.146844	-0.424970
6	6	0	0.846232	-1.706482	-1.045752

7	6	0	0.967369	-2.347893	-2.278231
8	6	0	2.031791	-0.492545	0.906629
9	6	0	2.609551	-1.178215	1.954374
10	6	0	2.760005	-0.641172	3.225150
11	6	0	2.359548	0.640420	3.510376
12	6	0	1.780071	1.365835	2.459637
13	6	0	1.599803	0.833038	1.184548
14	8	0	4.585399	-1.908762	-2.753149
15	6	0	5.291914	-1.136653	-1.794114
16	8	0	3.122800	-2.441651	1.932005
17	6	0	3.447066	-2.749768	3.277331
18	8	0	3.364041	-1.553342	4.036612
19	8	0	4.423123	-0.884134	-0.702739
20	15	0	-0.803062	-1.414723	-0.278973
21	15	0	0.699814	1.735946	-0.145460
22	1	0	2.264494	-2.974386	-3.912047
23	1	0	0.086400	-2.782513	-2.740952
24	1	0	2.486535	1.073140	4.497841
25	1	0	1.466366	2.384548	2.664750
26	1	0	5.595524	-0.179827	-2.248596
27	1	0	6.168172	-1.696618	-1.445123
28	1	0	4.467690	-3.147335	3.328122
29	1	0	2.720856	-3.481241	3.668965
30	29	0	-1.337355	0.755999	-0.582851
31	6	0	0.606298	3.462907	0.463166
32	6	0	1.169915	4.527266	-0.246168
33	6	0	-0.151017	3.745811	1.611968
34	6	0	1.005205	5.837799	0.193307
35	1	0	1.744290	4.334454	-1.149867
36	6	0	-0.302910	5.054853	2.052840
37	1	0	-0.647268	2.942162	2.158416
38	6	0	0.276804	6.104793	1.346653
39	1	0	1.453738	6.652764	-0.370585
40	1	0	-0.888648	5.251679	2.947565
41	1	0	0.152381	7.129084	1.690490
42	6	0	1.940696	1.824314	-1.490588
43	6	0	1.508599	1.612688	-2.801286
44	6	0	3.290130	2.099284	-1.247449
45	6	0	2.415235	1.661872	-3.856459
46	1	0	0.454903	1.389277	-2.982345
47	6	0	4.191938	2.162426	-2.303179
48	1	0	3.633040	2.254287	-0.224426
49	6	0	3.756286	1.934765	-3.608321
50	1	0	2.073277	1.484051	-4.873384
51	1	0	5.239050	2.388704	-2.108503
52	1	0	4.465455	1.975326	-4.432479
53	6	0	-1.876838	-2.622463	-1.150423
54	6	0	-2.372556	-3.781577	-0.552296
55	6	0	-2.278200	-2.312092	-2.456998
56	6	0	-3.238266	-4.621078	-1.249186
57	1	0	-2.099167	-4.027775	0.471363
58	6	0	-3.126629	-3.160229	-3.157481
59	1	0	-1.939063	-1.379372	-2.909685
60	6	0	-3.610775	-4.318345	-2.553291
61	1	0	-3.622446	-5.516726	-0.765987
62	1	0	-3.423375	-2.908456	-4.173306
63	1	0	-4.284334	-4.977030	-3.096803
64	6	0	-0.622117	-2.081474	1.413834
65	6	0	-1.113719	-1.315684	2.475316
66	6	0	0.015205	-3.298942	1.679883
67	6	0	-0.979196	-1.769161	3.784645
68	1	0	-1.587874	-0.349369	2.285486
69	6	0	0.133406	-3.755995	2.986913
70	1	0	0.431388	-3.883379	0.859009
71	6	0	-0.359320	-2.987599	4.041114
72	1	0	-1.359155	-1.160663	4.601806
73	1	0	0.614749	-4.712592	3.184954
74	1	0	-0.257781	-3.342199	5.064774
75	6	0	-3.493910	1.559455	1.435771

76	6	0	-4.906025	1.127934	1.095629
77	6	0	-2.664807	2.007630	0.337193
78	6	0	-3.016475	1.877949	-1.044623
79	6	0	-4.370541	1.262711	-1.353627
80	8	0	-3.139624	1.636330	2.614055
81	1	0	-5.501322	2.057268	1.098011
82	1	0	-5.294247	0.504410	1.912371
83	1	0	-4.338020	0.688815	-2.292246
84	1	0	-5.025748	2.130091	-1.557059
85	1	0	-2.009618	2.832686	0.608060
86	6	0	-2.693894	3.060071	-1.930796
87	1	0	-3.391869	3.880800	-1.704464
88	1	0	-1.675454	3.430268	-1.760920
89	1	0	-2.788952	2.806450	-2.993676
90	6	0	-5.062998	0.432830	-0.257419
91	6	0	-4.518111	-0.986772	-0.150437
92	6	0	-6.546662	0.338911	-0.611039
93	1	0	-5.124130	-1.571728	0.554523
94	1	0	-3.486806	-1.002956	0.219466
95	1	0	-4.538705	-1.499177	-1.120563
96	1	0	-7.007872	1.333436	-0.675300
97	1	0	-7.092070	-0.237154	0.147895
98	1	0	-6.688016	-0.161994	-1.578537
99	1	0	-0.791032	1.538218	4.557876
100	1	0	-1.331934	1.553948	4.039350

Zero-point correction= 0.796785 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.716552
Sum of electronic and zero-point Energies= -4514.703369
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.5232251 (a.u.)

R–in–TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.680189	-0.372498	-1.455970
2	6	0	-3.598493	1.772154	-0.524398
3	6	0	-3.926135	1.597615	0.933074
4	6	0	-4.441855	1.374340	-1.496413
5	6	0	-5.765302	0.711520	-1.240452
6	6	0	-6.179705	0.868039	0.220963
7	6	0	-5.042142	0.583511	1.205795
8	8	0	-2.422846	2.374821	-0.754513
9	6	0	-5.539942	0.744578	2.637268
10	6	0	-4.523995	-0.842018	1.018170
11	1	0	-4.206938	2.580300	1.349096
12	1	0	-3.003492	1.308397	1.465849
13	1	0	-7.038178	0.211787	0.441192
14	1	0	-6.526725	1.904580	0.378917
15	1	0	-4.160972	1.556241	-2.536800
16	6	0	-6.843520	1.267210	-2.164340
17	1	0	-6.969846	2.345643	-1.999393
18	1	0	-6.577075	1.123410	-3.219121
19	1	0	-7.812303	0.779782	-1.991395
20	1	0	-5.972098	1.741193	2.800850
21	1	0	-4.715733	0.611694	3.353464
22	1	0	-6.311495	-0.001091	2.872943
23	1	0	-4.023726	-0.966714	0.051010
24	1	0	-5.346725	-1.569439	1.069814
25	1	0	-3.798492	-1.103996	1.802077
26	6	0	2.041300	-2.549292	-2.985267
27	6	0	3.210055	-2.211621	-2.347968
28	6	0	3.210207	-1.606423	-1.097705
29	6	0	2.057863	-1.269434	-0.418303
30	6	0	0.837867	-1.645087	-1.051496
31	6	0	0.851702	-2.255206	-2.304530
32	6	0	2.177892	-0.598408	0.904263

33	6	0	2.649329	-1.313953	1.984512
34	6	0	2.801693	-0.765583	3.251889
35	6	0	2.500829	0.549072	3.510362
36	6	0	2.046355	1.312085	2.424676
37	6	0	1.893334	0.774917	1.147903
38	8	0	4.492912	-2.415606	-2.755559
39	6	0	5.318043	-1.810193	-1.772099
40	8	0	3.026902	-2.624251	2.009565
41	6	0	3.293678	-2.927484	3.368644
42	8	0	3.283267	-1.713842	4.103446
43	8	0	4.495701	-1.420652	-0.683997
44	15	0	-0.764494	-1.117570	-0.328011
45	15	0	1.214455	1.780736	-0.226470
46	1	0	2.041507	-3.026483	-3.960094
47	1	0	-0.094660	-2.516009	-2.773284
48	1	0	2.619553	0.975840	4.501381
49	1	0	1.809282	2.360480	2.591283
50	1	0	5.803418	-0.918337	-2.200551
51	1	0	6.066683	-2.532668	-1.423980
52	1	0	4.279894	-3.400139	3.453848
53	1	0	2.507105	-3.595778	3.755763
54	29	0	-0.745074	1.006790	-0.858052
55	6	0	1.196581	3.474235	0.450456
56	6	0	2.334577	4.275654	0.582061
57	6	0	-0.042129	3.953134	0.890161
58	6	0	2.238058	5.534091	1.163323
59	1	0	3.298134	3.916750	0.223004
60	6	0	-0.130779	5.210265	1.480787
61	1	0	-0.942774	3.357226	0.727058
62	6	0	1.006610	5.998209	1.620141
63	1	0	3.125311	6.156101	1.258538
64	1	0	-1.096312	5.579371	1.818393
65	1	0	0.933213	6.983765	2.074945
66	6	0	2.565555	1.720364	-1.456153
67	6	0	2.219809	1.655256	-2.808730
68	6	0	3.916569	1.702041	-1.095097
69	6	0	3.206757	1.562333	-3.784347
70	1	0	1.165400	1.659996	-3.087731
71	6	0	4.902799	1.630197	-2.072610
72	1	0	4.197662	1.708780	-0.042018
73	6	0	4.549151	1.551634	-3.417962
74	1	0	2.925898	1.497069	-4.832747
75	1	0	5.952069	1.624960	-1.782006
76	1	0	5.321791	1.480333	-4.180709
77	6	0	-2.033912	-2.165453	-1.134982
78	6	0	-2.496052	-3.379615	-0.620570
79	6	0	-2.651436	-1.631697	-2.272642
80	6	0	-3.553854	-4.045099	-1.230789
81	1	0	-2.058202	-3.796215	0.283668
82	6	0	-3.702891	-2.302788	-2.886330
83	1	0	-2.328467	-0.660468	-2.647960
84	6	0	-4.160030	-3.508139	-2.362277
85	1	0	-3.914041	-4.982042	-0.811765
86	1	0	-4.182654	-1.864786	-3.759082
87	1	0	-4.995547	-4.024116	-2.830018
88	6	0	-0.670370	-1.733031	1.391181
89	6	0	-1.106354	-0.908435	2.431203
90	6	0	-0.174820	-3.005192	1.697088
91	6	0	-1.070041	-1.352518	3.749418
92	1	0	-1.462305	0.097563	2.206387
93	6	0	-0.153047	-3.455860	3.012096
94	1	0	0.214397	-3.639680	0.900668
95	6	0	-0.599988	-2.628949	4.040558
96	1	0	-1.408561	-0.698192	4.549392
97	1	0	0.217001	-4.455207	3.235287
98	1	0	-0.577551	-2.979272	5.070086
99	1	0	-1.867656	1.914986	-1.833085
100	1	0	-1.274280	1.412862	-2.441184

Zero-point correction= 0.798450 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.716829
Sum of electronic and zero-point Energies= -4514.711241
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.5328813 (a.u.)

S−in−TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.023769	1.758430	-1.515241
2	6	0	4.558421	0.267414	-1.479608
3	6	0	2.437700	1.739988	1.213402
4	6	0	2.681294	2.484591	0.009852
5	6	0	4.115092	2.523643	-0.466750
6	6	0	3.388602	0.797091	1.751889
7	6	0	4.715477	0.594866	1.033951
8	8	0	3.204958	0.186812	2.811088
9	1	0	1.697877	2.107594	1.924383
10	1	0	4.600817	3.287032	0.169986
11	1	0	4.165533	2.904482	-1.498665
12	1	0	4.919047	-0.486758	1.012317
13	1	0	5.452705	1.009607	1.740285
14	6	0	2.012259	3.833180	-0.095981
15	1	0	2.556881	4.547405	0.538868
16	1	0	2.017869	4.214712	-1.124251
17	1	0	0.970813	3.812623	0.246720
18	6	0	4.926216	1.230166	-0.352914
19	6	0	6.406983	1.575287	-0.514907
20	1	0	3.498855	-0.007911	-1.454959
21	1	0	4.745003	0.737061	-2.455486
22	1	0	5.165707	-0.645477	-1.416379
23	1	0	6.602006	2.018453	-1.501004
24	1	0	7.027960	0.674092	-0.423235
25	1	0	6.737093	2.291526	0.249273
26	6	0	-3.327462	-0.599550	-3.004085
27	6	0	-3.490722	-1.746836	-2.267306
28	6	0	-2.930818	-1.887293	-1.004332
29	6	0	-2.142476	-0.921809	-0.420988
30	6	0	-1.962231	0.278386	-1.167593
31	6	0	-2.553466	0.415853	-2.421223
32	6	0	-1.612931	-1.096941	0.952944
33	6	0	-2.497544	-1.021331	2.009931
34	6	0	-2.094519	-0.947480	3.335049
35	6	0	-0.764090	-0.913197	3.677693
36	6	0	0.160355	-1.031668	2.630751
37	6	0	-0.237156	-1.195265	1.300505
38	8	0	-4.199247	-2.867615	-2.576610
39	6	0	-3.951466	-3.787463	-1.523028
40	8	0	-3.856299	-0.935466	1.939694
41	6	0	-4.307331	-0.736494	3.270177
42	8	0	-3.189092	-0.840072	4.138730
43	8	0	-3.280291	-3.096315	-0.483060
44	15	0	-0.897271	1.589409	-0.431040
45	15	0	1.037919	-1.243816	-0.014016
46	1	0	-3.780957	-0.482819	-3.983475
47	1	0	-2.419284	1.341940	-2.974483
48	1	0	-0.441148	-0.772476	4.704703
49	1	0	1.218186	-0.916656	2.864806
50	1	0	-3.308571	-4.601974	-1.895304
51	1	0	-4.903485	-4.181797	-1.147676
52	1	0	-5.045628	-1.507171	3.526807
53	1	0	-4.745798	0.270785	3.358402
54	29	0	1.377508	0.941714	-0.334422
55	6	0	0.326304	-2.325776	-1.317884
56	6	0	-0.061752	-3.636974	-1.025231
57	6	0	0.232934	-1.859822	-2.628945
58	6	0	-0.554701	-4.461090	-2.028704

59	1	0	0.022689	-4.010961	-0.004921
60	6	0	-0.272330	-2.681907	-3.632530
61	1	0	0.547356	-0.840116	-2.856496
62	6	0	-0.665661	-3.982293	-3.333801
63	1	0	-0.845927	-5.483936	-1.795620
64	1	0	-0.356730	-2.305334	-4.649445
65	1	0	-1.055796	-4.627232	-4.118468
66	6	0	2.399828	-2.357653	0.528886
67	6	0	2.588270	-2.924256	1.789362
68	6	0	3.322222	-2.658858	-0.482394
69	6	0	3.691054	-3.737271	2.040309
70	1	0	1.876955	-2.749755	2.589054
71	6	0	4.418475	-3.472331	-0.233623
72	1	0	3.171132	-2.257064	-1.483730
73	6	0	4.612798	-4.006892	1.037206
74	1	0	3.823850	-4.161155	3.032970
75	1	0	5.122269	-3.688029	-1.034897
76	1	0	5.475088	-4.637603	1.240792
77	6	0	-1.058425	3.006263	-1.582665
78	6	0	-1.623540	4.225302	-1.201311
79	6	0	-0.448002	2.910289	-2.841083
80	6	0	-1.580976	5.323156	-2.057035
81	1	0	-2.087338	4.326280	-0.222129
82	6	0	-0.424883	4.000679	-3.701042
83	1	0	0.032421	1.978835	-3.137877
84	6	0	-0.985770	5.213464	-3.307804
85	1	0	-2.015672	6.268421	-1.739676
86	1	0	0.047545	3.907548	-4.676361
87	1	0	-0.953590	6.071806	-3.974959
88	6	0	-1.914530	2.092637	1.014543
89	6	0	-1.282731	2.338917	2.234127
90	6	0	-3.307391	2.208212	0.935131
91	6	0	-2.022752	2.692712	3.358485
92	1	0	-0.204070	2.222108	2.312756
93	6	0	-4.046655	2.573875	2.053568
94	1	0	-3.811816	1.999835	-0.008441
95	6	0	-3.404826	2.814265	3.268601
96	1	0	-1.514846	2.863005	4.305567
97	1	0	-5.128651	2.667256	1.980171
98	1	0	-3.986299	3.091147	4.145663
99	1	0	1.165798	1.719938	4.594614
100	1	0	1.619814	1.301222	4.168833

Zero-point correction= 0.797247 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.718613
Sum of electronic and zero-point Energies= -4514.700412
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.522531 (a.u.)

S−in−TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.230944	0.400529	3.770025
2	6	0	2.036186	-0.682309	3.512125
3	6	0	2.374635	-1.045602	2.216036
4	6	0	1.935960	-0.360865	1.101537
5	6	0	1.194892	0.826485	1.356034
6	6	0	0.819731	1.151257	2.660178
7	6	0	2.173926	-0.918488	-0.254360
8	6	0	3.442703	-0.929914	-0.791088
9	6	0	3.721616	-1.387380	-2.072073
10	6	0	2.739479	-1.896710	-2.885631
11	6	0	1.443536	-1.940527	-2.350684
12	6	0	1.147952	-1.485375	-1.067043
13	8	0	2.579041	-1.568043	4.392227
14	6	0	3.249129	-2.545025	3.609973
15	8	0	4.592075	-0.494388	-0.202868

16	6	0	5.601266	-0.587631	-1.195164
17	8	0	5.053011	-1.251184	-2.323711
18	8	0	3.125279	-2.182245	2.244121
19	15	0	0.541778	1.778999	-0.062933
20	15	0	-0.600840	-1.455859	-0.492230
21	1	0	0.930443	0.657450	4.780956
22	1	0	0.180958	2.015465	2.828267
23	1	0	2.957584	-2.249079	-3.888870
24	1	0	0.640517	-2.341642	-2.965113
25	1	0	2.779452	-3.527835	3.771448
26	1	0	4.311846	-2.574246	3.887593
27	1	0	6.448082	-1.165731	-0.804039
28	1	0	5.921578	0.425229	-1.486430
29	6	0	-1.431426	-2.723814	-1.538058
30	6	0	-1.068781	-4.076204	-1.570639
31	6	0	-2.514961	-2.303385	-2.312506
32	6	0	-1.777637	-4.981258	-2.349762
33	1	0	-0.224954	-4.434076	-0.986458
34	6	0	-3.229564	-3.212050	-3.088890
35	1	0	-2.802029	-1.254829	-2.328632
36	6	0	-2.865046	-4.551822	-3.107476
37	1	0	-1.481501	-6.027944	-2.362859
38	1	0	-4.070896	-2.858535	-3.680868
39	1	0	-3.422565	-5.263668	-3.712379
40	6	0	-0.461835	-2.303065	1.139391
41	6	0	-1.207516	-1.829022	2.219191
42	6	0	0.350592	-3.426716	1.335516
43	6	0	-1.181789	-2.479433	3.449794
44	1	0	-1.800385	-0.924983	2.100620
45	6	0	0.366677	-4.088767	2.557038
46	1	0	1.011774	-3.765615	0.538984
47	6	0	-0.407415	-3.621382	3.617303
48	1	0	-1.768686	-2.088869	4.278143
49	1	0	0.990923	-4.971989	2.682924
50	1	0	-0.392351	-4.137334	4.574845
51	6	0	0.378387	3.519679	0.506291
52	6	0	-0.409334	4.333536	-0.314880
53	6	0	1.056727	4.110445	1.577145
54	6	0	-0.543672	5.692925	-0.058008
55	1	0	-0.909281	3.892641	-1.176871
56	6	0	0.917640	5.469526	1.838873
57	1	0	1.699645	3.509846	2.216873
58	6	0	0.113549	6.262860	1.027320
59	1	0	-1.163783	6.306448	-0.707640
60	1	0	1.447348	5.911660	2.680001
61	1	0	0.005251	7.324721	1.236113
62	6	0	1.987809	1.979151	-1.181354
63	6	0	1.814048	1.733811	-2.544082
64	6	0	3.227003	2.430700	-0.717267
65	6	0	2.872949	1.917339	-3.429617
66	1	0	0.843905	1.388598	-2.904139
67	6	0	4.278545	2.626668	-1.603845
68	1	0	3.374345	2.621740	0.345307
69	6	0	4.104059	2.363411	-2.962353
70	1	0	2.731659	1.713510	-4.488626
71	1	0	5.237643	2.987083	-1.235277
72	1	0	4.928760	2.512731	-3.656295
73	29	0	-1.242163	0.686269	-0.856733
74	1	0	-1.289460	0.713117	-2.593595
75	1	0	-2.304394	0.802352	-2.747583
76	6	0	-3.445012	2.271560	0.693515
77	6	0	-4.918556	0.317381	-0.832230
78	6	0	-2.959853	1.895081	-0.687662
79	6	0	-3.728162	1.006569	-1.433159
80	8	0	-3.514452	0.776583	-2.695206
81	1	0	-5.778866	0.935846	-1.139770
82	1	0	-5.064516	-0.643726	-1.346968
83	1	0	-2.547386	2.718542	-1.275742
84	6	0	-3.916787	1.022888	1.434480

85	1	0	-4.324733	1.297403	2.420018
86	1	0	-3.014085	0.429238	1.633581
87	6	0	-4.940440	0.120684	0.701931
88	6	0	-4.603510	-1.339787	1.007813
89	6	0	-6.353631	0.401804	1.215917
90	1	0	-3.646026	-1.627483	0.550890
91	1	0	-5.375715	-2.014807	0.614934
92	1	0	-4.524324	-1.509182	2.091203
93	1	0	-6.438010	0.154872	2.282847
94	1	0	-6.625695	1.458110	1.094369
95	1	0	-7.094088	-0.201377	0.672676
96	1	0	-2.589347	2.670601	1.266182
97	6	0	-4.493337	3.381145	0.629781
98	1	0	-4.859069	3.654774	1.628786
99	1	0	-5.359404	3.089153	0.021411
100	1	0	-4.071188	4.283706	0.169125

Zero-point correction= 0.798273 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.717367
Sum of electronic and zero-point Energies= -4514.710954
SCF- Energy:M06 (PCM, toluene)/6-31G(d, p) = -4515.5324748 (a.u.)

S8. Gibbs Energies (ΔG≠)* at the M06(PCM, toluene)/6-31G(d,p) Level

Species	$G^{\neq}$ (au.)	$\Delta G^{\neq}$ (kJ/mol)[a]	Configuration of product
R-out-**TS1**	-4514.818456	0.0	*R*
R-in-**TS1**	-4514.806671	31.0	*R*
S-out-**TS1**	-4514.814984	9.2	*S*
S-in-**TS1**	-4514.803918	38.2	*S*
Species	$G^{\neq}$ (au.)	$\Delta G^{\neq}$ (kJ/mol)[b]	Configuration of product
R-out-**TS2**	-4514.822386	0.0	*R*
R-in-**TS2**	-4514.816052	16.6	*R*
S-out-**TS2**	-4514.821204	3.1	*S*
S-in-**TS2**	-4514.815108	19.1	*S*

[a] with respect to *R-out*-**TS1** [b] with respect to *R-out*-**TS2**

S9. Reference 16 details

Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.