Supporting Information

Computational Investigation on the Enantioselective Copper(I)-Catalyzed Addition of Enynes to Ketones

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CONTENTS:

Part III :(S, S)- Me- BPE–CuMes system

Part I: Results and brief discussion on BPE–MesCu model reaction system

Unless Otherwise stated，the calculation all use 5d keyword in the optimized structures.

S1. The summarize energies of all species along reaction paths over the BPE-CuMes system in the gas-phase at the M06/6-31G(d, p) level.

1: the formation of the catalyst

M06/6-31G(d, p)

specises	***G***gas	Δ***G***gas	Δ*G*r(kJ mol^{-1})
BPE	-1075.206346		
CuMes	-1989.337100		
BPE+ CuMes	-3064.543446		
BPE-CuMes	-3064.617314		
1	-424.631200		
BPE +CuMes+1	-3489.174646	0.073868	193.9
BPE-CuMes+1	-3489.248514	0.0	0.0
TS1	-3489.227534	0.02098	55.1
IM2	-3139.515701		
MesH	-349.770592		
IM2+ MesH	-3489.286293	-0.037779	-99.2

2：the cycle of the teaction

M06/6-31G(d,p)

Species	***G***gas	**Δ*G***gas	Δ*G*r(kJ mol^{-1})
2	-384.511945		
1	-424.631200		
IM2+2+1	-3948.658846	0.007913	20.8
TS2+1	-3948.644989	0.02177	57.1
IM3+1	-3948.666759	0.0	0.0
IM31	-3948.665652	0.001107	2.9
TS3	-3948.647853	0.018906	49.6
Pro	-809.135470		
IM2+ Pro	-3948.65117	0.015588	40.9

S2. Cartesian coordinates and energies of all optimized structures over the BPE-CuMes system in the gas-phase at the M06/6-31G(d, p) level.

BPE:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.748856	-0.193126	-0.806717
2	6	0	-0.610127	-0.635808	0.616056
3	6	0	0.585072	0.295794	0.772147
4	15	0	1.727332	0.331337	-0.716216
5	6	0	3.120421	1.353629	0.048782
6	6	0	4.316412	0.413978	0.216229
7	6	0	3.764472	-0.949006	0.614509
8	6	0	2.660102	-1.269193	-0.389217
9	6	0	-2.563333	1.343308	-0.065436
10	6	0	-4.016532	0.969409	0.234211
11	6	0	-4.013390	-0.471279	0.728978
12	6	0	-3.207656	-1.267918	-0.293000
13	1	0	-0.265420	-1.663728	0.426478
14	1	0	-1.186676	-0.668884	1.553230
15	1	0	1.159917	0.027231	1.671737
16	1	0	0.246227	1.332306	0.922419
17	1	0	2.787878	1.736041	1.023860
18	1	0	5.042985	0.801740	0.941582
19	1	0	4.542953	-1.722698	0.634913
20	1	0	3.346417	-0.892421	1.631031
21	1	0	-2.482613	2.196545	-0.746093
22	1	0	-4.475623	1.660258	0.952793
23	1	0	-4.611626	1.028268	-0.689287
24	1	0	-3.524050	-0.518236	1.713602
25	1	0	-5.028331	-0.869070	0.859040
26	1	0	4.845561	0.317115	-0.743520
27	1	0	3.092233	-1.610572	-1.338541
28	1	0	-2.855132	-2.236507	0.082250
29	1	0	-3.814070	-1.468419	-1.185489
30	1	0	-2.039918	1.615027	0.862471
31	1	0	1.972987	-2.054630	-0.050869
32	1	0	3.356510	2.219980	-0.577173

Zero-point correction= 0.283496 (Hartree/Particle)
Thermal correction to Energy= 0.296924
Thermal correction to Enthalpy= 0.297868
Thermal correction to Gibbs Free Energy= 0.242603
Sum of electronic and zero-point Energies= -1075.165454
Sum of electronic and thermal Energies= -1075.152026
Sum of electronic and thermal Enthalpies= -1075.151082
Sum of electronic and thermal Free Energies= -1075.206346

CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.447817	0.000424	0.016916

2	6	0	-0.262455	1.207350	0.012622
3	6	0	-0.263942	-1.206748	0.012242
4	6	0	-1.657323	-1.196238	0.009647
5	6	0	0.478539	-2.510830	0.028790
6	6	0	0.479777	2.511507	0.028497
7	1	0	0.093824	-3.223721	-0.710635
8	1	0	1.536459	-2.314745	-0.190678
9	1	0	0.426472	-2.999635	1.010720
10	1	0	0.100133	3.220799	-0.717060
11	1	0	1.539100	2.314372	-0.183109
12	1	0	0.420682	3.005240	1.007553
13	6	0	-2.371989	0.001452	0.006265
14	6	0	-1.656802	1.197593	0.010137
15	6	0	-3.871216	-0.000415	-0.034129
16	1	0	-2.201783	-2.143348	0.005001
17	1	0	-2.200595	2.144940	0.005900
18	1	0	-4.243977	-0.112717	-1.060891
19	1	0	-4.285114	0.934472	0.359742
20	1	0	-4.289068	-0.828631	0.549762
21	29	0	2.247222	-0.000745	-0.021456

Zero-point correction= 0.171032 (Hartree/Particle)
Thermal correction to Energy= 0.182389
Thermal correction to Enthalpy= 0.183333
Thermal correction to Gibbs Free Energy= 0.132950
Sum of electronic and zero-point Energies= -1989.299019
Sum of electronic and thermal Energies= -1989.287661
Sum of electronic and thermal Enthalpies= -1989.286717
Sum of electronic and thermal Free Energies= -1989.337100

BPE-CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.912877	-0.238862	-0.070050
2	6	0	-2.745833	0.671554	-0.751869
3	6	0	-2.568101	-1.249081	0.664465
4	15	0	1.316947	1.696717	-0.049708
5	6	0	3.083155	1.091223	-0.092169
6	6	0	3.188824	-0.276991	0.574449
7	15	0	1.789884	-1.384107	0.024435
8	6	0	2.081762	-2.927094	1.017929
9	6	0	2.236234	-4.031710	-0.027383
10	6	0	3.088570	-3.452559	-1.154013
11	6	0	2.442248	-2.125125	-1.553395
12	6	0	1.251716	2.564089	1.591695
13	6	0	1.690642	4.001587	1.317857
14	6	0	1.069534	4.393110	-0.020451
15	6	0	1.410190	3.283866	-1.019098

16	1	0	3.352778	1.013034	-1.156399
17	1	0	3.769366	1.820198	0.362021
18	1	0	4.163222	-0.750980	0.388315
19	1	0	3.079499	-0.176656	1.665075
20	1	0	1.254804	-3.103155	1.712841
21	1	0	3.004029	-2.818137	1.605797
22	1	0	1.245351	-4.300953	-0.423938
23	1	0	2.669564	-4.942899	0.401644
24	1	0	3.174548	-4.137650	-2.005927
25	1	0	4.108473	-3.274683	-0.780122
26	1	0	1.591657	-2.290629	-2.225927
27	1	0	3.127804	-1.431721	-2.055552
28	1	0	1.866670	2.040125	2.333540
29	1	0	0.213079	2.531948	1.946210
30	1	0	2.787562	4.051743	1.240661
31	1	0	1.395381	4.681057	2.126586
32	1	0	1.412777	5.373659	-0.371166
33	1	0	-0.022479	4.457978	0.095896
34	1	0	2.429717	3.406549	-1.409709
35	1	0	0.724140	3.251940	-1.871614
36	29	0	-0.000044	-0.104279	-0.125077
37	6	0	-3.959730	-1.340118	0.708705
38	6	0	-1.761148	-2.263808	1.430357
39	6	0	-2.138853	1.801679	-1.540746
40	1	0	-2.397722	-2.990389	1.950530
41	1	0	-1.092514	-2.823789	0.759204
42	1	0	-1.120586	-1.783800	2.183614
43	1	0	-2.899621	2.400449	-2.056719
44	1	0	-1.431268	1.435474	-2.297418
45	1	0	-1.570856	2.480777	-0.884722
46	6	0	-4.767214	-0.436786	0.020637
47	6	0	-4.137662	0.571348	-0.705227
48	6	0	-6.261824	-0.561564	0.041211
49	1	0	-4.431902	-2.134575	1.292429
50	1	0	-4.750860	1.296379	-1.246615
51	1	0	-6.620906	-1.258995	-0.728070
52	1	0	-6.748217	0.402770	-0.147370
53	1	0	-6.622461	-0.938668	1.005813

Zero-point correction= 0.456769 (Hartree/Particle)
Thermal correction to Energy= 0.482393
Thermal correction to Enthalpy= 0.483337
Thermal correction to Gibbs Free Energy= 0.400066
Sum of electronic and zero-point Energies= -3064.560611
Sum of electronic and thermal Energies= -3064.534987
Sum of electronic and thermal Enthalpies= -3064.534043
Sum of electronic and thermal Free Energies= -3064.617314

1:

Standard orientation:

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

1	1	0	3.368137	0.872179	-1.619147
2	6	0	3.117740	-0.000015	-0.994760
3	6	0	1.689207	-0.000329	-0.716434
4	6	0	0.501381	-0.000588	-0.477481
5	6	0	4.003075	0.000193	0.222910
6	6	0	3.583440	0.000163	1.482563
7	1	0	2.521798	-0.000109	1.723083
8	1	0	4.285115	0.000366	2.312038
9	1	0	3.368469	-0.872081	-1.619177
10	1	0	5.071983	0.000428	0.004657
11	6	0	-0.901753	-0.000261	-0.213713
12	6	0	-1.601173	1.208124	-0.084394
13	6	0	-1.601638	-1.208335	-0.084046
14	6	0	-2.966452	1.204756	0.165937
15	1	0	-1.057421	2.144648	-0.184257
16	6	0	-2.966916	-1.204333	0.166299
17	1	0	-1.058271	-2.145100	-0.183717
18	6	0	-3.653494	0.000361	0.291495
19	1	0	-3.498181	2.148486	0.263975
20	1	0	-3.499023	-2.147834	0.264517
21	1	0	-4.723114	0.000601	0.487782

Zero-point correction= 0.171099 (Hartree/Particle)
Thermal correction to Energy= 0.181293
Thermal correction to Enthalpy= 0.182237
Thermal correction to Gibbs Free Energy= 0.133815
Sum of electronic and zero-point Energies= -424.593916
Sum of electronic and thermal Energies= -424.583722
Sum of electronic and thermal Enthalpies= -424.582778
Sum of electronic and thermal Free Energies= -424.631200

TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.944008	0.233455	0.824136
2	6	0	-2.531981	-1.049557	0.646818
3	6	0	-2.764369	1.335084	0.489358
4	15	0	0.205289	-0.386437	-1.802447
5	6	0	1.275528	0.823961	-2.726562
6	6	0	1.092783	2.230023	-2.161473
7	15	0	1.178491	2.247355	-0.294588
8	6	0	0.978865	4.073223	0.061620
9	6	0	2.277237	4.504354	0.742570
10	6	0	3.411160	3.776098	0.031986
11	6	0	3.020422	2.300065	0.001431
12	6	0	-1.388150	-0.299096	-2.749903
13	6	0	-1.286180	-1.373565	-3.829654
14	6	0	-0.596299	-2.565380	-3.171128
15	6	0	0.683218	-2.038031	-2.517772

16	1	0	2.315148	0.488841	-2.595337
17	1	0	1.061500	0.793359	-3.804712
18	1	0	1.821273	2.936136	-2.585685
19	1	0	0.090117	2.609430	-2.414468
20	1	0	0.095883	4.258196	0.679195
21	1	0	0.839359	4.609107	-0.887864
22	1	0	2.257056	4.197067	1.798851
23	1	0	2.402214	5.593630	0.727898
24	1	0	4.381057	3.933568	0.519542
25	1	0	3.502367	4.160377	-0.995421
26	1	0	3.216615	1.820757	0.970442
27	1	0	3.555778	1.726682	-0.765739
28	1	0	-1.558547	0.715647	-3.131241
29	1	0	-2.201740	-0.523863	-2.047207
30	1	0	-0.671830	-1.015262	-4.670534
31	1	0	-2.268857	-1.637082	-4.239383
32	1	0	-0.388589	-3.377411	-3.878091
33	1	0	-1.260300	-2.973350	-2.393374
34	1	0	1.477383	-1.894630	-3.264178
35	1	0	1.075225	-2.699743	-1.737978
36	29	0	0.072010	0.353032	0.306359
37	1	0	-1.262873	0.362583	2.112668
38	6	0	-4.044559	1.170041	-0.044824
39	6	0	-2.270229	2.740751	0.687701
40	6	0	-1.778178	-2.291572	1.030988
41	1	0	-3.098443	3.444374	0.836075
42	1	0	-1.600182	2.805478	1.554571
43	1	0	-1.701407	3.094116	-0.186340
44	1	0	-2.370602	-3.196118	0.849235
45	1	0	-1.503895	-2.272082	2.093817
46	1	0	-0.835355	-2.380839	0.469096
47	6	0	-4.584369	-0.094215	-0.252182
48	6	0	-3.806639	-1.198146	0.106239
49	6	0	-5.968086	-0.272807	-0.799411
50	1	0	-4.639671	2.050299	-0.300103
51	1	0	-4.221142	-2.200353	-0.029048
52	1	0	-6.294539	0.608019	-1.363647
53	1	0	-6.699174	-0.432931	0.004150
54	1	0	-6.028850	-1.144207	-1.462236
55	6	0	-0.425890	0.373227	3.234233
56	6	0	0.614134	-0.234976	2.490291
57	6	0	1.232496	-0.869819	1.620749
58	6	0	-0.996946	-0.362109	4.371246
59	6	0	-0.685820	-1.600932	4.770024
60	1	0	0.119158	-2.161790	4.295568
61	1	0	-1.218471	-2.088285	5.581675
62	1	0	-0.307492	1.451436	3.393480
63	1	0	-1.793215	0.170957	4.895115
64	6	0	2.141042	-1.819727	1.043589
65	6	0	1.988151	-3.185439	1.335067
66	6	0	3.157485	-1.438706	0.154480
67	6	0	2.815460	-4.131104	0.744246
68	1	0	1.202196	-3.491059	2.022661

69	6	0	3.982873	-2.389222	-0.432314
70	1	0	3.293651	-0.381790	-0.064840
71	6	0	3.813014	-3.741007	-0.146440
72	1	0	2.677592	-5.184177	0.979886
73	1	0	4.766728	-2.071001	-1.116788
74	1	0	4.456875	-4.485007	-0.609255

Zero-point correction= 0.624093 (Hartree/Particle)
Thermal correction to Energy= 0.660361
Thermal correction to Enthalpy= 0.661305
Thermal correction to Gibbs Free Energy= 0.557315
Sum of electronic and zero-point Energies= -3489.160756
Sum of electronic and thermal Energies= -3489.124488
Sum of electronic and thermal Enthalpies= -3489.123544
Sum of electronic and thermal Free Energies= -3489.227534

IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.118187	1.187434	-0.124497
2	6	0	1.479672	2.299542	0.478717
3	6	0	2.806153	1.879021	-0.149172
4	15	0	3.092000	0.047387	0.081571
5	6	0	4.664773	-0.215358	-0.887796
6	6	0	5.730204	-0.609050	0.138455
7	6	0	5.455751	0.195005	1.406895
8	6	0	3.972908	0.008459	1.719937
9	6	0	-0.553968	2.017691	-1.640710
10	6	0	-2.062945	2.013529	-1.399016
11	6	0	-2.281559	2.457234	0.045771
12	6	0	-1.348549	1.618385	0.926443
13	1	0	1.522464	2.168440	1.570534
14	1	0	1.250346	3.356736	0.285470
15	1	0	3.651272	2.457447	0.250687
16	1	0	2.777720	2.050885	-1.236418
17	1	0	4.931467	0.724593	-1.389906
18	1	0	6.744542	-0.449607	-0.246339
19	1	0	6.096798	-0.115693	2.241073
20	1	0	5.669958	1.258084	1.218959
21	1	0	-0.257775	1.471451	-2.541999
22	1	0	-2.597151	2.647832	-2.116351
23	1	0	-2.450849	0.990177	-1.519538
24	1	0	-2.024267	3.523609	0.137321
25	1	0	-3.330496	2.344990	0.348291
26	29	0	1.064178	-0.788285	-0.307090
27	1	0	5.640377	-1.680924	0.367930
28	1	0	3.788356	-0.972771	2.174959
29	1	0	-1.033030	2.131658	1.841883
30	6	0	0.008838	-2.493858	0.444913

31	6	0	-1.325819	-2.041410	0.481091
32	6	0	-2.480132	-1.636766	0.474693
33	6	0	0.684817	-2.675530	-0.803484
34	6	0	0.396864	-1.944325	-1.961310
35	1	0	-0.607979	-1.550451	-2.119428
36	1	0	0.981735	-2.134377	-2.856329
37	1	0	0.372735	-3.058396	1.300565
38	1	0	1.580781	-3.299075	-0.787865
39	1	0	-1.825042	0.674228	1.216419
40	1	0	-0.170276	3.046109	-1.712719
41	1	0	3.559103	0.764109	2.398889
42	1	0	4.513402	-0.972971	-1.662615
43	6	0	-3.773387	-1.057575	0.448148
44	6	0	-4.409725	-0.786903	-0.778347
45	6	0	-4.433129	-0.691019	1.635884
46	6	0	-5.644331	-0.154225	-0.811468
47	1	0	-3.911086	-1.082313	-1.700482
48	6	0	-5.671476	-0.065979	1.592689
49	1	0	-3.949660	-0.898404	2.588582
50	6	0	-6.282449	0.212453	0.371572
51	1	0	-6.116679	0.049912	-1.770361
52	1	0	-6.164429	0.211418	2.522413
53	1	0	-7.251353	0.705310	0.342439

Zero-point correction= 0.446090 (Hartree/Particle)
Thermal correction to Energy= 0.471598
Thermal correction to Enthalpy= 0.472542
Thermal correction to Gibbs Free Energy= 0.390983
Sum of electronic and zero-point Energies= -3139.460594
Sum of electronic and thermal Energies= -3139.435087
Sum of electronic and thermal Enthalpies= -3139.434142
Sum of electronic and thermal Free Energies= -3139.515701

MesH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.356087	-1.338002	-0.014925
2	6	0	1.354869	-0.370230	-0.006239
3	6	0	-0.997827	-0.988137	-0.007232
4	1	0	0.633778	-2.393494	-0.027365
5	6	0	-1.336785	0.360589	0.002468
6	6	0	-2.053993	-2.052797	0.006428
7	6	0	2.805251	-0.751775	0.005770
8	1	0	-3.046695	-1.637138	-0.195590
9	1	0	-1.853093	-2.827471	-0.743077
10	1	0	-2.099710	-2.556683	0.980578
11	1	0	3.371210	-0.201030	-0.755086
12	1	0	2.941974	-1.822023	-0.181337
13	1	0	3.269621	-0.524019	0.973842

14	6	0	-0.356759	1.357917	0.006563
15	6	0	0.980830	0.977214	0.003631
16	6	0	-0.751518	2.804773	-0.002914
17	1	0	-2.389911	0.647578	0.004939
18	1	0	1.755779	1.746001	0.006814
19	1	0	-1.183938	3.094894	-0.969079
20	1	0	0.108191	3.457233	0.182735
21	1	0	-1.508136	3.018855	0.761325

Zero-point correction= 0.181770 (Hartree/Particle)
Thermal correction to Energy= 0.190914
Thermal correction to Enthalpy= 0.191859
Thermal correction to Gibbs Free Energy= 0.146255
Sum of electronic and zero-point Energies= -349.735077
Sum of electronic and thermal Energies= -349.725932
Sum of electronic and thermal Enthalpies= -349.724988
Sum of electronic and thermal Free Energies= -349.770592

2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.579686	0.105860	-0.000018
2	6	0	-1.818728	1.270604	0.000035
3	8	0	2.204911	-1.304799	0.000076
4	6	0	1.691078	-0.201427	0.000007
5	6	0	2.539181	1.044761	-0.000079
6	6	0	0.206280	-0.050527	0.000028
7	6	0	-0.430656	1.193933	0.000050
8	6	0	-0.568035	-1.214467	-0.000023
9	6	0	-1.952409	-1.138733	-0.000043
10	1	0	-2.548495	-2.048248	-0.000075
11	1	0	-3.665560	0.168644	-0.000038
12	1	0	-2.307655	2.241971	0.000046
13	1	0	0.154624	2.111196	0.000101
14	1	0	-0.050033	-2.170302	-0.000047
15	1	0	3.590785	0.752555	-0.000360
16	1	0	2.332224	1.661346	-0.882766
17	1	0	2.332674	1.661211	0.882795

Zero-point correction= 0.137536 (Hartree/Particle)
Thermal correction to Energy= 0.145366
Thermal correction to Enthalpy= 0.146310
Thermal correction to Gibbs Free Energy= 0.104920
Sum of electronic and zero-point Energies= -384.479329
Sum of electronic and thermal Energies= -384.471498
Sum of electronic and thermal Enthalpies= -384.470554
Sum of electronic and thermal Free Energies= -384.511945

TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.784864	-1.996017	-0.566903
2	6	0	-2.424384	-2.652582	-1.152118
3	6	0	-3.351689	-1.485414	-1.486339
4	15	0	-3.384844	-0.221946	-0.110501
5	6	0	-4.490403	1.088639	-0.843034
6	6	0	-5.699305	1.161301	0.090497
7	6	0	-6.029951	-0.272439	0.495298
8	6	0	-4.725131	-0.891974	0.994281
9	6	0	0.204164	-1.770106	-2.126533
10	6	0	1.461776	-2.616373	-1.911745
11	6	0	1.022128	-3.906124	-1.222826
12	6	0	0.158637	-3.497241	-0.029743
13	1	0	-2.841936	-3.236970	-0.318158
14	1	0	-2.309973	-3.335863	-2.005355
15	1	0	-4.370607	-1.826439	-1.721329
16	1	0	-2.974993	-0.949790	-2.371884
17	1	0	-4.797410	0.779081	-1.851636
18	1	0	-6.548426	1.670735	-0.380539
19	1	0	-6.824998	-0.320885	1.249358
20	1	0	-6.390518	-0.822913	-0.387059
21	1	0	0.420237	-0.707680	-2.279528
22	1	0	1.986805	-2.807648	-2.855284
23	1	0	2.163081	-2.076590	-1.256133
24	1	0	0.423888	-4.509144	-1.923751
25	1	0	1.879662	-4.518806	-0.915985
26	29	0	-1.254712	-0.088210	0.506419
27	1	0	-5.436323	1.738579	0.989795
28	1	0	-4.506089	-0.572128	2.020820
29	1	0	-0.513737	-4.286606	0.325587
30	6	0	-0.328059	0.131440	2.330818
31	6	0	0.950759	-0.414112	2.039052
32	6	0	2.045282	-0.865003	1.741639
33	6	0	-0.477262	1.534747	2.465423
34	6	0	0.407486	2.490348	2.005061
35	1	0	1.442063	2.197390	1.832353
36	1	0	0.246333	3.536867	2.257544
37	1	0	-0.986664	-0.484815	2.949504
38	1	0	-1.443806	1.864904	2.856730
39	6	0	3.733978	4.144245	-1.332683
40	6	0	2.693168	4.999905	-0.988281
41	8	0	-0.225597	1.270843	-0.479027
42	6	0	-0.062964	2.492298	-0.192208
43	6	0	-1.290192	3.369157	-0.122891
44	6	0	1.240829	3.105291	-0.576838
45	6	0	1.456490	4.485573	-0.611631
46	6	0	2.294280	2.252353	-0.930119
47	6	0	3.528611	2.765754	-1.300674
48	1	0	4.335291	2.085312	-1.570413
49	1	0	4.700357	4.548451	-1.625749

50	1	0	2.843197	6.077243	-1.012281
51	1	0	0.654833	5.170309	-0.342155
52	1	0	2.116098	1.177832	-0.899802
53	1	0	-2.098050	2.805460	0.356639
54	1	0	-1.144364	4.306765	0.419839
55	1	0	-1.607057	3.611342	-1.148957
56	1	0	0.780983	-3.179767	0.817363
57	1	0	-0.377725	-2.134303	-2.986113
58	1	0	-4.722493	-1.988849	0.988114
59	1	0	-3.955257	2.039269	-0.934950
60	6	0	3.289709	-1.334675	1.247102
61	6	0	4.205279	-0.427838	0.681827
62	6	0	3.620501	-2.701062	1.254757
63	6	0	5.389122	-0.879591	0.117340
64	1	0	3.960089	0.633140	0.687685
65	6	0	4.807598	-3.143536	0.686720
66	1	0	2.927942	-3.410276	1.705645
67	6	0	5.695750	-2.238688	0.110271
68	1	0	6.081935	-0.162314	-0.319334
69	1	0	5.043399	-4.205903	0.696053
70	1	0	6.624037	-2.589973	-0.334073

Zero-point correction= 0.584896 (Hartree/Particle)
Thermal correction to Energy= 0.618853
Thermal correction to Enthalpy= 0.619797
Thermal correction to Gibbs Free Energy= 0.519005
Sum of electronic and zero-point Energies= -3523.947898
Sum of electronic and thermal Energies= -3523.913942
Sum of electronic and thermal Enthalpies= -3523.912997
Sum of electronic and thermal Free Energies= -3524.013789

IM3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.491984	-1.851059	0.832176
2	6	0	2.022825	-2.670887	1.474327
3	6	0	3.105018	-1.601520	1.611334
4	15	0	3.327832	-0.635612	0.027169
5	6	0	4.583770	0.633516	0.561993
6	6	0	5.818352	0.369145	-0.300861
7	6	0	5.957706	-1.146017	-0.424557
8	6	0	4.593142	-1.671649	-0.867890
9	6	0	-0.271648	-1.060425	2.317613
10	6	0	-1.742677	-1.448350	2.189661
11	6	0	-1.781788	-2.934726	1.838292
12	6	0	-0.818242	-3.153743	0.664543
13	1	0	2.327013	-3.433156	0.741669
14	1	0	1.835946	-3.182558	2.428835
15	1	0	4.064857	-2.029297	1.934889
16	1	0	2.804050	-0.862363	2.369905

17	1	0	4.813487	0.480628	1.625236
18	1	0	6.716414	0.838137	0.118542
19	1	0	6.757987	-1.436827	-1.116228
20	1	0	6.216305	-1.566345	0.559116
21	1	0	-0.096275	0.020972	2.274946
22	1	0	-2.307711	-1.221985	3.101715
23	1	0	-2.202653	-0.869288	1.372897
24	1	0	-1.443530	-3.517647	2.708386
25	1	0	-2.797213	-3.272118	1.593704
26	29	0	1.110508	-0.237304	-0.584925
27	1	0	5.669420	0.801263	-1.301895
28	1	0	4.449659	-1.526943	-1.946203
29	1	0	-0.383628	-4.159491	0.635065
30	6	0	0.196163	-0.450195	-2.433940
31	6	0	-1.148430	-0.784374	-2.114518
32	6	0	-2.283633	-1.074532	-1.786560
33	6	0	0.715225	0.830752	-2.262515
34	6	0	-0.081567	1.990629	-1.734921
35	1	0	-1.129165	1.677801	-1.624356
36	1	0	-0.060467	2.828551	-2.449216
37	1	0	0.752184	-1.168758	-3.037151
38	1	0	1.662666	1.043514	-2.760333
39	6	0	-2.749742	4.909428	1.287622
40	6	0	-1.832007	5.461052	0.400190
41	8	0	0.575771	1.298997	0.454752
42	6	0	0.423961	2.425886	-0.327449
43	6	0	1.760832	3.166460	-0.460583
44	6	0	-0.650942	3.344423	0.259021
45	6	0	-0.796506	4.683360	-0.110980
46	6	0	-1.584646	2.801568	1.144076
47	6	0	-2.623141	3.572516	1.654183
48	1	0	-3.336744	3.129195	2.347304
49	1	0	-3.558445	5.516814	1.689018
50	1	0	-1.920962	6.504116	0.101692
51	1	0	-0.094969	5.133787	-0.812285
52	1	0	-1.465731	1.755133	1.417465
53	1	0	2.504399	2.494755	-0.911170
54	1	0	1.710930	4.072230	-1.078564
55	1	0	2.116351	3.445500	0.538696
56	1	0	-1.322740	-2.976279	-0.293537
57	1	0	0.167985	-1.476227	3.236384
58	1	0	4.438133	-2.737972	-0.660809
59	1	0	4.179879	1.644877	0.453738
60	6	0	-3.576546	-1.375322	-1.277701
61	6	0	-4.164885	-2.632397	-1.485678
62	6	0	-4.257933	-0.421266	-0.502713
63	6	0	-5.399311	-2.928618	-0.923747
64	1	0	-3.635591	-3.370028	-2.085491
65	6	0	-5.491371	-0.727371	0.054604
66	1	0	-3.794882	0.551709	-0.340488
67	6	0	-6.065226	-1.980023	-0.151546
68	1	0	-5.845485	-3.906969	-1.088243
69	1	0	-6.008641	0.017069	0.655439

70	1	0	-7.031493	-2.215788	0.288158

Zero-point correction= 0.588138 (Hartree/Particle)
Thermal correction to Energy= 0.621510
Thermal correction to Enthalpy= 0.622454
Thermal correction to Gibbs Free Energy= 0.523074
Sum of electronic and zero-point Energies= -3523.970495
Sum of electronic and thermal Energies= -3523.937123
Sum of electronic and thermal Enthalpies= -3523.936178
Sum of electronic and thermal Free Energies= -3524.035559

IM31:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.805144	3.575744	-1.762227
2	6	0	-1.368109	2.174277	-2.076779
3	6	0	-2.443352	1.201536	-2.154214
4	6	0	-3.349435	0.393973	-2.185713
5	6	0	-3.038475	3.960581	-1.445917
6	1	0	-0.657503	1.846584	-1.283833
7	1	0	-0.782388	2.168002	-3.009317
8	1	0	-0.993157	4.306184	-1.774137
9	1	0	-3.264088	4.995559	-1.203603
10	1	0	-3.865905	3.251387	-1.427165
11	15	0	0.194446	-2.023926	0.246009
12	6	0	-1.482613	-2.771646	0.464996
13	6	0	-2.486452	-1.628249	0.568516
14	15	0	-1.994103	-0.351646	1.835099
15	6	0	-3.174026	1.028504	1.414339
16	6	0	-4.009850	1.235167	2.675875
17	6	0	-4.308968	-0.154568	3.233226
18	6	0	-2.964956	-0.873854	3.338241
19	6	0	0.265078	-1.506102	-1.528499
20	6	0	1.641575	-2.002160	-1.967796
21	6	0	1.781248	-3.431001	-1.447310
22	6	0	1.400293	-3.418795	0.038564
23	1	0	-1.463115	-3.368852	1.389141
24	1	0	-1.731837	-3.447763	-0.365939
25	1	0	-3.511315	-1.984969	0.752644
26	1	0	-2.509589	-1.079935	-0.383715
27	1	0	-3.803877	0.700039	0.575993
28	1	0	-4.922001	1.808140	2.470128
29	1	0	-4.835891	-0.118708	4.194886
30	1	0	-4.961785	-0.688948	2.525110
31	1	0	0.148709	-0.418540	-1.601330
32	1	0	1.772232	-1.941128	-3.054726
33	1	0	2.419187	-1.367853	-1.512242
34	1	0	1.089677	-4.082738	-2.002462
35	1	0	2.793888	-3.825686	-1.600382
36	29	0	0.325439	-0.209617	1.545609

37	1	0	-3.431063	1.808526	3.416973
38	1	0	-2.415564	-0.546420	4.230201
39	1	0	0.975399	-4.367108	0.387613
40	6	0	1.911408	-0.411865	2.868769
41	6	0	2.988464	-0.865489	2.058832
42	6	0	3.871401	-1.260508	1.321234
43	6	0	1.446311	0.899105	2.831386
44	6	0	2.032221	1.963963	1.947226
45	1	0	2.925620	1.564245	1.447556
46	1	0	2.347637	2.830850	2.548401
47	1	0	1.607279	-1.057174	3.693543
48	1	0	0.799397	1.213741	3.651621
49	6	0	3.223672	4.645743	-2.138502
50	6	0	2.831300	5.263894	-0.955807
51	8	0	0.524941	1.231109	0.252369
52	6	0	1.022336	2.379103	0.840397
53	6	0	-0.109974	3.207739	1.466652
54	6	0	1.780676	3.211408	-0.195985
55	6	0	2.120263	4.551789	0.005666
56	6	0	2.191831	2.599470	-1.383134
57	6	0	2.903339	3.307243	-2.346393
58	1	0	3.207153	2.812255	-3.267514
59	1	0	3.775369	5.203327	-2.892507
60	1	0	3.078585	6.309075	-0.778960
61	1	0	1.826786	5.055450	0.925571
62	1	0	1.922133	1.553673	-1.525849
63	1	0	-0.659988	2.590706	2.190585
64	1	0	0.244035	4.103015	1.994151
65	1	0	-0.818012	3.525487	0.689503
66	1	0	2.271641	-3.191934	0.664664
67	1	0	-0.535343	-1.998787	-2.100835
68	1	0	-3.045243	-1.967027	3.387289
69	1	0	-2.633871	1.921800	1.082243
70	6	0	4.808201	-1.693853	0.343660
71	6	0	5.423145	-2.952133	0.432736
72	6	0	5.083185	-0.874272	-0.764202
73	6	0	6.283589	-3.382017	-0.568375
74	1	0	5.208774	-3.584298	1.292032
75	6	0	5.943455	-1.314049	-1.760184
76	1	0	4.601310	0.101001	-0.829124
77	6	0	6.544485	-2.567538	-1.667346
78	1	0	6.753887	-4.359763	-0.491042
79	1	0	6.147439	-0.674365	-2.615706
80	1	0	7.217850	-2.908410	-2.450278
81	6	0	-4.370741	-0.600335	-2.136429
82	6	0	-5.574049	-0.355234	-1.457384
83	6	0	-4.154869	-1.868431	-2.696989
84	6	0	-6.528631	-1.356680	-1.336291
85	1	0	-5.742172	0.630256	-1.025249
86	6	0	-5.113975	-2.864068	-2.573513
87	1	0	-3.220311	-2.057735	-3.221810
88	6	0	-6.302125	-2.613697	-1.891045
89	1	0	-7.456930	-1.154586	-0.806520

90	1	0	-4.934631	-3.843246	-3.012124
91	1	0	-7.051207	-3.395887	-1.793421

Zero-point correction= 0.762078 (Hartree/Particle)
Thermal correction to Energy= 0.806627
Thermal correction to Enthalpy= 0.807571
Thermal correction to Gibbs Free Energy= 0.684084
Sum of electronic and zero-point Energies= -3948.587658
Sum of electronic and thermal Energies= -3948.543109
Sum of electronic and thermal Enthalpies= -3948.542165
Sum of electronic and thermal Free Energies= -3948.665652

TS3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.731465	-2.768286	2.703991
2	6	0	-0.447816	-1.353945	2.461730
3	6	0	-1.522227	-0.440306	2.454778
4	6	0	-2.455563	0.357348	2.425134
5	6	0	-1.921059	-3.393992	2.685491
6	1	0	0.215311	-1.342513	1.077266
7	1	0	0.436976	-0.986370	2.995646
8	1	0	0.164636	-3.376886	2.868235
9	1	0	-2.001173	-4.467386	2.836295
10	1	0	-2.848857	-2.834982	2.559104
11	15	0	-0.737803	1.700689	-1.118852
12	6	0	-2.570091	1.711379	-1.412524
13	6	0	-3.172532	0.380108	-0.976318
14	15	0	-2.235052	-1.091309	-1.596112
15	6	0	-3.006125	-2.468393	-0.622498
16	6	0	-3.527357	-3.445691	-1.674362
17	6	0	-4.129203	-2.606658	-2.800516
18	6	0	-3.072649	-1.570026	-3.186124
19	6	0	-0.458492	2.444453	0.553865
20	6	0	0.446080	3.651808	0.302683
21	6	0	-0.022550	4.299560	-0.997487
22	6	0	-0.094412	3.177644	-2.034409
23	1	0	-2.713626	1.871356	-2.492346
24	1	0	-3.050794	2.545063	-0.879712
25	1	0	-4.237486	0.306057	-1.239494
26	1	0	-3.095874	0.292581	0.116536
27	1	0	-3.835582	-2.045950	-0.036779
28	1	0	-4.249450	-4.151552	-1.248053
29	1	0	-4.437480	-3.216140	-3.658708
30	1	0	-5.030579	-2.097358	-2.427738
31	1	0	-0.036337	1.703263	1.240749
32	1	0	0.422813	4.350066	1.147492
33	1	0	1.489542	3.319685	0.188228
34	1	0	-1.022238	4.736160	-0.849668
35	1	0	0.640089	5.112354	-1.321187

36	29	0	-0.061261	-0.390387	-1.520464
37	1	0	-2.692349	-4.043397	-2.072413
38	1	0	-2.315313	-2.012554	-3.847347
39	1	0	-0.717568	3.409701	-2.905363
40	6	0	1.498013	-0.111294	-2.829558
41	6	0	2.451008	0.690481	-2.141639
42	6	0	3.230134	1.376693	-1.508218
43	6	0	1.333840	-1.469617	-2.572316
44	6	0	2.183589	-2.188639	-1.559127
45	1	0	3.053097	-1.562044	-1.321523
46	1	0	2.565621	-3.131890	-1.974318
47	1	0	1.058903	0.313771	-3.734497
48	1	0	0.790585	-2.058405	-3.312194
49	6	0	4.486516	-3.238324	2.748395
50	6	0	3.854809	-4.308566	2.127972
51	8	0	0.764136	-1.283128	0.098480
52	6	0	1.439512	-2.482990	-0.235604
53	6	0	0.444873	-3.620662	-0.446444
54	6	0	2.477338	-2.787495	0.837309
55	6	0	2.860442	-4.084487	1.178199
56	6	0	3.122896	-1.717109	1.466961
57	6	0	4.116008	-1.938201	2.412035
58	1	0	4.598115	-1.089382	2.894706
59	1	0	5.259453	-3.414029	3.493213
60	1	0	4.131556	-5.329009	2.384617
61	1	0	2.378104	-4.939582	0.709531
62	1	0	2.817604	-0.702796	1.211362
63	1	0	-0.287073	-3.320864	-1.207866
64	1	0	0.936751	-4.533631	-0.801844
65	1	0	-0.099267	-3.847504	0.478434
66	1	0	0.912903	2.925745	-2.394560
67	1	0	-1.431846	2.752308	0.960069
68	1	0	-3.476477	-0.687163	-3.697167
69	1	0	-2.301537	-2.904525	0.096138
70	6	0	4.125680	2.145020	-0.714771
71	6	0	4.138119	3.545825	-0.801351
72	6	0	4.992231	1.506266	0.186763
73	6	0	4.996428	4.287729	-0.001740
74	1	0	3.463201	4.037388	-1.500740
75	6	0	5.845981	2.256869	0.982341
76	1	0	4.978233	0.419530	0.252451
77	6	0	5.851612	3.646718	0.891040
78	1	0	4.998561	5.372689	-0.074437
79	1	0	6.512309	1.754064	1.679479
80	1	0	6.521559	4.231143	1.517093
81	6	0	-3.511858	1.299772	2.419521
82	6	0	-4.816161	0.932891	2.028475
83	6	0	-3.288899	2.647812	2.770137
84	6	0	-5.834403	1.872588	1.968469
85	1	0	-5.009259	-0.108805	1.773351
86	6	0	-4.314199	3.581581	2.703974
87	1	0	-2.296698	2.940703	3.109594
88	6	0	-5.592045	3.205533	2.297008

89	1	0	-6.832019	1.561576	1.663530
90	1	0	-4.114146	4.615107	2.981035
91	1	0	-6.392631	3.939587	2.246280

Zero-point correction= 0.757727 (Hartree/Particle)
Thermal correction to Energy= 0.801600
Thermal correction to Enthalpy= 0.802544
Thermal correction to Gibbs Free Energy= 0.680932
Sum of electronic and zero-point Energies= -3948.571059
Sum of electronic and thermal Energies= -3948.527186
Sum of electronic and thermal Enthalpies= -3948.526242
Sum of electronic and thermal Free Energies= -3948.647853

Pro:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.870122	-0.762654	2.224617
2	6	0	-0.094505	-3.274899	-0.444077
3	6	0	-1.136215	-2.323289	-0.314069
4	6	0	-2.000868	-1.473804	-0.217278
5	6	0	1.176773	-2.926192	-0.707704
6	6	0	1.611666	-1.511140	-0.882063
7	1	0	0.727311	-0.893009	-1.083099
8	1	0	2.285646	-1.405394	-1.744798
9	1	0	-0.353442	-4.325669	-0.318173
10	1	0	1.925533	-3.715017	-0.782820
11	6	0	2.372053	3.371057	-0.204440
12	6	0	3.508327	2.632189	-0.512522
13	8	0	1.522053	-1.243170	1.464695
14	6	0	2.336154	-0.919423	0.347487
15	6	0	3.705718	-1.561123	0.532717
16	6	0	2.398421	0.591150	0.171035
17	6	0	3.520535	1.251744	-0.328251
18	6	0	1.258455	1.344057	0.474474
19	6	0	1.243684	2.720160	0.288355
20	1	0	0.346590	3.286745	0.532174
21	1	0	2.364760	4.449146	-0.347748
22	1	0	4.394962	3.131102	-0.897968
23	1	0	4.419304	0.690174	-0.576116
24	1	0	0.379901	0.828707	0.861170
25	1	0	3.571906	-2.623539	0.761083
26	1	0	4.334214	-1.478679	-0.361464
27	1	0	4.243550	-1.097031	1.369305
28	6	0	-2.969059	-0.437110	-0.115766
29	6	0	-4.275304	-0.703710	0.321804
30	6	0	-2.621497	0.880385	-0.457007
31	6	0	-5.204710	0.322348	0.418262
32	1	0	-4.544691	-1.724125	0.584090
33	6	0	-3.556374	1.900380	-0.356415
34	1	0	-1.610344	1.084358	-0.805915

35	6	0	-4.849985	1.626017	0.081267
36	1	0	-6.214417	0.103774	0.758421
37	1	0	-3.275417	2.916749	-0.623816
38	1	0	-5.581520	2.426951	0.158656

Zero-point correction= 0.314234 (Hartree/Particle)
Thermal correction to Energy= 0.332180
Thermal correction to Enthalpy= 0.333125
Thermal correction to Gibbs Free Energy= 0.267102
Sum of electronic and zero-point Energies= -809.088339
Sum of electronic and thermal Energies= -809.070392
Sum of electronic and thermal Enthalpies= -809.069448
Sum of electronic and thermal Free Energies= -809.135470

S3: The summarize energies of all species along reaction paths over the BPE-CuMes systemin the gas-phase at the B3LYP/6-31G(d, p) level.

1: the formation of the catalyst

B3LYP /6-31G(d, p)

specises	***G***gas	Δ***G***gas	Δ*G*r(kJ mol^{-1})
BPE	-1075.594274		
CuMes	-1989.706107		
BPE+ CuMes	-3065.300381		
BPE-CuMes	-3065.359188		
1	-424.981901		
BPE +CuMes+1	-3490.282282	0.058807	154.4
BPE-CuMes+1	-3490.341089	0.0	0.0
TS1	-3490.289268	0.051821	136.0
IM2	-3140.305549		
MesH	-350.065447		
IM2+ MesH	-3490.370996	-0.029907	-78.5

2.the cycle of the teaction

B3LYP/6-31G(d,p)

Species	*G*gas	Δ*G*gas	Δ*G*r(kJ mol^{-1})
2	-384.794742		
1	-424.981901		
IM2+2+1	-3950.082192	0.001881	4.9
TS2+1	-3950.060247	0.020064	52.7
IM3+1	-3950.080311	0.0	0.0
IM31	-3950.071039	0.009272	24.3
TS3	-3950.043583	0.036728	96.4
Pro	-809.758909		
IM2+ Pro	-3950.064458	0.015853	41.6

S4. Cartesian coordinates and energies of all optimized structures over the BPE-CuMes system in the gas-phase at the B3LYP /6-31G(d, p) level.

BPE:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.838112	0.109117	-0.789105
2	6	0	-0.624364	0.449343	0.615713
3	6	0	0.624403	-0.449604	0.615685
4	15	0	1.838141	-0.109289	-0.789119
5	6	0	3.221216	-1.305976	-0.273440
6	6	0	4.428142	-0.446272	0.154476
7	6	0	3.878598	0.806570	0.851781
8	6	0	2.769574	1.366444	-0.056173
9	6	0	-2.769782	-1.366438	-0.056100
10	6	0	-3.878730	-0.806343	0.851810
11	6	0	-4.428082	0.446536	0.154424
12	6	0	-3.221027	1.306037	-0.273535
13	1	0	-0.332365	1.503746	0.525706
14	1	0	-1.142532	0.357039	1.579401
15	1	0	1.142579	-0.357341	1.579373
16	1	0	0.332416	-1.504005	0.525628
17	1	0	3.469506	-1.982299	-1.095946
18	1	0	2.870218	-1.922911	0.561702
19	1	0	4.997489	-0.142709	-0.733562
20	1	0	5.116814	-1.007957	0.796448
21	1	0	4.664606	1.547080	1.043266
22	1	0	3.458688	0.528960	1.827276
23	1	0	3.204437	1.932826	-0.887313

24	1	0	2.084480	2.042743	0.465888
25	1	0	-2.084802	-2.042818	0.466003
26	1	0	-3.204722	-1.932791	-0.887219
27	1	0	-3.458786	-0.528737	1.827291
28	1	0	-4.664850	-1.546725	1.043335
29	1	0	-5.116676	1.008361	0.796358
30	1	0	-4.997468	0.143003	-0.733599
31	1	0	-2.869954	1.922984	0.561567
32	1	0	-3.469208	1.982336	-1.096094

Zero-point correction= 0.284487 (Hartree/Particle)
Thermal correction to Energy= 0.298277
Thermal correction to Enthalpy= 0.299221
Thermal correction to Gibbs Free Energy= 0.242476
Sum of electronic and zero-point Energies= -1075.552263
Sum of electronic and thermal Energies= -1075.538473
Sum of electronic and thermal Enthalpies= -1075.537529
Sum of electronic and thermal Free Energies= -1075.594274

CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.447914	0.000000	-0.010379
2	6	0	-0.259070	-1.214685	-0.008591
3	6	0	-0.259058	1.214677	-0.008601
4	29	0	2.249670	-0.000001	0.015008
5	6	0	-1.658295	1.200550	-0.010479
6	6	0	0.483544	2.531919	-0.018739
7	6	0	0.483550	-2.531916	-0.018743
8	1	0	0.130169	3.213008	0.763509
9	1	0	1.549118	2.340488	0.144980
10	1	0	0.379113	3.053159	-0.978359
11	1	0	0.379221	-3.053091	-0.978410
12	1	0	0.130109	-3.213065	0.763421
13	1	0	1.549106	-2.340478	0.145087
14	6	0	-2.376080	0.000010	-0.009144
15	6	0	-1.658292	-1.200548	-0.010472
16	6	0	-3.886892	-0.000006	0.027551
17	1	0	-2.200369	2.145076	-0.009569
18	1	0	-2.200388	-2.145061	-0.009558
19	1	0	-4.260289	-0.000051	1.059785
20	1	0	-4.300062	-0.885605	-0.465296
21	1	0	-4.300083	0.885621	-0.465227

Zero-point correction= 0.171923 (Hartree/Particle)
Thermal correction to Energy= 0.183359
Thermal correction to Enthalpy= 0.184304
Thermal correction to Gibbs Free Energy= 0.132917
Sum of electronic and zero-point Energies= -1989.667102

Sum of electronic and thermal Energies= -1989.655665
Sum of electronic and thermal Enthalpies= -1989.654721
Sum of electronic and thermal Free Energies= -1989.706107

BPE-CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.966533	-0.000979	0.002820
2	6	0	-2.715981	-0.180215	1.186651
3	6	0	-2.715882	0.175386	-1.184679
4	15	0	1.555154	-1.581790	0.117976
5	6	0	3.183616	-0.671540	0.372300
6	6	0	3.182183	0.673768	-0.374888
7	15	0	1.553794	1.583107	-0.116258
8	6	0	1.725357	3.065593	-1.254673
9	6	0	1.766911	4.308033	-0.338261
10	6	0	2.502843	3.913513	0.953003
11	6	0	1.886743	2.584823	1.429579
12	6	0	1.884062	-2.580721	-1.430521
13	6	0	2.504199	-3.908978	-0.958123
14	6	0	1.773191	-4.306916	0.334907
15	6	0	1.731825	-3.065962	1.253427
16	1	0	3.270956	-0.497715	1.452466
17	1	0	4.041194	-1.287636	0.076820
18	1	0	4.040091	1.290496	-0.081704
19	1	0	3.266751	0.500068	-1.455292
20	1	0	0.894164	3.098561	-1.962961
21	1	0	2.651931	2.972243	-1.832483
22	1	0	0.742893	4.612788	-0.090857
23	1	0	2.242364	5.158136	-0.839370
24	1	0	2.426253	4.691984	1.720298
25	1	0	3.571191	3.776280	0.741144
26	1	0	0.929479	2.760625	1.930666
27	1	0	2.524164	2.032752	2.127293
28	1	0	2.517902	-2.026588	-2.129864
29	1	0	0.925246	-2.757543	-1.928275
30	1	0	3.572984	-3.770075	-0.749598
31	1	0	2.426516	-4.686373	-1.726400
32	1	0	2.251990	-5.156769	0.833249
33	1	0	0.749050	-4.613467	0.090276
34	1	0	2.659603	-2.972013	1.829203
35	1	0	0.902358	-3.101406	1.963623
36	29	0	-0.030451	0.000074	0.002791
37	6	0	-4.115294	0.171239	-1.182840
38	6	0	-1.990133	0.359805	-2.503040
39	6	0	-1.994538	-0.365538	2.507309
40	1	0	-2.672025	0.613373	-3.322486
41	1	0	-1.240828	1.159306	-2.431787
42	1	0	-1.452038	-0.551615	-2.797909

43	1	0	-2.676100	-0.642524	3.319465
44	1	0	-1.477360	0.553190	2.816880
45	1	0	-1.228535	-1.148510	2.431269
46	6	0	-4.842041	-0.006054	-0.000301
47	6	0	-4.117994	-0.182630	1.180883
48	6	0	-6.353735	0.008365	-0.004302
49	1	0	-4.653605	0.306616	-2.121303
50	1	0	-4.658639	-0.325386	2.116602
51	1	0	-6.750609	1.013386	-0.199686
52	1	0	-6.757967	-0.320273	0.958494
53	1	0	-6.763327	-0.649744	-0.779960

Zero-point correction= 0.457885 (Hartree/Particle)
Thermal correction to Energy= 0.483680
Thermal correction to Enthalpy= 0.484624
Thermal correction to Gibbs Free Energy= 0.398864
Sum of electronic and zero-point Energies= -3065.300167
Sum of electronic and thermal Energies= -3065.274372
Sum of electronic and thermal Enthalpies= -3065.273428
Sum of electronic and thermal Free Energies= -3065.359188

1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.370764	0.369674	-1.802291
2	6	0	3.121198	-0.288940	-0.956297
3	6	0	1.686624	-0.206846	-0.687958
4	6	0	0.496319	-0.138457	-0.466121
5	6	0	4.026400	0.056152	0.210688
6	6	0	3.630316	0.416260	1.429177
7	1	0	2.577068	0.490994	1.683247
8	1	0	4.349756	0.646872	2.208770
9	1	0	3.367804	-1.303190	-1.305504
10	1	0	5.089723	-0.011078	-0.017327
11	6	0	-0.908860	-0.060792	-0.211808
12	6	0	-1.590532	1.166880	-0.322205
13	6	0	-1.635495	-1.210707	0.154000
14	6	0	-2.959059	1.238153	-0.073390
15	1	0	-1.034801	2.055733	-0.603326
16	6	0	-3.003872	-1.131038	0.400901
17	1	0	-1.114429	-2.158772	0.241032
18	6	0	-3.670404	0.091580	0.288531
19	1	0	-3.472219	2.191486	-0.162023
20	1	0	-3.551942	-2.025716	0.682315
21	1	0	-4.737541	0.150520	0.482003

Zero-point correction= 0.171731 (Hartree/Particle)
Thermal correction to Energy= 0.181954
Thermal correction to Enthalpy= 0.182899
Thermal correction to Gibbs Free Energy= 0.133424

Sum of electronic and zero-point Energies= -424.943594
Sum of electronic and thermal Energies= -424.933371
Sum of electronic and thermal Enthalpies= -424.932427
Sum of electronic and thermal Free Energies= -424.981901

TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.346246	-0.349469	-0.209913
2	6	0	2.516310	-1.759002	-0.100263
3	6	0	3.520828	0.447703	-0.112317
4	15	0	-0.915136	-0.393270	1.883356
5	6	0	-2.184085	0.981096	2.017157
6	6	0	-1.518366	2.364859	1.916851
7	15	0	-0.350517	2.467458	0.451234
8	6	0	0.464859	4.135127	0.703126
9	6	0	0.160781	4.935285	-0.578614
10	6	0	-1.283066	4.603208	-0.988957
11	6	0	-1.430342	3.069208	-0.952793
12	6	0	-0.398477	-0.676271	3.659796
13	6	0	-1.363689	-1.740045	4.218309
14	6	0	-1.631211	-2.742601	3.083160
15	6	0	-1.971883	-1.936797	1.812193
16	1	0	-2.876111	0.830651	1.179740
17	1	0	-2.766962	0.890985	2.941276
18	1	0	-2.270478	3.162032	1.878132
19	1	0	-0.902216	2.547328	2.806953
20	1	0	1.535686	4.024748	0.885383
21	1	0	0.023418	4.625777	1.578476
22	1	0	0.847512	4.627080	-1.376902
23	1	0	0.309125	6.009534	-0.424550
24	1	0	-1.530791	5.005622	-1.977060
25	1	0	-1.977021	5.060965	-0.272259
26	1	0	-1.075953	2.603561	-1.876404
27	1	0	-2.463941	2.742348	-0.809117
28	1	0	-0.404671	0.260017	4.226904
29	1	0	0.631184	-1.048557	3.657814
30	1	0	-2.306881	-1.266419	4.520073
31	1	0	-0.952711	-2.229388	5.108346
32	1	0	-2.434121	-3.443278	3.335965
33	1	0	-0.727967	-3.340925	2.909575
34	1	0	-3.027141	-1.644233	1.799171
35	1	0	-1.780660	-2.489714	0.891223
36	29	0	0.595152	0.424509	0.418003
37	1	0	1.561109	0.013226	-1.258441
38	6	0	4.764789	-0.131227	0.148329
39	6	0	3.454920	1.948111	-0.299170
40	6	0	1.333854	-2.690763	-0.251746

41	1	0	4.415482	2.350265	-0.637272
42	1	0	2.690311	2.220866	-1.033755
43	1	0	3.202324	2.461979	0.637276
44	1	0	1.645618	-3.666861	-0.636479
45	1	0	0.581381	-2.280540	-0.929311
46	1	0	0.843237	-2.864954	0.716100
47	6	0	4.912427	-1.513947	0.297716
48	6	0	3.771323	-2.311818	0.160664
49	6	0	6.268909	-2.131454	0.539558
50	1	0	5.644205	0.506399	0.227772
51	1	0	3.869070	-3.392983	0.249305
52	1	0	6.754333	-2.408617	-0.405341
53	1	0	6.192857	-3.043099	1.141038
54	1	0	6.939509	-1.437491	1.056139
55	6	0	0.965806	0.200866	-2.672892
56	6	0	-0.377953	-0.178362	-2.452115
57	6	0	-1.504887	-0.569257	-2.156236
58	6	0	1.826247	-0.609800	-3.545359
59	6	0	1.574268	-1.824481	-4.062197
60	1	0	0.614815	-2.315377	-3.924462
61	1	0	2.323177	-2.355030	-4.641443
62	1	0	1.120650	1.278928	-2.775576
63	1	0	2.805667	-0.166798	-3.732205
64	6	0	-2.805811	-1.050995	-1.863396
65	6	0	-3.097724	-2.435663	-1.934334
66	6	0	-3.854412	-0.179213	-1.481887
67	6	0	-4.367382	-2.915353	-1.628742
68	1	0	-2.310960	-3.120068	-2.236143
69	6	0	-5.120806	-0.671116	-1.174070
70	1	0	-3.664075	0.889138	-1.455218
71	6	0	-5.388580	-2.041112	-1.241288
72	1	0	-4.563586	-3.982440	-1.694724
73	1	0	-5.908360	0.022346	-0.889636
74	1	0	-6.378013	-2.420902	-1.004713

Zero-point correction= 0.625373 (Hartree/Particle)
Thermal correction to Energy= 0.663338
Thermal correction to Enthalpy= 0.664283
Thermal correction to Gibbs Free Energy= 0.550708
Sum of electronic and zero-point Energies= -3490.214604
Sum of electronic and thermal Energies= -3490.176638
Sum of electronic and thermal Enthalpies= -3490.175694
Sum of electronic and thermal Free Energies= -3490.289268

IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.277643	1.382154	0.084218

2	6	0	-1.708701	2.234703	-0.778441
3	6	0	-3.060714	1.762818	-0.214797
4	15	0	-3.148018	-0.111361	-0.120808
5	6	0	-4.742287	-0.386286	0.839104
6	6	0	-5.729258	-1.069103	-0.131675
7	6	0	-5.457638	-0.517798	-1.541863
8	6	0	-3.935104	-0.578754	-1.756259
9	6	0	0.235125	2.569864	1.445038
10	6	0	1.692949	2.965218	1.124694
11	6	0	1.826167	3.061456	-0.404748
12	6	0	1.192646	1.785855	-0.990018
13	1	0	-1.632541	1.956525	-1.836682
14	1	0	-1.620569	3.325896	-0.723591
15	1	0	-3.894041	2.166189	-0.802471
16	1	0	-3.184488	2.127232	0.812494
17	1	0	-5.129052	0.582483	1.174780
18	1	0	-6.768643	-0.913255	0.177134
19	1	0	-6.000811	-1.079210	-2.310509
20	1	0	-5.802272	0.522751	-1.603013
21	1	0	0.133802	2.094293	2.422884
22	1	0	1.972762	3.900038	1.622743
23	1	0	2.372697	2.187429	1.493291
24	1	0	1.290778	3.949336	-0.766309
25	1	0	2.871935	3.167158	-0.712740
26	29	0	-1.050231	-0.653595	0.489166
27	1	0	-5.555197	-2.152408	-0.129857
28	1	0	-3.615527	-1.598094	-1.997440
29	1	0	0.895911	1.885018	-2.038291
30	6	0	0.159348	-2.386582	-0.131503
31	6	0	1.496200	-1.939066	-0.189688
32	6	0	2.660172	-1.563729	-0.252577
33	6	0	-0.562173	-2.506915	1.101211
34	6	0	-0.354268	-1.710999	2.236315
35	1	0	0.619301	-1.265762	2.417952
36	1	0	-0.966181	-1.889898	3.113506
37	1	0	-0.177021	-3.013468	-0.953206
38	1	0	-1.424820	-3.172257	1.088173
39	1	0	1.881091	0.937886	-0.922122
40	1	0	-0.421739	3.447559	1.429449
41	1	0	-3.577766	0.069761	-2.562377
42	1	0	-4.548144	-0.987124	1.730640
43	6	0	4.006673	-1.120661	-0.317911
44	6	0	4.666619	-0.620877	0.829474
45	6	0	4.729084	-1.159232	-1.533290
46	6	0	5.984359	-0.178622	0.757436
47	1	0	4.130245	-0.595204	1.773259
48	6	0	6.047152	-0.716458	-1.592962
49	1	0	4.238778	-1.543086	-2.422609
50	6	0	6.684803	-0.221688	-0.451556
51	1	0	6.470593	0.199271	1.653177

52	1	0	6.581945	-0.757937	-2.538370
53	1	0	7.713666	0.122375	-0.502752

Zero-point correction= 0.447597 (Hartree/Particle)
Thermal correction to Energy= 0.473919
Thermal correction to Enthalpy= 0.474863
Thermal correction to Gibbs Free Energy= 0.388291
Sum of electronic and zero-point Energies= -3140.246244
Sum of electronic and thermal Energies= -3140.219921
Sum of electronic and thermal Enthalpies= -3140.218977
Sum of electronic and thermal Free Energies= -3140.305549

MesH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.369027	0.233242	-0.025965
2	6	0	0.490093	1.321833	-0.011702
3	6	0	0.899504	-1.085576	-0.011800
4	1	0	2.441762	0.415812	-0.047561
5	6	0	-0.482622	-1.302440	0.006899
6	6	0	1.865045	-2.248417	0.009973
7	6	0	1.014989	2.739151	0.009829
8	1	0	1.430332	-3.139770	-0.452565
9	1	0	2.792098	-2.009543	-0.520482
10	1	0	2.140186	-2.517095	1.037925
11	1	0	0.335666	3.426717	-0.503564
12	1	0	1.995665	2.810560	-0.470409
13	1	0	1.129665	3.104716	1.038336
14	6	0	-1.389847	-0.236280	0.014113
15	6	0	-0.886778	1.069280	0.007173
16	6	0	-2.879755	-0.490834	-0.006960
17	1	0	-0.861202	-2.322899	0.011723
18	1	0	-1.581417	1.907210	0.012024
19	1	0	-3.253169	-0.580770	-1.035047
20	1	0	-3.432555	0.325314	0.468245
21	1	0	-3.134967	-1.420011	0.512009

Zero-point correction= 0.182668 (Hartree/Particle)
Thermal correction to Energy= 0.191796
Thermal correction to Enthalpy= 0.192741
Thermal correction to Gibbs Free Energy= 0.147042
Sum of electronic and zero-point Energies= -350.029821
Sum of electronic and thermal Energies= -350.020692
Sum of electronic and thermal Enthalpies= -350.019748
Sum of electronic and thermal Free Energies= -350.065447

2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.212165	-1.311391	-0.000071
2	6	0	-2.592804	0.110772	-0.000009
3	6	0	-1.965134	-1.139042	0.000032
4	6	0	-0.576222	-1.219545	0.000049
5	6	0	0.205165	-0.052979	-0.000009
6	6	0	-0.432959	1.196667	-0.000003
7	6	0	1.697839	-0.202954	-0.000022
8	6	0	2.562035	1.047313	0.000053
9	1	0	-2.561652	-2.046784	0.000043
10	1	0	-3.677310	0.174754	-0.000032
11	1	0	0.151961	2.110926	-0.000021
12	1	0	-0.064558	-2.176205	0.000072
13	6	0	-1.825668	1.277226	-0.000035
14	1	0	-2.311406	2.248660	-0.000078
15	1	0	2.361192	1.664673	-0.882449
16	1	0	2.361129	1.664481	0.882689
17	1	0	3.609806	0.745874	0.000007

Zero-point correction= 0.138211 (Hartree/Particle)
Thermal correction to Energy= 0.145996
Thermal correction to Enthalpy= 0.146940
Thermal correction to Gibbs Free Energy= 0.105592
Sum of electronic and zero-point Energies= -384.762123
Sum of electronic and thermal Energies= -384.754338
Sum of electronic and thermal Enthalpies= -384.753393
Sum of electronic and thermal Free Energies= -384.794742

TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.912844	-2.018501	0.911395
2	6	0	2.640029	-2.744725	0.964576
3	6	0	3.696714	-1.636812	1.116374
4	15	0	3.408831	-0.235852	-0.102967
5	6	0	4.712726	1.013110	0.430125
6	6	0	5.698975	1.138082	-0.749730
7	6	0	5.832062	-0.251934	-1.393348
8	6	0	4.402912	-0.786394	-1.595749
9	6	0	0.367972	-2.007159	2.709277
10	6	0	-0.857376	-2.943789	2.782839
11	6	0	-0.620780	-4.104930	1.802935
12	6	0	-0.165771	-3.478853	0.471678
13	1	0	2.784484	-3.266005	0.009922
14	1	0	2.741097	-3.492849	1.759438
15	1	0	4.710806	-2.042232	1.017057
16	1	0	3.625850	-1.188716	2.115535

17	1	0	5.222983	0.642102	1.326343
18	1	0	6.666533	1.534986	-0.423590
19	1	0	6.389525	-0.214739	-2.336146
20	1	0	6.387833	-0.916863	-0.719445
21	1	0	0.133012	-0.989038	3.027263
22	1	0	-1.030118	-3.296394	3.805635
23	1	0	-1.754435	-2.392260	2.476558
24	1	0	0.163425	-4.766088	2.194943
25	1	0	-1.521607	-4.715109	1.673909
26	29	0	1.139916	-0.066467	-0.200603
27	1	0	5.298509	1.841576	-1.490588
28	1	0	3.945633	-0.340604	-2.485658
29	1	0	0.361298	-4.178791	-0.183998
30	6	0	0.161113	0.001027	-2.077395
31	6	0	-1.141505	-0.515290	-1.827656
32	6	0	-2.256946	-0.968624	-1.625246
33	6	0	0.364749	1.383991	-2.316908
34	6	0	-0.467733	2.422233	-1.914707
35	1	0	-1.506660	2.196176	-1.701851
36	1	0	-0.270981	3.424810	-2.281443
37	1	0	0.821533	-0.671515	-2.627697
38	1	0	1.334077	1.642277	-2.744853
39	6	0	-3.543036	4.634622	1.478027
40	6	0	-2.497708	5.378903	0.929382
41	8	0	0.193153	1.418350	0.640287
42	6	0	0.076805	2.627013	0.234755
43	6	0	1.357085	3.435989	0.062674
44	6	0	-1.168909	3.357979	0.648265
45	6	0	-1.322439	4.748125	0.519176
46	6	0	-2.228209	2.620508	1.206290
47	6	0	-3.400937	3.250392	1.614590
48	1	0	-4.206307	2.661822	2.046532
49	1	0	-4.457422	5.127005	1.797100
50	1	0	-2.594859	6.455889	0.820875
51	1	0	-0.524836	5.349073	0.094924
52	1	0	-2.102506	1.548744	1.311180
53	1	0	2.117062	2.805384	-0.402337
54	1	0	1.233916	4.336965	-0.540584
55	1	0	1.722475	3.736423	1.054911
56	1	0	-1.019642	-3.084512	-0.088145
57	1	0	1.184453	-2.377054	3.340797
58	1	0	4.356155	-1.872940	-1.721074
59	1	0	4.245258	1.965949	0.688693
60	6	0	-3.562668	-1.459129	-1.347632
61	6	0	-4.545803	-0.609873	-0.792219
62	6	0	-3.911631	-2.801476	-1.613755
63	6	0	-5.821767	-1.090968	-0.513381
64	1	0	-4.289013	0.424216	-0.584177
65	6	0	-5.190532	-3.273087	-1.328967
66	1	0	-3.168732	-3.461864	-2.050835
67	6	0	-6.152947	-2.423135	-0.777895
68	1	0	-6.563996	-0.421590	-0.086691
69	1	0	-5.439019	-4.309394	-1.542354

70	1	0	-7.150363	-2.793591	-0.559646

Zero-point correction= 0.586877 (Hartree/Particle)
Thermal correction to Energy= 0.621773
Thermal correction to Enthalpy= 0.622718
Thermal correction to Gibbs Free Energy= 0.515090
Sum of electronic and zero-point Energies= -3525.006559
Sum of electronic and thermal Energies= -3524.971662
Sum of electronic and thermal Enthalpies= -3524.970718
Sum of electronic and thermal Free Energies= -3525.078346

IM3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.469513	-1.774947	1.171902
2	6	0	2.040016	-2.659170	1.664092
3	6	0	3.250900	-1.724406	1.492012
4	15	0	3.305302	-0.941599	-0.214957
5	6	0	4.748718	0.247501	-0.033757
6	6	0	5.838311	-0.241761	-1.009631
7	6	0	5.794059	-1.778752	-1.023364
8	6	0	4.318217	-2.181384	-1.199553
9	6	0	-0.138572	-0.937367	2.727096
10	6	0	-1.555223	-1.500430	2.963502
11	6	0	-1.542654	-2.987130	2.566866
12	6	0	-0.865750	-3.078378	1.185094
13	1	0	2.137770	-3.528863	1.002222
14	1	0	1.982922	-3.038619	2.690947
15	1	0	4.187639	-2.251417	1.709712
16	1	0	3.176923	-0.890169	2.200425
17	1	0	5.109446	0.216854	1.000320
18	1	0	6.826900	0.137869	-0.729254
19	1	0	6.428192	-2.200516	-1.811646
20	1	0	6.173123	-2.164196	-0.067980
21	1	0	-0.126883	0.143208	2.569045
22	1	0	-1.874360	-1.355362	4.001333
23	1	0	-2.270892	-0.963576	2.329066
24	1	0	-0.965652	-3.560591	3.304174
25	1	0	-2.552461	-3.411615	2.546814
26	29	0	0.973545	-0.296123	-0.459943
27	1	0	5.626933	0.135347	-2.018436
28	1	0	4.018708	-2.100492	-2.250277
29	1	0	-0.462353	-4.070440	0.960342
30	6	0	-0.166600	-0.624894	-2.212454
31	6	0	-1.528841	-0.845189	-1.861982
32	6	0	-2.694134	-1.077276	-1.591407
33	6	0	0.460332	0.623000	-2.193243
34	6	0	-0.179584	1.906044	-1.716596
35	1	0	-1.209353	1.703128	-1.408317

36	1	0	-0.219571	2.626943	-2.544506
37	1	0	0.302586	-1.421374	-2.788125
38	1	0	1.368257	0.712487	-2.786040
39	6	0	-1.719179	5.632609	1.434695
40	6	0	-1.428454	5.709377	0.070834
41	8	0	0.801818	1.414361	0.416835
42	6	0	0.598861	2.466685	-0.475476
43	6	0	1.956397	3.068289	-0.925363
44	6	0	-0.225296	3.591910	0.180389
45	6	0	-0.686462	4.700966	-0.546064
46	6	0	-0.524315	3.528372	1.545873
47	6	0	-1.260764	4.537928	2.169204
48	1	0	-1.478671	4.468721	3.232506
49	1	0	-2.295275	6.417642	1.917466
50	1	0	-1.778868	6.556160	-0.514192
51	1	0	-0.467358	4.783460	-1.607744
52	1	0	-0.159804	2.670837	2.099135
53	1	0	2.562962	2.305059	-1.425753
54	1	0	1.842747	3.919990	-1.606079
55	1	0	2.502411	3.408587	-0.040300
56	1	0	-1.570441	-2.818698	0.388890
57	1	0	0.527744	-1.176694	3.564141
58	1	0	4.106145	-3.207856	-0.883261
59	1	0	4.422572	1.269794	-0.235554
60	6	0	-4.057024	-1.310805	-1.248490
61	6	0	-4.686711	-2.529548	-1.576923
62	6	0	-4.803027	-0.324733	-0.568426
63	6	0	-6.017700	-2.751518	-1.233693
64	1	0	-4.120462	-3.291241	-2.103793
65	6	0	-6.133348	-0.556842	-0.229762
66	1	0	-4.325503	0.616383	-0.315013
67	6	0	-6.746704	-1.768521	-0.559352
68	1	0	-6.488875	-3.694980	-1.494874
69	1	0	-6.694581	0.212307	0.293278
70	1	0	-7.785022	-1.944682	-0.293910

Zero-point correction= 0.589514 (Hartree/Particle)
Thermal correction to Energy= 0.624057
Thermal correction to Enthalpy= 0.625001
Thermal correction to Gibbs Free Energy= 0.518524
Sum of electronic and zero-point Energies= -3525.027420
Sum of electronic and thermal Energies= -3524.992877
Sum of electronic and thermal Enthalpies= -3524.991933
Sum of electronic and thermal Free Energies= -3525.098410

IM31:

Standard orientation:

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

1	6	0	-2.099734	3.777782	-1.305966
2	6	0	-1.910729	2.309553	-1.624947
3	6	0	-3.129219	1.503499	-1.607527
4	6	0	-4.150056	0.844528	-1.596373
5	6	0	-3.247554	4.386086	-1.010452
6	1	0	-1.164739	1.894417	-0.918294
7	1	0	-1.440338	2.224203	-2.616993
8	1	0	-1.170168	4.344663	-1.316535
9	1	0	-3.278011	5.447138	-0.782070
10	1	0	-4.190120	3.846190	-0.989349
11	15	0	0.356850	-1.944902	-0.696504
12	6	0	-1.212092	-2.942882	-0.506406
13	6	0	-2.316605	-2.098147	0.153399
14	15	0	-1.709054	-1.233791	1.702148
15	6	0	-3.191619	-0.179501	2.166295
16	6	0	-3.671770	-0.693377	3.538475
17	6	0	-3.478484	-2.218489	3.555585
18	6	0	-2.048180	-2.493377	3.053993
19	6	0	0.208493	-1.111747	-2.365393
20	6	0	1.385112	-1.650473	-3.207748
21	6	0	1.614678	-3.119991	-2.815681
22	6	0	1.634667	-3.173822	-1.276199
23	1	0	-0.960389	-3.799826	0.131263
24	1	0	-1.550458	-3.344222	-1.468836
25	1	0	-3.200898	-2.709469	0.368761
26	1	0	-2.637268	-1.299194	-0.525756
27	1	0	-3.969458	-0.304764	1.405907
28	1	0	-4.712539	-0.409869	3.729423
29	1	0	-3.648795	-2.642960	4.551665
30	1	0	-4.205088	-2.686329	2.879128
31	1	0	0.247791	-0.029334	-2.228803
32	1	0	1.193000	-1.537115	-4.280227
33	1	0	2.288533	-1.071899	-2.980221
34	1	0	0.793162	-3.738140	-3.200845
35	1	0	2.542903	-3.514610	-3.243697
36	29	0	0.481125	-0.512618	1.053146
37	1	0	-3.066762	-0.242659	4.335719
38	1	0	-1.319861	-2.332970	3.856832
39	1	0	1.440702	-4.171693	-0.871003
40	6	0	2.151416	-0.984315	2.286310
41	6	0	3.320852	-1.145451	1.491643
42	6	0	4.334883	-1.332140	0.842210
43	6	0	1.575936	0.246082	2.602485
44	6	0	2.057236	1.576279	2.074606
45	1	0	2.950770	1.417156	1.464045
46	1	0	2.342343	2.229092	2.910713
47	1	0	1.876407	-1.846285	2.892464
48	1	0	0.909829	0.260512	3.462271
49	6	0	2.858898	5.503027	-1.031991
50	6	0	2.693410	5.600032	0.351378
51	8	0	0.491704	1.272104	0.277298
52	6	0	0.962645	2.240921	1.167413
53	6	0	-0.196997	2.782538	2.041731

54	6	0	1.618185	3.412287	0.407181
55	6	0	2.079920	4.566134	1.060339
56	6	0	1.800766	3.324884	-0.978394
57	6	0	2.410123	4.358918	-1.693249
58	1	0	2.537061	4.268960	-2.769590
59	1	0	3.333363	6.308927	-1.585497
60	1	0	3.041410	6.483597	0.880628
61	1	0	1.963133	4.665006	2.136339
62	1	0	1.455585	2.423899	-1.472073
63	1	0	-0.650421	1.963979	2.610965
64	1	0	0.122150	3.551588	2.753898
65	1	0	-0.969761	3.214738	1.399277
66	1	0	2.602700	-2.843335	-0.886324
67	1	0	-0.756540	-1.365532	-2.817763
68	1	0	-1.904254	-3.515306	2.688517
69	1	0	-2.916428	0.877180	2.180373
70	6	0	5.516746	-1.509515	0.066962
71	6	0	6.147849	-2.768643	-0.011079
72	6	0	6.077680	-0.425338	-0.640759
73	6	0	7.300700	-2.934239	-0.774009
74	1	0	5.724265	-3.606423	0.534011
75	6	0	7.230829	-0.601576	-1.400437
76	1	0	5.597341	0.546211	-0.584187
77	6	0	7.847210	-1.853850	-1.471498
78	1	0	7.775891	-3.909990	-0.823346
79	1	0	7.651080	0.242776	-1.939465
80	1	0	8.747194	-1.986360	-2.064830
81	6	0	-5.350649	0.068140	-1.579678
82	6	0	-6.340767	0.296332	-0.602226
83	6	0	-5.569386	-0.942732	-2.537256
84	6	0	-7.507329	-0.465215	-0.585057
85	1	0	-6.183724	1.079318	0.133003
86	6	0	-6.738148	-1.700005	-2.512864
87	1	0	-4.815471	-1.120208	-3.297809
88	6	0	-7.711039	-1.466490	-1.537653
89	1	0	-8.261605	-0.274210	0.173171
90	1	0	-6.891955	-2.473954	-3.259685
91	1	0	-8.622016	-2.057653	-1.522451

Zero-point correction= 0.762266 (Hartree/Particle)
Thermal correction to Energy= 0.809083
Thermal correction to Enthalpy= 0.810027
Thermal correction to Gibbs Free Energy= 0.671182
Sum of electronic and zero-point Energies= -3949.979955
Sum of electronic and thermal Energies= -3949.933138
Sum of electronic and thermal Enthalpies= -3949.932194
Sum of electronic and thermal Free Energies= -3950.071039

TS3:

Standard orientation:

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

1	6	0	-1.439069	3.339715	-2.075018
2	6	0	-1.117819	1.908990	-2.177281
3	6	0	-2.175605	0.973281	-2.173032
4	6	0	-3.106046	0.169683	-2.141350
5	6	0	-2.597497	3.922534	-1.704542
6	1	0	-0.161442	1.635570	-0.918669
7	1	0	-0.348357	1.693585	-2.925010
8	1	0	-0.592457	3.994832	-2.289872
9	1	0	-2.684434	5.001926	-1.627328
10	1	0	-3.492102	3.337592	-1.507920
11	15	0	-0.400011	-2.120974	0.483531
12	6	0	-2.027954	-2.529657	1.301692
13	6	0	-2.956062	-1.303283	1.316040
14	15	0	-2.098179	0.214820	1.988896
15	6	0	-3.271724	1.606552	1.557518
16	6	0	-3.704846	2.223500	2.902476
17	6	0	-3.832947	1.077971	3.921238
18	6	0	-2.549455	0.232624	3.808178
19	6	0	-0.653004	-2.429423	-1.340015
20	6	0	0.415357	-3.472032	-1.725383
21	6	0	0.528790	-4.470221	-0.560678
22	6	0	0.656128	-3.640797	0.733372
23	1	0	-1.791652	-2.843986	2.326476
24	1	0	-2.513474	-3.376400	0.803838
25	1	0	-3.872557	-1.513641	1.878792
26	1	0	-3.253135	-1.051005	0.292849
27	1	0	-4.129144	1.180759	1.026154
28	1	0	-4.638937	2.785377	2.797876
29	1	0	-3.984580	1.448198	4.941342
30	1	0	-4.705484	0.461764	3.669793
31	1	0	-0.580669	-1.496893	-1.901725
32	1	0	0.160805	-3.968416	-2.667894
33	1	0	1.381892	-2.974997	-1.874586
34	1	0	-0.376018	-5.089933	-0.519904
35	1	0	1.379624	-5.148878	-0.684767
36	29	0	0.128272	-0.056173	1.271961
37	1	0	-2.942756	2.934055	3.247640
38	1	0	-1.728203	0.703708	4.360009
39	1	0	0.356954	-4.188454	1.632267
40	6	0	1.837802	-0.369718	2.485339
41	6	0	2.918757	-0.912444	1.735118
42	6	0	3.856018	-1.391826	1.122509
43	6	0	1.466616	0.973415	2.454549
44	6	0	2.143497	1.981433	1.555787
45	1	0	2.993153	1.501171	1.063941
46	1	0	2.539211	2.811839	2.153264
47	1	0	1.488502	-0.977490	3.319063
48	1	0	0.888824	1.346317	3.296497
49	6	0	3.784803	4.438736	-2.500669
50	6	0	3.364572	5.154917	-1.379853
51	8	0	0.560092	1.390312	-0.113415
52	6	0	1.201529	2.545270	0.452443

53	6	0	0.150143	3.484504	1.068573
54	6	0	2.069428	3.243088	-0.604961
55	6	0	2.516448	4.562318	-0.442214
56	6	0	2.505542	2.531681	-1.732539
57	6	0	3.350298	3.123392	-2.672348
58	1	0	3.664367	2.555799	-3.544333
59	1	0	4.439861	4.901567	-3.233329
60	1	0	3.692581	6.180446	-1.233281
61	1	0	2.204529	5.142999	0.419934
62	1	0	2.160384	1.513552	-1.869831
63	1	0	-0.436196	2.938878	1.814192
64	1	0	0.613090	4.337699	1.573022
65	1	0	-0.536655	3.857507	0.305425
66	1	0	1.686616	-3.303389	0.879624
67	1	0	-1.662489	-2.824239	-1.496017
68	1	0	-2.660289	-0.783717	4.199608
69	1	0	-2.797102	2.322108	0.882939
70	6	0	4.950989	-1.907366	0.370174
71	6	0	5.515737	-3.161375	0.679869
72	6	0	5.487285	-1.164075	-0.702191
73	6	0	6.584155	-3.654633	-0.064199
74	1	0	5.109715	-3.735615	1.506708
75	6	0	6.555831	-1.666554	-1.439353
76	1	0	5.055344	-0.198191	-0.944512
77	6	0	7.108031	-2.911191	-1.124923
78	1	0	7.011014	-4.621834	0.185196
79	1	0	6.959797	-1.084427	-2.262527
80	1	0	7.942126	-3.298903	-1.702288
81	6	0	-4.205947	-0.720587	-2.219106
82	6	0	-5.452181	-0.404162	-1.621185
83	6	0	-4.105416	-1.963988	-2.893483
84	6	0	-6.525162	-1.287824	-1.685237
85	1	0	-5.562590	0.553657	-1.121119
86	6	0	-5.185063	-2.840825	-2.948876
87	1	0	-3.172074	-2.215809	-3.387610
88	6	0	-6.402442	-2.515905	-2.342949
89	1	0	-7.469419	-1.013803	-1.220985
90	1	0	-5.078164	-3.784455	-3.478514
91	1	0	-7.242897	-3.201917	-2.391321

Zero-point correction= 0.759305 (Hartree/Particle)
Thermal correction to Energy= 0.804773
Thermal correction to Enthalpy= 0.805717
Thermal correction to Gibbs Free Energy= 0.674090
Sum of electronic and zero-point Energies= -3949.958368
Sum of electronic and thermal Energies= -3949.912900
Sum of electronic and thermal Enthalpies= -3949.911956
Sum of electronic and thermal Free Energies= -3950.043583

Pro:

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	2.441338	-0.955490	2.324922
2	6	0	-0.620897	-2.965511	-0.347052
3	6	0	-1.620561	-1.962151	-0.264302
4	6	0	-2.512825	-1.136509	-0.192536
5	6	0	0.698173	-2.745891	-0.518952
6	6	0	1.341880	-1.400423	-0.672632
7	1	0	0.577922	-0.620453	-0.613246
8	1	0	1.804776	-1.323958	-1.666136
9	1	0	-0.971654	-3.993877	-0.269521
10	1	0	1.343519	-3.619828	-0.574040
11	6	0	3.753684	3.021647	-0.333710
12	6	0	4.307001	1.975163	-1.073613
13	8	0	1.787383	-1.166257	1.643878
14	6	0	2.442630	-1.070808	0.374871
15	6	0	3.599955	-2.085757	0.338871
16	6	0	2.933271	0.364453	0.127388
17	6	0	3.900106	0.660016	-0.844998
18	6	0	2.377900	1.424965	0.856469
19	6	0	2.785813	2.740767	0.631102
20	1	0	2.344200	3.547006	1.210599
21	1	0	4.072937	4.044927	-0.509592
22	1	0	5.059576	2.180933	-1.829861
23	1	0	4.343581	-0.137153	-1.433951
24	1	0	1.618828	1.205784	1.599738
25	1	0	3.236910	-3.068641	0.648162
26	1	0	4.045813	-2.181088	-0.655387
27	1	0	4.393969	-1.782444	1.030261
28	6	0	-3.543318	-0.156863	-0.108345
29	6	0	-4.897164	-0.542480	-0.025066
30	6	0	-3.228524	1.217893	-0.107019
31	6	0	-5.900479	0.419265	0.056175
32	1	0	-5.145736	-1.598933	-0.025409
33	6	0	-4.238688	2.172222	-0.025162
34	1	0	-2.188179	1.520522	-0.169696
35	6	0	-5.576974	1.778624	0.056468
36	1	0	-6.939123	0.107346	0.119601
37	1	0	-3.981229	3.227606	-0.025097
38	1	0	-6.362420	2.526077	0.119900

Zero-point correction= 0.314404 (Hartree/Particle)
Thermal correction to Energy= 0.332730
Thermal correction to Enthalpy= 0.333674
Thermal correction to Gibbs Free Energy= 0.263958
Sum of electronic and zero-point Energies= -809.708463
Sum of electronic and thermal Energies= -809.690137
Sum of electronic and thermal Enthalpies= -809.689193
Sum of electronic and thermal Free Energies= -809.758909

S5. The summarize energies of all species along reaction paths over the BPE-CuMes system in the THF solvent at the M06/6-311+G(d, p) level.

1: the formation of the catalyst

M06(SMD,THF) /6-311+G(d, p)

species	SCF_{SMD}	G^*_{gas}	G_{sol}	ΔG_{sol}	ΔG_{sol}(kJ mol^{-1})
BPE	-1075.58977032	0.242603	-1075.347167		
CuMes	-1989.78779467	0.132950	-1989.654844		
BPE+ CuMes			-3065.002011		
BPE-CuMes	-3065.45009418	0.400066	-3065.050028		
1	-424.882657537	0.133815	-424.748825		
BPE +CuMes+1			-3489.750854	0.048017	126.05
BPE-CuMes+1			-3489.798871	0.0	0.0
TS1	-3490.31341594	0.557315	-3489.7561	0.042771	112.27
IM2	-3140.35876075	0.390983	-3139.967777		
MesH	-350.003515782	0.146255	-349.8572607		
IM2+ MesH			-3489.825038	-0.0261667	-68.69

2: the cycle of the teaction

species	SCF_{SMD}	G^*_{gas}	G_{sol}	ΔG_{sol}	ΔG_{sol}(kJ.mol^{-1})
2	-384.724253926	0.104920	-384.6193339		
1	-424.882657537	0.133815	-424.7488425		
IM2+2+1			-3949.335953	-0.004799	-12.597
TS2	-3525.08326388	0.519005	-3524.564258		
TS2+1			-3949.313101	0.018053	47.389
IM3	-3525.10538531	0.523074	-3524.582311		
IM3+1			-3949.331154	0.0	0.0
IM31	-3950.00464093	0.684084	-3949.320556	0.010598	27.820
TS3	-3949.98578045	0.680932	-3949.304848	0.026306	69.053
Pro	-809.628847004	0.267102	-809.361745		
IM2+Pro			-3949.329522	0.001632	4.284

S6. Cartesian coordinates and energies of all optimized structures over the BPE-CuMes system in the THF solvent at the M06 /6-311+G(d, p) level.

BPE:

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	15	0	-1.597889	-0.038224	-0.371819
2	6	0	-0.583392	-0.565873	1.093337
3	6	0	0.707687	0.247087	1.147123
4	15	0	1.581693	0.203716	-0.503313
5	6	0	3.007435	1.370708	-0.207386
6	6	0	4.273872	0.513674	-0.279043
7	6	0	3.939896	-0.840294	0.342071
8	6	0	2.648343	-1.310036	-0.323494
9	6	0	-2.699358	1.314059	0.259221
10	6	0	-4.082200	0.896757	-0.239299
11	6	0	-4.226663	-0.595436	0.051550
12	6	0	-2.965391	-1.287202	-0.477951
13	1	0	-0.350979	-1.630368	0.938806
14	1	0	-1.156822	-0.489019	2.027671
15	1	0	1.375980	-0.096307	1.949575
16	1	0	0.476522	1.305251	1.344533
17	1	0	2.894180	1.821404	0.787993
18	1	0	5.123689	1.001272	0.213240
19	1	0	4.754920	-1.564196	0.220252
20	1	0	3.782158	-0.716797	1.424289
21	1	0	-2.374696	2.285974	-0.125829
22	1	0	-4.882144	1.491087	0.218235
23	1	0	-4.142995	1.054480	-1.327237
24	1	0	-4.306197	-0.743588	1.139540
25	1	0	-5.135069	-1.009572	-0.403825
26	1	0	4.556774	0.364522	-1.331270
27	1	0	2.845256	-1.701090	-1.329633
28	1	0	-2.702865	-2.198071	0.071989
29	1	0	-3.077336	-1.552495	-1.536019
30	1	0	-2.670822	1.345695	1.358397
31	1	0	2.116844	-2.093175	0.230899
32	1	0	2.995162	2.181941	-0.941410

SCF Done: E(RM06) = -1075.58977032 A.U.

CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.385303	0.002273	-0.001347
2	6	0	-0.294993	1.215286	0.003023
3	6	0	-0.299118	-1.217196	0.002008
4	6	0	-1.689713	-1.200067	0.002889
5	6	0	0.460031	-2.510457	0.020484
6	6	0	0.444593	2.519918	0.019721
7	1	0	-0.194319	-3.363898	-0.185686
8	1	0	1.265060	-2.514293	-0.723930
9	1	0	0.929295	-2.683480	0.997630
10	1	0	0.061681	3.207872	-0.743580

11	1	0	1.515392	2.378471	-0.160598
12	1	0	0.336992	3.027085	0.987129
13	6	0	-2.403348	0.002371	0.002456
14	6	0	-1.693318	1.198173	0.004025
15	6	0	-3.902954	-0.009358	-0.016531
16	1	0	-2.236417	-2.144819	0.001894
17	1	0	-2.238437	2.143919	0.003750
18	1	0	-4.287853	-0.353234	-0.985156
19	1	0	-4.315102	0.988591	0.166506
20	1	0	-4.308201	-0.686095	0.745154
21	29	0	2.325277	-0.000199	-0.011155

SCF Done: E(RM06) = -1989.78779467 A.U.

BPE-CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.912877	-0.238862	-0.070050
2	6	0	-2.745833	0.671554	-0.751869
3	6	0	-2.568101	-1.249081	0.664465
4	15	0	1.316947	1.696717	-0.049708
5	6	0	3.083155	1.091223	-0.092169
6	6	0	3.188824	-0.276991	0.574449
7	15	0	1.789884	-1.384107	0.024435
8	6	0	2.081762	-2.927094	1.017929
9	6	0	2.236234	-4.031710	-0.027383
10	6	0	3.088570	-3.452559	-1.154013
11	6	0	2.442248	-2.125125	-1.553395
12	6	0	1.251716	2.564089	1.591695
13	6	0	1.690642	4.001587	1.317857
14	6	0	1.069534	4.393110	-0.020451
15	6	0	1.410190	3.283866	-1.019098
16	1	0	3.352778	1.013034	-1.156399
17	1	0	3.769366	1.820198	0.362021
18	1	0	4.163222	-0.750980	0.388315
19	1	0	3.079499	-0.176656	1.665075
20	1	0	1.254804	-3.103155	1.712841
21	1	0	3.004029	-2.818137	1.605797
22	1	0	1.245351	-4.300953	-0.423938
23	1	0	2.669564	-4.942899	0.401644
24	1	0	3.174548	-4.137650	-2.005927
25	1	0	4.108473	-3.274683	-0.780122
26	1	0	1.591657	-2.290629	-2.225927
27	1	0	3.127804	-1.431721	-2.055552
28	1	0	1.866670	2.040125	2.333540
29	1	0	0.213079	2.531948	1.946210
30	1	0	2.787562	4.051743	1.240661
31	1	0	1.395381	4.681057	2.126586
32	1	0	1.412777	5.373659	-0.371166
33	1	0	-0.022479	4.457978	0.095896

34	1	0	2.429717	3.406549	-1.409709
35	1	0	0.724140	3.251940	-1.871614
36	29	0	-0.000044	-0.104279	-0.125077
37	6	0	-3.959730	-1.340118	0.708705
38	6	0	-1.761148	-2.263808	1.430357
39	6	0	-2.138853	1.801679	-1.540746
40	1	0	-2.397722	-2.990389	1.950530
41	1	0	-1.092514	-2.823789	0.759204
42	1	0	-1.120586	-1.783800	2.183614
43	1	0	-2.899621	2.400449	-2.056719
44	1	0	-1.431268	1.435474	-2.297418
45	1	0	-1.570856	2.480777	-0.884722
46	6	0	-4.767214	-0.436786	0.020637
47	6	0	-4.137662	0.571348	-0.705227
48	6	0	-6.261824	-0.561564	0.041211
49	1	0	-4.431902	-2.134575	1.292429
50	1	0	-4.750860	1.296379	-1.246615
51	1	0	-6.620906	-1.258995	-0.728070
52	1	0	-6.748217	0.402770	-0.147370
53	1	0	-6.622461	-0.938668	1.005813

SCF Done: E(RM06) = -3065.45009418 A.U.

1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.368137	0.872179	-1.619147
2	6	0	3.117740	-0.000015	-0.994760
3	6	0	1.689207	-0.000329	-0.716434
4	6	0	0.501381	-0.000588	-0.477481
5	6	0	4.003075	0.000193	0.222910
6	6	0	3.583440	0.000163	1.482563
7	1	0	2.521798	-0.000109	1.723083
8	1	0	4.285115	0.000366	2.312038
9	1	0	3.368469	-0.872081	-1.619177
10	1	0	5.071983	0.000428	0.004657
11	6	0	-0.901753	-0.000261	-0.213713
12	6	0	-1.601173	1.208124	-0.084394
13	6	0	-1.601638	-1.208335	-0.084046
14	6	0	-2.966452	1.204756	0.165937
15	1	0	-1.057421	2.144648	-0.184257
16	6	0	-2.966916	-1.204333	0.166299
17	1	0	-1.058271	-2.145100	-0.183717
18	6	0	-3.653494	0.000361	0.291495
19	1	0	-3.498181	2.148486	0.263975
20	1	0	-3.499023	-2.147834	0.264517
21	1	0	-4.723114	0.000601	0.487782

SCF Done: E(RM06) = -424.882657537 A.U.

TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.944008	0.233455	0.824136
2	6	0	-2.531981	-1.049557	0.646818
3	6	0	-2.764369	1.335084	0.489358
4	15	0	0.205289	-0.386437	-1.802447
5	6	0	1.275528	0.823961	-2.726562
6	6	0	1.092783	2.230023	-2.161473
7	15	0	1.178491	2.247355	-0.294588
8	6	0	0.978865	4.073223	0.061620
9	6	0	2.277237	4.504354	0.742570
10	6	0	3.411160	3.776098	0.031986
11	6	0	3.020422	2.300065	0.001431
12	6	0	-1.388150	-0.299096	-2.749903
13	6	0	-1.286180	-1.373565	-3.829654
14	6	0	-0.596299	-2.565380	-3.171128
15	6	0	0.683218	-2.038031	-2.517772
16	1	0	2.315148	0.488841	-2.595337
17	1	0	1.061500	0.793359	-3.804712
18	1	0	1.821273	2.936136	-2.585685
19	1	0	0.090117	2.609430	-2.414468
20	1	0	0.095883	4.258196	0.679195
21	1	0	0.839359	4.609107	-0.887864
22	1	0	2.257056	4.197067	1.798851
23	1	0	2.402214	5.593630	0.727898
24	1	0	4.381057	3.933568	0.519542
25	1	0	3.502367	4.160377	-0.995421
26	1	0	3.216615	1.820757	0.970442
27	1	0	3.555778	1.726682	-0.765739
28	1	0	-1.558547	0.715647	-3.131241
29	1	0	-2.201740	-0.523863	-2.047207
30	1	0	-0.671830	-1.015262	-4.670534
31	1	0	-2.268857	-1.637082	-4.239383
32	1	0	-0.388589	-3.377411	-3.878091
33	1	0	-1.260300	-2.973350	-2.393374
34	1	0	1.477383	-1.894630	-3.264178
35	1	0	1.075225	-2.699743	-1.737978
36	29	0	0.072010	0.353032	0.306359
37	1	0	-1.262873	0.362583	2.112668
38	6	0	-4.044559	1.170041	-0.044824
39	6	0	-2.270229	2.740751	0.687701
40	6	0	-1.778178	-2.291572	1.030988
41	1	0	-3.098443	3.444374	0.836075
42	1	0	-1.600182	2.805478	1.554571
43	1	0	-1.701407	3.094116	-0.186340
44	1	0	-2.370602	-3.196118	0.849235
45	1	0	-1.503895	-2.272082	2.093817
46	1	0	-0.835355	-2.380839	0.469096
47	6	0	-4.584369	-0.094215	-0.252182

48	6	0	-3.806639	-1.198146	0.106239
49	6	0	-5.968086	-0.272807	-0.799411
50	1	0	-4.639671	2.050299	-0.300103
51	1	0	-4.221142	-2.200353	-0.029048
52	1	0	-6.294539	0.608019	-1.363647
53	1	0	-6.699174	-0.432931	0.004150
54	1	0	-6.028850	-1.144207	-1.462236
55	6	0	-0.425890	0.373227	3.234233
56	6	0	0.614134	-0.234976	2.490291
57	6	0	1.232496	-0.869819	1.620749
58	6	0	-0.996946	-0.362109	4.371246
59	6	0	-0.685820	-1.600932	4.770024
60	1	0	0.119158	-2.161790	4.295568
61	1	0	-1.218471	-2.088285	5.581675
62	1	0	-0.307492	1.451436	3.393480
63	1	0	-1.793215	0.170957	4.895115
64	6	0	2.141042	-1.819727	1.043589
65	6	0	1.988151	-3.185439	1.335067
66	6	0	3.157485	-1.438706	0.154480
67	6	0	2.815460	-4.131104	0.744246
68	1	0	1.202196	-3.491059	2.022661
69	6	0	3.982873	-2.389222	-0.432314
70	1	0	3.293651	-0.381790	-0.064840
71	6	0	3.813014	-3.741007	-0.146440
72	1	0	2.677592	-5.184177	0.979886
73	1	0	4.766728	-2.071001	-1.116788
74	1	0	4.456875	-4.485007	-0.609255

SCF Done: E(RM06) = -3490.31341594 A.U.

IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.118187	1.187434	-0.124497
2	6	0	1.479672	2.299542	0.478717
3	6	0	2.806153	1.879021	-0.149172
4	15	0	3.092000	0.047387	0.081571
5	6	0	4.664773	-0.215358	-0.887796
6	6	0	5.730204	-0.609050	0.138455
7	6	0	5.455751	0.195005	1.406895
8	6	0	3.972908	0.008459	1.719937
9	6	0	-0.553968	2.017691	-1.640710
10	6	0	-2.062945	2.013529	-1.399016
11	6	0	-2.281559	2.457234	0.045771
12	6	0	-1.348549	1.618385	0.926443
13	1	0	1.522464	2.168440	1.570534
14	1	0	1.250346	3.356736	0.285470
15	1	0	3.651272	2.457447	0.250687
16	1	0	2.777720	2.050885	-1.236418
17	1	0	4.931467	0.724593	-1.389906

18	1	0	6.744542	-0.449607	-0.246339
19	1	0	6.096798	-0.115693	2.241073
20	1	0	5.669958	1.258084	1.218959
21	1	0	-0.257775	1.471451	-2.541999
22	1	0	-2.597151	2.647832	-2.116351
23	1	0	-2.450849	0.990177	-1.519538
24	1	0	-2.024267	3.523609	0.137321
25	1	0	-3.330496	2.344990	0.348291
26	29	0	1.064178	-0.788285	-0.307090
27	1	0	5.640377	-1.680924	0.367930
28	1	0	3.788356	-0.972771	2.174959
29	1	0	-1.033030	2.131658	1.841883
30	6	0	0.008838	-2.493858	0.444913
31	6	0	-1.325819	-2.041410	0.481091
32	6	0	-2.480132	-1.636766	0.474693
33	6	0	0.684817	-2.675530	-0.803484
34	6	0	0.396864	-1.944325	-1.961310
35	1	0	-0.607979	-1.550451	-2.119428
36	1	0	0.981735	-2.134377	-2.856329
37	1	0	0.372735	-3.058396	1.300565
38	1	0	1.580781	-3.299075	-0.787865
39	1	0	-1.825042	0.674228	1.216419
40	1	0	-0.170276	3.046109	-1.712719
41	1	0	3.559103	0.764109	2.398889
42	1	0	4.513402	-0.972971	-1.662615
43	6	0	-3.773387	-1.057575	0.448148
44	6	0	-4.409725	-0.786903	-0.778347
45	6	0	-4.433129	-0.691019	1.635884
46	6	0	-5.644331	-0.154225	-0.811468
47	1	0	-3.911086	-1.082313	-1.700482
48	6	0	-5.671476	-0.065979	1.592689
49	1	0	-3.949660	-0.898404	2.588582
50	6	0	-6.282449	0.212453	0.371572
51	1	0	-6.116679	0.049912	-1.770361
52	1	0	-6.164429	0.211418	2.522413
53	1	0	-7.251353	0.705310	0.342439

SCF Done: E(RM06) = -3140.35876075 A.U.

MesH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.356080	-1.338004	-0.014925
2	6	0	1.354867	-0.370238	-0.006239
3	6	0	-0.997832	-0.988132	-0.007232
4	1	0	0.633765	-2.393498	-0.027365
5	6	0	-1.336783	0.360596	0.002468
6	6	0	-2.054004	-2.052786	0.006428
7	6	0	2.805247	-0.751791	0.005770
8	1	0	-3.046704	-1.637122	-0.195590

9	1	0	-1.853108	-2.827461	-0.743077
10	1	0	-2.099724	-2.556672	0.980578
11	1	0	3.371209	-0.201049	-0.755086
12	1	0	2.941964	-1.822039	-0.181337
13	1	0	3.269618	-0.524037	0.973842
14	6	0	-0.356752	1.357919	0.006563
15	6	0	0.980835	0.977208	0.003631
16	6	0	-0.751503	2.804777	-0.002914
17	1	0	-2.389907	0.647591	0.004939
18	1	0	1.755789	1.745991	0.006814
19	1	0	-1.183921	3.094900	-0.969079
20	1	0	0.108210	3.457232	0.182735
21	1	0	-1.508120	3.018863	0.761325

SCF Done: E(RM06) = -350.003515782 A.U.

2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.579686	0.105860	-0.000018
2	6	0	-1.818728	1.270604	0.000035
3	8	0	2.204911	-1.304799	0.000076
4	6	0	1.691078	-0.201427	0.000007
5	6	0	2.539181	1.044761	-0.000079
6	6	0	0.206280	-0.050527	0.000028
7	6	0	-0.430656	1.193933	0.000050
8	6	0	-0.568035	-1.214467	-0.000023
9	6	0	-1.952409	-1.138733	-0.000043
10	1	0	-2.548495	-2.048248	-0.000075
11	1	0	-3.665560	0.168644	-0.000038
12	1	0	-2.307655	2.241971	0.000046
13	1	0	0.154624	2.111196	0.000101
14	1	0	-0.050033	-2.170302	-0.000047
15	1	0	3.590785	0.752555	-0.000360
16	1	0	2.332224	1.661346	-0.882766
17	1	0	2.332674	1.661211	0.882795

SCF Done: E(RM06) = -384.724253926 A.U.

TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.784864	-1.996017	-0.566903
2	6	0	-2.424384	-2.652582	-1.152118
3	6	0	-3.351689	-1.485414	-1.486339
4	15	0	-3.384844	-0.221946	-0.110501
5	6	0	-4.490403	1.088639	-0.843034

6	6	0	-5.699305	1.161301	0.090497
7	6	0	-6.029951	-0.272439	0.495298
8	6	0	-4.725131	-0.891974	0.994281
9	6	0	0.204164	-1.770106	-2.126533
10	6	0	1.461776	-2.616373	-1.911745
11	6	0	1.022128	-3.906124	-1.222826
12	6	0	0.158637	-3.497241	-0.029743
13	1	0	-2.841936	-3.236970	-0.318158
14	1	0	-2.309973	-3.335863	-2.005355
15	1	0	-4.370607	-1.826439	-1.721329
16	1	0	-2.974993	-0.949790	-2.371884
17	1	0	-4.797410	0.779081	-1.851636
18	1	0	-6.548426	1.670735	-0.380539
19	1	0	-6.824998	-0.320885	1.249358
20	1	0	-6.390518	-0.822913	-0.387059
21	1	0	0.420237	-0.707680	-2.279528
22	1	0	1.986805	-2.807648	-2.855284
23	1	0	2.163081	-2.076590	-1.256133
24	1	0	0.423888	-4.509144	-1.923751
25	1	0	1.879662	-4.518806	-0.915985
26	29	0	-1.254712	-0.088210	0.506419
27	1	0	-5.436323	1.738579	0.989795
28	1	0	-4.506089	-0.572128	2.020820
29	1	0	-0.513737	-4.286606	0.325587
30	6	0	-0.328059	0.131440	2.330818
31	6	0	0.950759	-0.414112	2.039052
32	6	0	2.045282	-0.865003	1.741639
33	6	0	-0.477262	1.534747	2.465423
34	6	0	0.407486	2.490348	2.005061
35	1	0	1.442063	2.197390	1.832353
36	1	0	0.246333	3.536867	2.257544
37	1	0	-0.986664	-0.484815	2.949504
38	1	0	-1.443806	1.864904	2.856730
39	6	0	3.733978	4.144245	-1.332683
40	6	0	2.693168	4.999905	-0.988281
41	8	0	-0.225597	1.270843	-0.479027
42	6	0	-0.062964	2.492298	-0.192208
43	6	0	-1.290192	3.369157	-0.122891
44	6	0	1.240829	3.105291	-0.576838
45	6	0	1.456490	4.485573	-0.611631
46	6	0	2.294280	2.252353	-0.930119
47	6	0	3.528611	2.765754	-1.300674
48	1	0	4.335291	2.085312	-1.570413
49	1	0	4.700357	4.548451	-1.625749
50	1	0	2.843197	6.077243	-1.012281
51	1	0	0.654833	5.170309	-0.342155
52	1	0	2.116098	1.177832	-0.899802
53	1	0	-2.098050	2.805460	0.356639
54	1	0	-1.144364	4.306765	0.419839
55	1	0	-1.607057	3.611342	-1.148957
56	1	0	0.780983	-3.179767	0.817363
57	1	0	-0.377725	-2.134303	-2.986113
58	1	0	-4.722493	-1.988849	0.988114

59	1	0	-3.955257	2.039269	-0.934950
60	6	0	3.289709	-1.334675	1.247102
61	6	0	4.205279	-0.427838	0.681827
62	6	0	3.620501	-2.701062	1.254757
63	6	0	5.389122	-0.879591	0.117340
64	1	0	3.960089	0.633140	0.687685
65	6	0	4.807598	-3.143536	0.686720
66	1	0	2.927942	-3.410276	1.705645
67	6	0	5.695750	-2.238688	0.110271
68	1	0	6.081935	-0.162314	-0.319334
69	1	0	5.043399	-4.205903	0.696053
70	1	0	6.624037	-2.589973	-0.334073

SCF Done: E(RM06) = -3525.08326388 A.U.

IM3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.491984	-1.851059	0.832176
2	6	0	2.022825	-2.670887	1.474327
3	6	0	3.105018	-1.601520	1.611334
4	15	0	3.327832	-0.635612	0.027169
5	6	0	4.583770	0.633516	0.561993
6	6	0	5.818352	0.369145	-0.300861
7	6	0	5.957706	-1.146017	-0.424557
8	6	0	4.593142	-1.671649	-0.867890
9	6	0	-0.271648	-1.060425	2.317613
10	6	0	-1.742677	-1.448350	2.189661
11	6	0	-1.781788	-2.934726	1.838292
12	6	0	-0.818242	-3.153743	0.664543
13	1	0	2.327013	-3.433156	0.741669
14	1	0	1.835946	-3.182558	2.428835
15	1	0	4.064857	-2.029297	1.934889
16	1	0	2.804050	-0.862363	2.369905
17	1	0	4.813487	0.480628	1.625236
18	1	0	6.716414	0.838137	0.118542
19	1	0	6.757987	-1.436827	-1.116228
20	1	0	6.216305	-1.566345	0.559116
21	1	0	-0.096275	0.020972	2.274946
22	1	0	-2.307711	-1.221985	3.101715
23	1	0	-2.202653	-0.869288	1.372897
24	1	0	-1.443530	-3.517647	2.708386
25	1	0	-2.797213	-3.272118	1.593704
26	29	0	1.110508	-0.237304	-0.584925
27	1	0	5.669420	0.801263	-1.301895
28	1	0	4.449659	-1.526943	-1.946203
29	1	0	-0.383628	-4.159491	0.635065
30	6	0	0.196163	-0.450195	-2.433940
31	6	0	-1.148430	-0.784374	-2.114518
32	6	0	-2.283633	-1.074532	-1.786560

33	6	0	0.715225	0.830752	-2.262515
34	6	0	-0.081567	1.990629	-1.734921
35	1	0	-1.129165	1.677801	-1.624356
36	1	0	-0.060467	2.828551	-2.449216
37	1	0	0.752184	-1.168758	-3.037151
38	1	0	1.662666	1.043514	-2.760333
39	6	0	-2.749742	4.909428	1.287622
40	6	0	-1.832007	5.461052	0.400190
41	8	0	0.575771	1.298997	0.454752
42	6	0	0.423961	2.425886	-0.327449
43	6	0	1.760832	3.166460	-0.460583
44	6	0	-0.650942	3.344423	0.259021
45	6	0	-0.796506	4.683360	-0.110980
46	6	0	-1.584646	2.801568	1.144076
47	6	0	-2.623141	3.572516	1.654183
48	1	0	-3.336744	3.129195	2.347304
49	1	0	-3.558445	5.516814	1.689018
50	1	0	-1.920962	6.504116	0.101692
51	1	0	-0.094969	5.133787	-0.812285
52	1	0	-1.465731	1.755133	1.417465
53	1	0	2.504399	2.494755	-0.911170
54	1	0	1.710930	4.072230	-1.078564
55	1	0	2.116351	3.445500	0.538696
56	1	0	-1.322740	-2.976279	-0.293537
57	1	0	0.167985	-1.476227	3.236384
58	1	0	4.438133	-2.737972	-0.660809
59	1	0	4.179879	1.644877	0.453738
60	6	0	-3.576546	-1.375322	-1.277701
61	6	0	-4.164885	-2.632397	-1.485678
62	6	0	-4.257933	-0.421266	-0.502713
63	6	0	-5.399311	-2.928618	-0.923747
64	1	0	-3.635591	-3.370028	-2.085491
65	6	0	-5.491371	-0.727371	0.054604
66	1	0	-3.794882	0.551709	-0.340488
67	6	0	-6.065226	-1.980023	-0.151546
68	1	0	-5.845485	-3.906969	-1.088243
69	1	0	-6.008641	0.017069	0.655439
70	1	0	-7.031493	-2.215789	0.288158

SCF Done: E(RM06) = -3525.10538531 A.U.

IM31:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.805144	3.575744	-1.762227
2	6	0	-1.368109	2.174277	-2.076779
3	6	0	-2.443352	1.201536	-2.154214
4	6	0	-3.349435	0.393973	-2.185713
5	6	0	-3.038475	3.960581	-1.445917
6	1	0	-0.657503	1.846584	-1.283833

7	1	0	-0.782388	2.168002	-3.009317
8	1	0	-0.993157	4.306184	-1.774137
9	1	0	-3.264088	4.995559	-1.203603
10	1	0	-3.865905	3.251387	-1.427165
11	15	0	0.194446	-2.023926	0.246009
12	6	0	-1.482613	-2.771646	0.464996
13	6	0	-2.486452	-1.628249	0.568516
14	15	0	-1.994103	-0.351646	1.835099
15	6	0	-3.174026	1.028504	1.414339
16	6	0	-4.009850	1.235167	2.675875
17	6	0	-4.308968	-0.154568	3.233226
18	6	0	-2.964956	-0.873854	3.338241
19	6	0	0.265078	-1.506102	-1.528499
20	6	0	1.641575	-2.002160	-1.967796
21	6	0	1.781248	-3.431001	-1.447310
22	6	0	1.400293	-3.418795	0.038564
23	1	0	-1.463115	-3.368852	1.389141
24	1	0	-1.731837	-3.447763	-0.365939
25	1	0	-3.511315	-1.984969	0.752644
26	1	0	-2.509589	-1.079935	-0.383715
27	1	0	-3.803877	0.700039	0.575993
28	1	0	-4.922001	1.808140	2.470128
29	1	0	-4.835891	-0.118708	4.194886
30	1	0	-4.961785	-0.688948	2.525110
31	1	0	0.148709	-0.418540	-1.601330
32	1	0	1.772232	-1.941128	-3.054726
33	1	0	2.419187	-1.367853	-1.512242
34	1	0	1.089677	-4.082738	-2.002462
35	1	0	2.793888	-3.825686	-1.600382
36	29	0	0.325439	-0.209617	1.545609
37	1	0	-3.431063	1.808526	3.416973
38	1	0	-2.415564	-0.546420	4.230201
39	1	0	0.975399	-4.367108	0.387613
40	6	0	1.911408	-0.411865	2.868769
41	6	0	2.988464	-0.865489	2.058832
42	6	0	3.871401	-1.260508	1.321234
43	6	0	1.446311	0.899105	2.831386
44	6	0	2.032221	1.963963	1.947226
45	1	0	2.925620	1.564245	1.447556
46	1	0	2.347637	2.830850	2.548401
47	1	0	1.607279	-1.057174	3.693543
48	1	0	0.799397	1.213741	3.651621
49	6	0	3.223672	4.645743	-2.138502
50	6	0	2.831300	5.263894	-0.955807
51	8	0	0.524941	1.231109	0.252369
52	6	0	1.022336	2.379103	0.840397
53	6	0	-0.109974	3.207739	1.466652
54	6	0	1.780676	3.211408	-0.195985
55	6	0	2.120263	4.551789	0.005666
56	6	0	2.191831	2.599470	-1.383134
57	6	0	2.903339	3.307243	-2.346393
58	1	0	3.207153	2.812255	-3.267514
59	1	0	3.775369	5.203327	-2.892507

60	1	0	3.078585	6.309075	-0.778960
61	1	0	1.826786	5.055450	0.925571
62	1	0	1.922133	1.553673	-1.525849
63	1	0	-0.659988	2.590706	2.190585
64	1	0	0.244035	4.103015	1.994151
65	1	0	-0.818012	3.525487	0.689503
66	1	0	2.271641	-3.191934	0.664664
67	1	0	-0.535343	-1.998787	-2.100835
68	1	0	-3.045243	-1.967027	3.387289
69	1	0	-2.633871	1.921800	1.082243
70	6	0	4.808201	-1.693853	0.343660
71	6	0	5.423145	-2.952133	0.432736
72	6	0	5.083185	-0.874272	-0.764202
73	6	0	6.283589	-3.382017	-0.568375
74	1	0	5.208774	-3.584298	1.292032
75	6	0	5.943455	-1.314049	-1.760184
76	1	0	4.601310	0.101001	-0.829124
77	6	0	6.544485	-2.567538	-1.667346
78	1	0	6.753887	-4.359763	-0.491042
79	1	0	6.147439	-0.674365	-2.615706
80	1	0	7.217850	-2.908410	-2.450278
81	6	0	-4.370741	-0.600335	-2.136429
82	6	0	-5.574049	-0.355234	-1.457384
83	6	0	-4.154869	-1.868431	-2.696989
84	6	0	-6.528631	-1.356680	-1.336291
85	1	0	-5.742172	0.630256	-1.025249
86	6	0	-5.113975	-2.864068	-2.573513
87	1	0	-3.220311	-2.057735	-3.221810
88	6	0	-6.302125	-2.613697	-1.891045
89	1	0	-7.456930	-1.154586	-0.806520
90	1	0	-4.934631	-3.843246	-3.012124
91	1	0	-7.051207	-3.395887	-1.793421

SCF Done: E(RM06) = -3950.00464093 A.U.

TS3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.731465	-2.768286	2.703991
2	6	0	-0.447816	-1.353945	2.461730
3	6	0	-1.522227	-0.440306	2.454778
4	6	0	-2.455563	0.357348	2.425134
5	6	0	-1.921059	-3.393992	2.685491
6	1	0	0.215311	-1.342513	1.077266
7	1	0	0.436976	-0.986370	2.995646
8	1	0	0.164636	-3.376886	2.868235
9	1	0	-2.001173	-4.467386	2.836295
10	1	0	-2.848857	-2.834982	2.559104
11	15	0	-0.737803	1.700689	-1.118852
12	6	0	-2.570091	1.711379	-1.412524

13	6	0	-3.172532	0.380108	-0.976318
14	15	0	-2.235052	-1.091309	-1.596112
15	6	0	-3.006125	-2.468393	-0.622498
16	6	0	-3.527357	-3.445691	-1.674362
17	6	0	-4.129203	-2.606658	-2.800516
18	6	0	-3.072649	-1.570026	-3.186124
19	6	0	-0.458492	2.444453	0.553865
20	6	0	0.446080	3.651808	0.302683
21	6	0	-0.022550	4.299560	-0.997487
22	6	0	-0.094412	3.177644	-2.034409
23	1	0	-2.713626	1.871356	-2.492346
24	1	0	-3.050794	2.545063	-0.879712
25	1	0	-4.237486	0.306057	-1.239494
26	1	0	-3.095874	0.292581	0.116536
27	1	0	-3.835582	-2.045950	-0.036779
28	1	0	-4.249450	-4.151552	-1.248053
29	1	0	-4.437480	-3.216140	-3.658708
30	1	0	-5.030579	-2.097358	-2.427738
31	1	0	-0.036337	1.703263	1.240749
32	1	0	0.422813	4.350066	1.147492
33	1	0	1.489542	3.319685	0.188228
34	1	0	-1.022238	4.736160	-0.849668
35	1	0	0.640089	5.112354	-1.321187
36	29	0	-0.061261	-0.390387	-1.520464
37	1	0	-2.692349	-4.043397	-2.072413
38	1	0	-2.315313	-2.012554	-3.847347
39	1	0	-0.717568	3.409701	-2.905363
40	6	0	1.498013	-0.111294	-2.829558
41	6	0	2.451008	0.690481	-2.141639
42	6	0	3.230134	1.376693	-1.508218
43	6	0	1.333840	-1.469617	-2.572316
44	6	0	2.183589	-2.188639	-1.559127
45	1	0	3.053097	-1.562044	-1.321523
46	1	0	2.565621	-3.131890	-1.974318
47	1	0	1.058903	0.313771	-3.734497
48	1	0	0.790585	-2.058405	-3.312194
49	6	0	4.486516	-3.238324	2.748395
50	6	0	3.854809	-4.308566	2.127972
51	8	0	0.764136	-1.283128	0.098480
52	6	0	1.439512	-2.482990	-0.235604
53	6	0	0.444873	-3.620662	-0.446444
54	6	0	2.477338	-2.787495	0.837309
55	6	0	2.860442	-4.084487	1.178199
56	6	0	3.122896	-1.717109	1.466961
57	6	0	4.116008	-1.938201	2.412035
58	1	0	4.598115	-1.089382	2.894706
59	1	0	5.259453	-3.414029	3.493213
60	1	0	4.131556	-5.329009	2.384617
61	1	0	2.378104	-4.939582	0.709531
62	1	0	2.817604	-0.702796	1.211362
63	1	0	-0.287073	-3.320864	-1.207866
64	1	0	0.936751	-4.533631	-0.801844
65	1	0	-0.099267	-3.847504	0.478434

66	1	0	0.912903	2.925745	-2.394560
67	1	0	-1.431846	2.752308	0.960069
68	1	0	-3.476477	-0.687163	-3.697167
69	1	0	-2.301537	-2.904525	0.096138
70	6	0	4.125680	2.145020	-0.714771
71	6	0	4.138119	3.545825	-0.801351
72	6	0	4.992231	1.506266	0.186763
73	6	0	4.996428	4.287729	-0.001740
74	1	0	3.463201	4.037388	-1.500740
75	6	0	5.845981	2.256869	0.982341
76	1	0	4.978233	0.419530	0.252451
77	6	0	5.851612	3.646718	0.891040
78	1	0	4.998561	5.372689	-0.074437
79	1	0	6.512309	1.754064	1.679479
80	1	0	6.521559	4.231143	1.517093
81	6	0	-3.511858	1.299772	2.419521
82	6	0	-4.816161	0.932891	2.028475
83	6	0	-3.288899	2.647812	2.770137
84	6	0	-5.834403	1.872588	1.968469
85	1	0	-5.009259	-0.108805	1.773351
86	6	0	-4.314199	3.581581	2.703974
87	1	0	-2.296698	2.940703	3.109594
88	6	0	-5.592045	3.205533	2.297008
89	1	0	-6.832019	1.561576	1.663530
90	1	0	-4.114146	4.615107	2.981035
91	1	0	-6.392631	3.939587	2.246280

SCF Done: E(RM06) = -3949.98578045 A.U.

Pro:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.870122	-0.762654	2.224617
2	6	0	-0.094505	-3.274899	-0.444077
3	6	0	-1.136215	-2.323289	-0.314069
4	6	0	-2.000868	-1.473804	-0.217278
5	6	0	1.176773	-2.926192	-0.707704
6	6	0	1.611666	-1.511140	-0.882063
7	1	0	0.727311	-0.893009	-1.083099
8	1	0	2.285646	-1.405394	-1.744798
9	1	0	-0.353442	-4.325669	-0.318173
10	1	0	1.925533	-3.715017	-0.782820
11	6	0	2.372053	3.371057	-0.204440
12	6	0	3.508327	2.632189	-0.512522
13	8	0	1.522053	-1.243170	1.464695
14	6	0	2.336154	-0.919423	0.347487
15	6	0	3.705718	-1.561123	0.532717
16	6	0	2.398421	0.591150	0.171035
17	6	0	3.520535	1.251744	-0.328251
18	6	0	1.258455	1.344057	0.474474

19	6	0	1.243684	2.720160	0.288355
20	1	0	0.346590	3.286745	0.532174
21	1	0	2.364760	4.449146	-0.347748
22	1	0	4.394962	3.131102	-0.897968
23	1	0	4.419304	0.690174	-0.576116
24	1	0	0.379901	0.828707	0.861170
25	1	0	3.571906	-2.623539	0.761083
26	1	0	4.334214	-1.478679	-0.361464
27	1	0	4.243550	-1.097031	1.369305
28	6	0	-2.969059	-0.437110	-0.115766
29	6	0	-4.275304	-0.703710	0.321804
30	6	0	-2.621497	0.880385	-0.457007
31	6	0	-5.204710	0.322348	0.418262
32	1	0	-4.544691	-1.724125	0.584090
33	6	0	-3.556374	1.900380	-0.356415
34	1	0	-1.610344	1.084358	-0.805915
35	6	0	-4.849985	1.626017	0.081267
36	1	0	-6.214417	0.103774	0.758421
37	1	0	-3.275417	2.916749	-0.623816
38	1	0	-5.581520	2.426951	0.158656

SCF Done: E(RM06) = -809.628847004 A.U.

S7: The summarize energies of all species along reaction paths over the BPE-CuMes system in the THF solvent at the B3LYP/6-311+G(d, p) level.

1: the formation of the catalyst

B3LYP(SMD,THF) /6-311+G(d, p)

species	**SCF_{SMD}**	***G^*_{gas}***	**G_{sol}**	ΔG_{sol}	ΔG_{sol}(kJ mol^{-1})
BPE	-1075.99634977	0.242476	-1075.753873		
CuMes	-1990.1759460	0.132917	-1990.042877		
BPE+ CuMes			-3065.79675		
BPE-CuMes	-3066.22553807	0.398864	-3065.826674		
1	-425.238883574	0.133424	-425.1054595		
BPE +CuMes+1			-3490.90221	0.0299245	78.55
BPE-CuMes+1			-3490.932134	0.0	0.0
TS1	-3491.41813350	0.550708	-3490.867425	0.064709	169.86
IM2	-3141.18388963	0.388291	-3140.795598		
MesH	-350.303503484	0.147042	-350.1564614		
IM2+ MesH			-3490.952059	-0.019925	-52.30

2.the cycle of the teaction

B3LYP(SMD,THF)/6-311+G(d, p)

species	SCF_{PCM}	G^*_{THF}	G_{sol}	ΔG_{sol}	ΔG_{sol}(kJ.mol^{-1})
2	-385.018099507	0.105592	-384.9125075		
1	-425.238883574	0.133424	-425.1054595		
IM2+2+1			-3950.813565	-0.019532	-51.27
TS2	-3526.18824283	0.515090	-3525.673152		
TS2+1			-3950.778612	0.015421	40.48
IM3	-	0.518524			
IM3+1				0.0	0.0
IM31	-3951.4407430	0.671182	-3950.772892	0.021141	55.5
TS3	-3951.42315413	0.674090	-3950.749064	0.044969	118.04
Pro	-810.263718401	0.263958	-809.9997604		
IM2+Pro			-3950.795358	-0.001325	-3.48

G^*_{THF} =Thermal correction to Gibbs Free Energy in gas .

S8. Cartesian coordinates and energies of all optimized structures over the BPE-CuMes system at the B3LYP /6-311+G(d, p) level.

BPE:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.838112	0.109117	-0.789105
2	6	0	-0.624364	0.449343	0.615713
3	6	0	0.624403	-0.449604	0.615685
4	15	0	1.838141	-0.109289	-0.789119
5	6	0	3.221216	-1.305976	-0.273440
6	6	0	4.428142	-0.446272	0.154476
7	6	0	3.878598	0.806570	0.851781
8	6	0	2.769574	1.366444	-0.056173
9	6	0	-2.769782	-1.366438	-0.056100
10	6	0	-3.878730	-0.806343	0.851810
11	6	0	-4.428082	0.446536	0.154424
12	6	0	-3.221027	1.306037	-0.273535
13	1	0	-0.332365	1.503746	0.525706
14	1	0	-1.142532	0.357039	1.579401
15	1	0	1.142579	-0.357341	1.579373

16	1	0	0.332416	-1.504005	0.525628
17	1	0	3.469506	-1.982299	-1.095946
18	1	0	2.870218	-1.922911	0.561702
19	1	0	4.997489	-0.142709	-0.733562
20	1	0	5.116814	-1.007957	0.796448
21	1	0	4.664606	1.547080	1.043266
22	1	0	3.458688	0.528960	1.827276
23	1	0	3.204437	1.932826	-0.887313
24	1	0	2.084480	2.042743	0.465888
25	1	0	-2.084802	-2.042818	0.466003
26	1	0	-3.204722	-1.932791	-0.887219
27	1	0	-3.458786	-0.528737	1.827291
28	1	0	-4.664850	-1.546725	1.043335
29	1	0	-5.116676	1.008361	0.796358
30	1	0	-4.997468	0.143003	-0.733599
31	1	0	-2.869954	1.922984	0.561567
32	1	0	-3.469208	1.982336	-1.096094

SCF Done: E(RB3LYP) = -1075.99634977 A.U.

CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.447914	0.000000	-0.010379
2	6	0	-0.259070	-1.214685	-0.008591
3	6	0	-0.259058	1.214677	-0.008601
4	29	0	2.249670	0.000000	0.015008
5	6	0	-1.658295	1.200550	-0.010479
6	6	0	0.483544	2.531919	-0.018739
7	6	0	0.483550	-2.531916	-0.018743
8	1	0	0.130169	3.213008	0.763509
9	1	0	1.549118	2.340488	0.144980
10	1	0	0.379113	3.053159	-0.978359
11	1	0	0.379221	-3.053091	-0.978410
12	1	0	0.130109	-3.213065	0.763421
13	1	0	1.549106	-2.340478	0.145087
14	6	0	-2.376080	0.000010	-0.009144
15	6	0	-1.658292	-1.200548	-0.010472
16	6	0	-3.886892	-0.000006	0.027551
17	1	0	-2.200369	2.145076	-0.009569
18	1	0	-2.200388	-2.145061	-0.009558
19	1	0	-4.260289	-0.000051	1.059785
20	1	0	-4.300062	-0.885605	-0.465296
21	1	0	-4.300083	0.885621	-0.465227

SCF Done: E(RB3LYP) = -1990.17579460 A.U.

BPE-CuMes:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.966533	-0.000979	0.002820
2	6	0	-2.715981	-0.180215	1.186651
3	6	0	-2.715882	0.175386	-1.184679
4	15	0	1.555154	-1.581790	0.117976
5	6	0	3.183616	-0.671540	0.372300
6	6	0	3.182183	0.673768	-0.374888
7	15	0	1.553794	1.583107	-0.116258
8	6	0	1.725357	3.065593	-1.254673
9	6	0	1.766911	4.308033	-0.338261
10	6	0	2.502843	3.913513	0.953003
11	6	0	1.886743	2.584823	1.429579
12	6	0	1.884062	-2.580721	-1.430521
13	6	0	2.504199	-3.908978	-0.958123
14	6	0	1.773191	-4.306916	0.334907
15	6	0	1.731825	-3.065962	1.253427
16	1	0	3.270956	-0.497715	1.452466
17	1	0	4.041194	-1.287636	0.076820
18	1	0	4.040091	1.290496	-0.081704
19	1	0	3.266751	0.500068	-1.455292
20	1	0	0.894164	3.098561	-1.962961
21	1	0	2.651931	2.972243	-1.832483
22	1	0	0.742893	4.612788	-0.090857
23	1	0	2.242364	5.158136	-0.839370
24	1	0	2.426253	4.691984	1.720298
25	1	0	3.571191	3.776280	0.741144
26	1	0	0.929479	2.760625	1.930666
27	1	0	2.524164	2.032752	2.127293
28	1	0	2.517902	-2.026588	-2.129864
29	1	0	0.925246	-2.757543	-1.928275
30	1	0	3.572984	-3.770075	-0.749598
31	1	0	2.426516	-4.686373	-1.726400
32	1	0	2.251990	-5.156769	0.833249
33	1	0	0.749050	-4.613467	0.090276
34	1	0	2.659603	-2.972013	1.829203
35	1	0	0.902358	-3.101406	1.963623
36	29	0	-0.030451	0.000074	0.002791
37	6	0	-4.115294	0.171239	-1.182840
38	6	0	-1.990133	0.359805	-2.503040
39	6	0	-1.994538	-0.365538	2.507309
40	1	0	-2.672025	0.613373	-3.322486
41	1	0	-1.240828	1.159306	-2.431787
42	1	0	-1.452038	-0.551615	-2.797909
43	1	0	-2.676100	-0.642524	3.319465
44	1	0	-1.477360	0.553190	2.816880
45	1	0	-1.228535	-1.148510	2.431269
46	6	0	-4.842041	-0.006054	-0.000301
47	6	0	-4.117994	-0.182630	1.180883
48	6	0	-6.353735	0.008365	-0.004302

49	1	0	-4.653605	0.306616	-2.121303
50	1	0	-4.658639	-0.325386	2.116602
51	1	0	-6.750609	1.013386	-0.199686
52	1	0	-6.757967	-0.320273	0.958494
53	1	0	-6.763327	-0.649744	-0.779960

SCF Done: E(RB3LYP) = -3066.22553807 A.U

1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.370764	0.369674	-1.802291
2	6	0	3.121198	-0.288940	-0.956297
3	6	0	1.686624	-0.206846	-0.687958
4	6	0	0.496319	-0.138457	-0.466121
5	6	0	4.026400	0.056152	0.210688
6	6	0	3.630316	0.416260	1.429177
7	1	0	2.577068	0.490994	1.683247
8	1	0	4.349756	0.646872	2.208770
9	1	0	3.367804	-1.303190	-1.305504
10	1	0	5.089723	-0.011078	-0.017327
11	6	0	-0.908860	-0.060792	-0.211808
12	6	0	-1.590532	1.166880	-0.322205
13	6	0	-1.635495	-1.210707	0.154000
14	6	0	-2.959059	1.238153	-0.073390
15	1	0	-1.034801	2.055733	-0.603326
16	6	0	-3.003872	-1.131038	0.400901
17	1	0	-1.114429	-2.158772	0.241032
18	6	0	-3.670404	0.091580	0.288531
19	1	0	-3.472219	2.191486	-0.162023
20	1	0	-3.551942	-2.025716	0.682315
21	1	0	-4.737541	0.150520	0.482003

SCF Done: E(RB3LYP) = -425.238883574 A.U.

TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.346246	-0.349469	-0.209913
2	6	0	2.516310	-1.759002	-0.100263
3	6	0	3.520828	0.447703	-0.112317
4	15	0	-0.915136	-0.393270	1.883356
5	6	0	-2.184085	0.981096	2.017157
6	6	0	-1.518366	2.364859	1.916851
7	15	0	-0.350517	2.467458	0.451234

8	6	0	0.464859	4.135127	0.703126
9	6	0	0.160781	4.935285	-0.578614
10	6	0	-1.283066	4.603208	-0.988957
11	6	0	-1.430342	3.069208	-0.952793
12	6	0	-0.398477	-0.676271	3.659796
13	6	0	-1.363689	-1.740045	4.218309
14	6	0	-1.631211	-2.742601	3.083160
15	6	0	-1.971883	-1.936797	1.812193
16	1	0	-2.876111	0.830651	1.179740
17	1	0	-2.766962	0.890985	2.941276
18	1	0	-2.270478	3.162032	1.878132
19	1	0	-0.902216	2.547328	2.806953
20	1	0	1.535686	4.024748	0.885383
21	1	0	0.023418	4.625777	1.578476
22	1	0	0.847512	4.627080	-1.376902
23	1	0	0.309125	6.009534	-0.424550
24	1	0	-1.530791	5.005622	-1.977060
25	1	0	-1.977021	5.060965	-0.272259
26	1	0	-1.075953	2.603561	-1.876404
27	1	0	-2.463941	2.742348	-0.809117
28	1	0	-0.404671	0.260017	4.226904
29	1	0	0.631184	-1.048557	3.657814
30	1	0	-2.306881	-1.266419	4.520073
31	1	0	-0.952711	-2.229388	5.108346
32	1	0	-2.434121	-3.443278	3.335965
33	1	0	-0.727967	-3.340925	2.909575
34	1	0	-3.027141	-1.644233	1.799171
35	1	0	-1.780660	-2.489714	0.891223
36	29	0	0.595152	0.424509	0.418003
37	1	0	1.561109	0.013226	-1.258441
38	6	0	4.764789	-0.131227	0.148329
39	6	0	3.454920	1.948111	-0.299170
40	6	0	1.333854	-2.690763	-0.251746
41	1	0	4.415482	2.350265	-0.637272
42	1	0	2.690311	2.220866	-1.033755
43	1	0	3.202324	2.461979	0.637276
44	1	0	1.645618	-3.666861	-0.636479
45	1	0	0.581381	-2.280540	-0.929311
46	1	0	0.843237	-2.864954	0.716100
47	6	0	4.912427	-1.513947	0.297716
48	6	0	3.771323	-2.311818	0.160664
49	6	0	6.268909	-2.131454	0.539558
50	1	0	5.644205	0.506399	0.227772
51	1	0	3.869070	-3.392983	0.249305
52	1	0	6.754333	-2.408617	-0.405341
53	1	0	6.192857	-3.043099	1.141038
54	1	0	6.939509	-1.437491	1.056139
55	6	0	0.965806	0.200866	-2.672892
56	6	0	-0.377953	-0.178362	-2.452115
57	6	0	-1.504887	-0.569257	-2.156236
58	6	0	1.826247	-0.609800	-3.545359
59	6	0	1.574268	-1.824481	-4.062197
60	1	0	0.614815	-2.315377	-3.924462

61	1	0	2.323177	-2.355030	-4.641443
62	1	0	1.120650	1.278928	-2.775576
63	1	0	2.805667	-0.166798	-3.732205
64	6	0	-2.805811	-1.050995	-1.863396
65	6	0	-3.097724	-2.435663	-1.934334
66	6	0	-3.854412	-0.179213	-1.481887
67	6	0	-4.367382	-2.915353	-1.628742
68	1	0	-2.310960	-3.120068	-2.236143
69	6	0	-5.120806	-0.671116	-1.174070
70	1	0	-3.664075	0.889138	-1.455218
71	6	0	-5.388580	-2.041112	-1.241288
72	1	0	-4.563586	-3.982440	-1.694724
73	1	0	-5.908360	0.022346	-0.889636
74	1	0	-6.378013	-2.420902	-1.004713

SCF Done: E(RB3LYP) = -3491.41813350 A.U.

IM2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.277643	1.382154	0.084218
2	6	0	-1.708701	2.234703	-0.778441
3	6	0	-3.060714	1.762818	-0.214797
4	15	0	-3.148018	-0.111361	-0.120808
5	6	0	-4.742287	-0.386286	0.839104
6	6	0	-5.729258	-1.069103	-0.131675
7	6	0	-5.457638	-0.517798	-1.541863
8	6	0	-3.935104	-0.578754	-1.756259
9	6	0	0.235125	2.569864	1.445038
10	6	0	1.692949	2.965218	1.124694
11	6	0	1.826167	3.061456	-0.404748
12	6	0	1.192646	1.785855	-0.990018
13	1	0	-1.632541	1.956525	-1.836682
14	1	0	-1.620569	3.325896	-0.723591
15	1	0	-3.894041	2.166189	-0.802471
16	1	0	-3.184488	2.127232	0.812494
17	1	0	-5.129052	0.582483	1.174780
18	1	0	-6.768643	-0.913255	0.177134
19	1	0	-6.000811	-1.079210	-2.310509
20	1	0	-5.802272	0.522751	-1.603013
21	1	0	0.133802	2.094293	2.422884
22	1	0	1.972762	3.900038	1.622743
23	1	0	2.372697	2.187429	1.493291
24	1	0	1.290778	3.949336	-0.766309
25	1	0	2.871935	3.167158	-0.712740
26	29	0	-1.050231	-0.653595	0.489166
27	1	0	-5.555197	-2.152408	-0.129857
28	1	0	-3.615527	-1.598094	-1.997440
29	1	0	0.895911	1.885018	-2.038291

30	6	0	0.159348	-2.386582	-0.131503
31	6	0	1.496200	-1.939066	-0.189688
32	6	0	2.660172	-1.563729	-0.252577
33	6	0	-0.562173	-2.506915	1.101211
34	6	0	-0.354268	-1.710999	2.236315
35	1	0	0.619301	-1.265762	2.417952
36	1	0	-0.966181	-1.889898	3.113506
37	1	0	-0.177021	-3.013468	-0.953206
38	1	0	-1.424820	-3.172257	1.088173
39	1	0	1.881091	0.937886	-0.922122
40	1	0	-0.421739	3.447559	1.429449
41	1	0	-3.577766	0.069761	-2.562377
42	1	0	-4.548144	-0.987124	1.730640
43	6	0	4.006673	-1.120661	-0.317911
44	6	0	4.666619	-0.620877	0.829474
45	6	0	4.729084	-1.159232	-1.533290
46	6	0	5.984359	-0.178622	0.757436
47	1	0	4.130245	-0.595204	1.773259
48	6	0	6.047152	-0.716458	-1.592962
49	1	0	4.238778	-1.543086	-2.422609
50	6	0	6.684803	-0.221688	-0.451556
51	1	0	6.470593	0.199271	1.653177
52	1	0	6.581945	-0.757937	-2.538370
53	1	0	7.713666	0.122375	-0.502752

SCF Done: E(RB3LYP) = -3141.18388963 A.U.

MesH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.369032	0.233211	-0.025965
2	6	0	0.490123	1.321822	-0.011702
3	6	0	0.899479	-1.085597	-0.011800
4	1	0	2.441772	0.415756	-0.047561
5	6	0	-0.482652	-1.302429	0.006899
6	6	0	1.864993	-2.248460	0.009973
7	6	0	1.015052	2.739128	0.009829
8	1	0	1.430260	-3.139803	-0.452565
9	1	0	2.792052	-2.009607	-0.520482
10	1	0	2.140128	-2.517144	1.037925
11	1	0	0.335745	3.426709	-0.503564
12	1	0	1.995730	2.810514	-0.470409
13	1	0	1.129736	3.104690	1.038336
14	6	0	-1.389852	-0.236248	0.014113
15	6	0	-0.886753	1.069300	0.007173
16	6	0	-2.879766	-0.490768	-0.006960
17	1	0	-0.861255	-2.322879	0.011723
18	1	0	-1.581373	1.907246	0.012024
19	1	0	-3.253182	-0.580695	-1.035047

20	1	0	-3.432548	0.325393	0.468245
21	1	0	-3.135000	-1.419939	0.512009

SCF Done: E(RB3LYP) = -350.303503484 A.U.

2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.212165	-1.311391	-0.000071
2	6	0	-2.592804	0.110772	-0.000009
3	6	0	-1.965134	-1.139042	0.000032
4	6	0	-0.576222	-1.219545	0.000049
5	6	0	0.205165	-0.052979	-0.000009
6	6	0	-0.432959	1.196667	-0.000003
7	6	0	1.697839	-0.202954	-0.000022
8	6	0	2.562035	1.047313	0.000053
9	1	0	-2.561652	-2.046784	0.000043
10	1	0	-3.677310	0.174754	-0.000032
11	1	0	0.151961	2.110926	-0.000021
12	1	0	-0.064558	-2.176205	0.000072
13	6	0	-1.825668	1.277226	-0.000035
14	1	0	-2.311406	2.248660	-0.000078
15	1	0	2.361192	1.664673	-0.882449
16	1	0	2.361129	1.664481	0.882689
17	1	0	3.609806	0.745874	0.000007

SCF Done: E(RB3LYP) = -385.018099507 A.U.

TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.912844	-2.018501	0.911395
2	6	0	2.640029	-2.744725	0.964576
3	6	0	3.696714	-1.636812	1.116374
4	15	0	3.408831	-0.235852	-0.102967
5	6	0	4.712726	1.013110	0.430125
6	6	0	5.698975	1.138082	-0.749730
7	6	0	5.832062	-0.251934	-1.393348
8	6	0	4.402912	-0.786394	-1.595749
9	6	0	0.367972	-2.007159	2.709277
10	6	0	-0.857376	-2.943789	2.782839
11	6	0	-0.620780	-4.104930	1.802935
12	6	0	-0.165771	-3.478853	0.471678
13	1	0	2.784484	-3.266005	0.009922
14	1	0	2.741097	-3.492849	1.759438

15	1	0	4.710806	-2.042232	1.017057
16	1	0	3.625850	-1.188716	2.115535
17	1	0	5.222983	0.642102	1.326343
18	1	0	6.666533	1.534986	-0.423590
19	1	0	6.389525	-0.214739	-2.336146
20	1	0	6.387833	-0.916863	-0.719445
21	1	0	0.133012	-0.989038	3.027263
22	1	0	-1.030118	-3.296394	3.805635
23	1	0	-1.754435	-2.392260	2.476558
24	1	0	0.163425	-4.766088	2.194943
25	1	0	-1.521607	-4.715109	1.673909
26	29	0	1.139916	-0.066467	-0.200603
27	1	0	5.298509	1.841576	-1.490588
28	1	0	3.945633	-0.340604	-2.485658
29	1	0	0.361298	-4.178791	-0.183998
30	6	0	0.161113	0.001027	-2.077395
31	6	0	-1.141505	-0.515290	-1.827656
32	6	0	-2.256946	-0.968624	-1.625246
33	6	0	0.364749	1.383991	-2.316908
34	6	0	-0.467733	2.422233	-1.914707
35	1	0	-1.506660	2.196176	-1.701851
36	1	0	-0.270981	3.424810	-2.281443
37	1	0	0.821533	-0.671515	-2.627697
38	1	0	1.334077	1.642277	-2.744853
39	6	0	-3.543036	4.634622	1.478027
40	6	0	-2.497708	5.378903	0.929382
41	8	0	0.193153	1.418350	0.640287
42	6	0	0.076805	2.627013	0.234755
43	6	0	1.357085	3.435989	0.062674
44	6	0	-1.168909	3.357979	0.648265
45	6	0	-1.322439	4.748125	0.519176
46	6	0	-2.228209	2.620508	1.206290
47	6	0	-3.400937	3.250392	1.614590
48	1	0	-4.206307	2.661822	2.046532
49	1	0	-4.457422	5.127005	1.797100
50	1	0	-2.594859	6.455889	0.820875
51	1	0	-0.524836	5.349073	0.094924
52	1	0	-2.102506	1.548744	1.311180
53	1	0	2.117062	2.805384	-0.402337
54	1	0	1.233916	4.336965	-0.540584
55	1	0	1.722475	3.736423	1.054911
56	1	0	-1.019642	-3.084512	-0.088145
57	1	0	1.184453	-2.377054	3.340797
58	1	0	4.356155	-1.872940	-1.721074
59	1	0	4.245258	1.965949	0.688693
60	6	0	-3.562668	-1.459129	-1.347632
61	6	0	-4.545803	-0.609873	-0.792219
62	6	0	-3.911631	-2.801476	-1.613755
63	6	0	-5.821767	-1.090968	-0.513381
64	1	0	-4.289013	0.424216	-0.584177
65	6	0	-5.190532	-3.273087	-1.328967
66	1	0	-3.168732	-3.461864	-2.050835
67	6	0	-6.152947	-2.423135	-0.777895

68	1	0	-6.563996	-0.421590	-0.086691
69	1	0	-5.439019	-4.309394	-1.542354
70	1	0	-7.150363	-2.793591	-0.559646

SCF Done: E(RB3LYP) = -3526.18824283 A.U

IM3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.469513	-1.774947	1.171902
2	6	0	2.040016	-2.659170	1.664092
3	6	0	3.250900	-1.724406	1.492012
4	15	0	3.305302	-0.941599	-0.214957
5	6	0	4.748718	0.247501	-0.033757
6	6	0	5.838311	-0.241761	-1.009631
7	6	0	5.794059	-1.778752	-1.023364
8	6	0	4.318217	-2.181384	-1.199553
9	6	0	-0.138572	-0.937367	2.727096
10	6	0	-1.555223	-1.500430	2.963502
11	6	0	-1.542654	-2.987130	2.566866
12	6	0	-0.865750	-3.078378	1.185094
13	1	0	2.137770	-3.528863	1.002222
14	1	0	1.982922	-3.038619	2.690947
15	1	0	4.187639	-2.251417	1.709712
16	1	0	3.176923	-0.890169	2.200425
17	1	0	5.109446	0.216854	1.000320
18	1	0	6.826900	0.137869	-0.729254
19	1	0	6.428192	-2.200516	-1.811646
20	1	0	6.173123	-2.164196	-0.067980
21	1	0	-0.126883	0.143208	2.569045
22	1	0	-1.874360	-1.355362	4.001333
23	1	0	-2.270892	-0.963576	2.329066
24	1	0	-0.965652	-3.560591	3.304174
25	1	0	-2.552461	-3.411615	2.546814
26	29	0	0.973545	-0.296123	-0.459943
27	1	0	5.626933	0.135347	-2.018436
28	1	0	4.018708	-2.100492	-2.250277
29	1	0	-0.462353	-4.070440	0.960342
30	6	0	-0.166600	-0.624894	-2.212454
31	6	0	-1.528841	-0.845189	-1.861982
32	6	0	-2.694134	-1.077276	-1.591407
33	6	0	0.460332	0.623000	-2.193243
34	6	0	-0.179584	1.906044	-1.716596
35	1	0	-1.209353	1.703128	-1.408317
36	1	0	-0.219571	2.626943	-2.544506
37	1	0	0.302586	-1.421374	-2.788125
38	1	0	1.368257	0.712487	-2.786040
39	6	0	-1.719179	5.632609	1.434695
40	6	0	-1.428454	5.709377	0.070834

41	8	0	0.801818	1.414361	0.416835
42	6	0	0.598861	2.466685	-0.475476
43	6	0	1.956397	3.068289	-0.925363
44	6	0	-0.225296	3.591910	0.180389
45	6	0	-0.686462	4.700966	-0.546064
46	6	0	-0.524315	3.528372	1.545873
47	6	0	-1.260764	4.537928	2.169204
48	1	0	-1.478671	4.468721	3.232506
49	1	0	-2.295275	6.417642	1.917466
50	1	0	-1.778868	6.556160	-0.514192
51	1	0	-0.467358	4.783460	-1.607744
52	1	0	-0.159804	2.670837	2.099135
53	1	0	2.562962	2.305059	-1.425753
54	1	0	1.842747	3.919990	-1.606079
55	1	0	2.502411	3.408587	-0.040300
56	1	0	-1.570441	-2.818698	0.388890
57	1	0	0.527744	-1.176694	3.564141
58	1	0	4.106145	-3.207856	-0.883261
59	1	0	4.422572	1.269794	-0.235554
60	6	0	-4.057024	-1.310805	-1.248490
61	6	0	-4.686711	-2.529548	-1.576923
62	6	0	-4.803027	-0.324733	-0.568426
63	6	0	-6.017700	-2.751518	-1.233693
64	1	0	-4.120462	-3.291241	-2.103793
65	6	0	-6.133348	-0.556842	-0.229762
66	1	0	-4.325503	0.616383	-0.315013
67	6	0	-6.746704	-1.768521	-0.559352
68	1	0	-6.488875	-3.694980	-1.494874
69	1	0	-6.694581	0.212307	0.293278
70	1	0	-7.785022	-1.944682	-0.293910

SCF Done: E(RB3LYP) = -3526.20709794 A.U.

IM31:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.099734	3.777782	-1.305966
2	6	0	-1.910729	2.309553	-1.624947
3	6	0	-3.129219	1.503499	-1.607527
4	6	0	-4.150056	0.844528	-1.596373
5	6	0	-3.247554	4.386086	-1.010452
6	1	0	-1.164739	1.894417	-0.918294
7	1	0	-1.440338	2.224203	-2.616993
8	1	0	-1.170168	4.344663	-1.316535
9	1	0	-3.278011	5.447138	-0.782070
10	1	0	-4.190120	3.846190	-0.989349
11	15	0	0.356850	-1.944902	-0.696504
12	6	0	-1.212092	-2.942882	-0.506406
13	6	0	-2.316605	-2.098147	0.153399

14	15	0	-1.709054	-1.233791	1.702148
15	6	0	-3.191619	-0.179501	2.166295
16	6	0	-3.671770	-0.693377	3.538475
17	6	0	-3.478484	-2.218489	3.555585
18	6	0	-2.048180	-2.493377	3.053993
19	6	0	0.208493	-1.111747	-2.365393
20	6	0	1.385112	-1.650473	-3.207748
21	6	0	1.614678	-3.119991	-2.815681
22	6	0	1.634667	-3.173822	-1.276199
23	1	0	-0.960389	-3.799826	0.131263
24	1	0	-1.550458	-3.344222	-1.468836
25	1	0	-3.200898	-2.709469	0.368761
26	1	0	-2.637268	-1.299194	-0.525756
27	1	0	-3.969458	-0.304764	1.405907
28	1	0	-4.712539	-0.409869	3.729423
29	1	0	-3.648795	-2.642960	4.551665
30	1	0	-4.205088	-2.686329	2.879128
31	1	0	0.247791	-0.029334	-2.228803
32	1	0	1.193000	-1.537115	-4.280227
33	1	0	2.288533	-1.071899	-2.980221
34	1	0	0.793162	-3.738140	-3.200845
35	1	0	2.542903	-3.514610	-3.243697
36	29	0	0.481125	-0.512618	1.053146
37	1	0	-3.066762	-0.242659	4.335719
38	1	0	-1.319861	-2.332970	3.856832
39	1	0	1.440702	-4.171693	-0.871003
40	6	0	2.151416	-0.984315	2.286310
41	6	0	3.320852	-1.145451	1.491643
42	6	0	4.334883	-1.332140	0.842210
43	6	0	1.575936	0.246082	2.602485
44	6	0	2.057236	1.576279	2.074606
45	1	0	2.950770	1.417156	1.464045
46	1	0	2.342343	2.229092	2.910713
47	1	0	1.876407	-1.846285	2.892464
48	1	0	0.909829	0.260512	3.462271
49	6	0	2.858898	5.503027	-1.031991
50	6	0	2.693410	5.600032	0.351378
51	8	0	0.491704	1.272104	0.277298
52	6	0	0.962645	2.240921	1.167413
53	6	0	-0.196997	2.782538	2.041731
54	6	0	1.618185	3.412287	0.407181
55	6	0	2.079920	4.566134	1.060339
56	6	0	1.800766	3.324884	-0.978394
57	6	0	2.410123	4.358918	-1.693249
58	1	0	2.537061	4.268960	-2.769590
59	1	0	3.333363	6.308927	-1.585497
60	1	0	3.041410	6.483597	0.880628
61	1	0	1.963133	4.665006	2.136339
62	1	0	1.455585	2.423899	-1.472073
63	1	0	-0.650421	1.963979	2.610965
64	1	0	0.122150	3.551588	2.753898
65	1	0	-0.969761	3.214738	1.399277
66	1	0	2.602700	-2.843335	-0.886324

67	1	0	-0.756540	-1.365532	-2.817763
68	1	0	-1.904254	-3.515306	2.688517
69	1	0	-2.916428	0.877180	2.180373
70	6	0	5.516746	-1.509515	0.066962
71	6	0	6.147849	-2.768643	-0.011079
72	6	0	6.077680	-0.425338	-0.640759
73	6	0	7.300700	-2.934239	-0.774009
74	1	0	5.724265	-3.606423	0.534011
75	6	0	7.230829	-0.601576	-1.400437
76	1	0	5.597341	0.546211	-0.584187
77	6	0	7.847210	-1.853850	-1.471498
78	1	0	7.775891	-3.909990	-0.823346
79	1	0	7.651080	0.242776	-1.939465
80	1	0	8.747194	-1.986360	-2.064830
81	6	0	-5.350649	0.068140	-1.579678
82	6	0	-6.340767	0.296332	-0.602226
83	6	0	-5.569386	-0.942732	-2.537256
84	6	0	-7.507329	-0.465215	-0.585057
85	1	0	-6.183724	1.079318	0.133003
86	6	0	-6.738148	-1.700005	-2.512864
87	1	0	-4.815471	-1.120208	-3.297809
88	6	0	-7.711039	-1.466490	-1.537653
89	1	0	-8.261605	-0.274210	0.173171
90	1	0	-6.891955	-2.473954	-3.259685
91	1	0	-8.622016	-2.057653	-1.522451

SCF Done: E(RB3LYP) = -3951.44407430 A.U.

TS3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.439069	3.339715	-2.075018
2	6	0	-1.117819	1.908990	-2.177281
3	6	0	-2.175605	0.973281	-2.173032
4	6	0	-3.106046	0.169683	-2.141350
5	6	0	-2.597497	3.922534	-1.704542
6	1	0	-0.161442	1.635570	-0.918669
7	1	0	-0.348357	1.693585	-2.925010
8	1	0	-0.592457	3.994832	-2.289872
9	1	0	-2.684434	5.001926	-1.627328
10	1	0	-3.492102	3.337592	-1.507920
11	15	0	-0.400011	-2.120974	0.483531
12	6	0	-2.027954	-2.529657	1.301692
13	6	0	-2.956062	-1.303283	1.316040
14	15	0	-2.098179	0.214820	1.988896
15	6	0	-3.271724	1.606552	1.557518
16	6	0	-3.704846	2.223500	2.902476
17	6	0	-3.832947	1.077971	3.921238
18	6	0	-2.549455	0.232624	3.808178

19	6	0	-0.653004	-2.429423	-1.340015
20	6	0	0.415357	-3.472032	-1.725383
21	6	0	0.528790	-4.470221	-0.560678
22	6	0	0.656128	-3.640797	0.733372
23	1	0	-1.791652	-2.843986	2.326476
24	1	0	-2.513474	-3.376400	0.803838
25	1	0	-3.872557	-1.513641	1.878792
26	1	0	-3.253135	-1.051005	0.292849
27	1	0	-4.129144	1.180759	1.026154
28	1	0	-4.638937	2.785377	2.797876
29	1	0	-3.984580	1.448198	4.941342
30	1	0	-4.705484	0.461764	3.669793
31	1	0	-0.580669	-1.496893	-1.901725
32	1	0	0.160805	-3.968416	-2.667894
33	1	0	1.381892	-2.974997	-1.874586
34	1	0	-0.376018	-5.089933	-0.519904
35	1	0	1.379624	-5.148878	-0.684767
36	29	0	0.128272	-0.056173	1.271961
37	1	0	-2.942756	2.934055	3.247640
38	1	0	-1.728203	0.703708	4.360009
39	1	0	0.356954	-4.188454	1.632267
40	6	0	1.837802	-0.369718	2.485339
41	6	0	2.918757	-0.912444	1.735118
42	6	0	3.856018	-1.391826	1.122509
43	6	0	1.466616	0.973415	2.454549
44	6	0	2.143497	1.981433	1.555787
45	1	0	2.993153	1.501171	1.063941
46	1	0	2.539211	2.811839	2.153264
47	1	0	1.488502	-0.977490	3.319063
48	1	0	0.888824	1.346317	3.296497
49	6	0	3.784803	4.438736	-2.500669
50	6	0	3.364572	5.154917	-1.379853
51	8	0	0.560092	1.390312	-0.113415
52	6	0	1.201529	2.545270	0.452443
53	6	0	0.150143	3.484504	1.068573
54	6	0	2.069428	3.243088	-0.604961
55	6	0	2.516448	4.562318	-0.442214
56	6	0	2.505542	2.531681	-1.732539
57	6	0	3.350298	3.123392	-2.672348
58	1	0	3.664367	2.555799	-3.544333
59	1	0	4.439861	4.901567	-3.233329
60	1	0	3.692581	6.180446	-1.233281
61	1	0	2.204529	5.142999	0.419934
62	1	0	2.160384	1.513552	-1.869831
63	1	0	-0.436196	2.938878	1.814192
64	1	0	0.613090	4.337699	1.573022
65	1	0	-0.536655	3.857507	0.305425
66	1	0	1.686616	-3.303389	0.879624
67	1	0	-1.662489	-2.824239	-1.496017
68	1	0	-2.660289	-0.783717	4.199608
69	1	0	-2.797102	2.322108	0.882939
70	6	0	4.950989	-1.907366	0.370174
71	6	0	5.515737	-3.161375	0.679869

72	6	0	5.487285	-1.164075	-0.702191
73	6	0	6.584155	-3.654633	-0.064199
74	1	0	5.109715	-3.735615	1.506708
75	6	0	6.555831	-1.666554	-1.439353
76	1	0	5.055344	-0.198191	-0.944512
77	6	0	7.108031	-2.911191	-1.124923
78	1	0	7.011014	-4.621834	0.185196
79	1	0	6.959797	-1.084427	-2.262527
80	1	0	7.942126	-3.298903	-1.702288
81	6	0	-4.205947	-0.720587	-2.219106
82	6	0	-5.452181	-0.404162	-1.621185
83	6	0	-4.105416	-1.963988	-2.893483
84	6	0	-6.525162	-1.287824	-1.685237
85	1	0	-5.562590	0.553657	-1.121119
86	6	0	-5.185063	-2.840825	-2.948876
87	1	0	-3.172074	-2.215809	-3.387610
88	6	0	-6.402442	-2.515905	-2.342949
89	1	0	-7.469419	-1.013803	-1.220985
90	1	0	-5.078164	-3.784455	-3.478514
91	1	0	-7.242897	-3.201917	-2.391321

SCF Done: E(RB3LYP) = -3951.42315413 A.U.

Pro:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.441338	-0.955490	2.324922
2	6	0	-0.620897	-2.965511	-0.347052
3	6	0	-1.620561	-1.962151	-0.264302
4	6	0	-2.512825	-1.136509	-0.192536
5	6	0	0.698173	-2.745891	-0.518952
6	6	0	1.341880	-1.400423	-0.672632
7	1	0	0.577922	-0.620453	-0.613246
8	1	0	1.804776	-1.323958	-1.666136
9	1	0	-0.971654	-3.993877	-0.269521
10	1	0	1.343519	-3.619828	-0.574040
11	6	0	3.753684	3.021647	-0.333710
12	6	0	4.307001	1.975163	-1.073613
13	8	0	1.787383	-1.166257	1.643878
14	6	0	2.442630	-1.070808	0.374871
15	6	0	3.599955	-2.085757	0.338871
16	6	0	2.933271	0.364453	0.127388
17	6	0	3.900106	0.660016	-0.844998
18	6	0	2.377900	1.424965	0.856469
19	6	0	2.785813	2.740767	0.631102
20	1	0	2.344200	3.547006	1.210599
21	1	0	4.072937	4.044927	-0.509592
22	1	0	5.059576	2.180933	-1.829861
23	1	0	4.343581	-0.137153	-1.433951

24	1	0	1.618828	1.205784	1.599738
25	1	0	3.236910	-3.068641	0.648162
26	1	0	4.045813	-2.181088	-0.655387
27	1	0	4.393969	-1.782444	1.030261
28	6	0	-3.543318	-0.156863	-0.108345
29	6	0	-4.897164	-0.542480	-0.025066
30	6	0	-3.228524	1.217893	-0.107019
31	6	0	-5.900479	0.419265	0.056175
32	1	0	-5.145736	-1.598933	-0.025409
33	6	0	-4.238688	2.172222	-0.025162
34	1	0	-2.188179	1.520522	-0.169696
35	6	0	-5.576974	1.778624	0.056468
36	1	0	-6.939123	0.107346	0.119601
37	1	0	-3.981229	3.227606	-0.025097
38	1	0	-6.362420	2.526077	0.119900

SCF Done: E(RB3LYP) = -810.263718401 A.U.

Part II :(S,S)- Ph- BPE–CuMes system

S9: The summarize energies of TS2s in the (*S, S*)-Ph-BPE-CuMes system in the gas-phase at the M06/6-31G (d, p).

M06/6-31G (d, p)

specises	***G*gas**	**Δ*G*gas**	**Δ*G*r(kJ mol^{-1})**
L_{ph}-*right-si*-TS2	-4447.213330	0.002362	6.2
L_{ph}-*right-re*-TS2	-4447.205442	0.01025	26.9
L_{ph}-*left-si*-TS2	-4447.208314	0.007378	19.4
L_{ph}-*left-re*-TS2	-4447.215692	0.0	0.0

S10: Cartesian coordinates and energies of TS2s optimized stationary points of (*S, S*)-Ph-BPE-MesCu reaction system at the M06 /6-31G (d, p) level.

L_{ph}-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.314626	1.254866	1.276408
2	6	0	-2.014708	1.986365	1.432974
3	6	0	-3.096726	1.138346	0.768825
4	15	0	-2.530770	0.331712	-0.810929
5	6	0	-4.064615	-0.681716	-1.264879
6	6	0	-4.565485	-0.079100	-2.583776
7	6	0	-4.357821	1.422051	-2.501990
8	6	0	-2.891397	1.635228	-2.133983
9	6	0	-0.070700	0.152042	2.800871

10	6	0	0.736045	0.991436	3.793134
11	6	0	1.647567	1.888445	2.969316
12	6	0	0.736753	2.636826	1.988668
13	1	0	-1.944176	2.967997	0.941600
14	1	0	-2.259964	2.165871	2.489127
15	1	0	-4.011506	1.725967	0.606060
16	1	0	-3.363032	0.292928	1.421325
17	1	0	-4.803985	-0.444332	-0.483924
18	1	0	-5.610654	-0.358114	-2.765889
19	1	0	-4.614177	1.939041	-3.435957
20	1	0	-5.013673	1.831919	-1.719836
21	1	0	0.580517	-0.640291	2.404156
22	1	0	0.075110	1.627651	4.400627
23	1	0	1.288604	0.348380	4.489377
24	1	0	2.226577	2.592541	3.580421
25	1	0	2.370850	1.278695	2.401004
26	29	0	-0.372886	-0.143514	-0.513556
27	1	0	-3.981175	-0.472690	-3.427693
28	6	0	-2.467408	3.021899	-1.747740
29	1	0	0.054616	3.266381	2.584957
30	6	0	1.465465	3.510839	1.013101
31	6	0	-1.344015	-0.484056	3.277925
32	6	0	-3.859068	-2.168191	-1.273072
33	6	0	-4.257140	-2.928897	-0.171025
34	6	0	-4.111914	-4.312346	-0.163942
35	6	0	-3.563555	-4.962705	-1.264632
36	6	0	-3.143505	-4.215376	-2.361122
37	6	0	-3.284732	-2.832449	-2.361871
38	6	0	-3.365348	3.970316	-1.249544
39	6	0	-1.119560	3.383088	-1.856584
40	6	0	-0.678922	4.639701	-1.464908
41	6	0	-1.580491	5.567705	-0.950633
42	6	0	-2.925322	5.230701	-0.851370
43	6	0	1.500914	4.893719	1.203094
44	6	0	2.166371	2.964567	-0.064927
45	6	0	2.883612	3.781558	-0.932233
46	6	0	2.915452	5.160444	-0.731938
47	6	0	2.221308	5.714456	0.340090
48	6	0	-1.753720	-1.692312	2.700274
49	6	0	-2.945785	-2.299594	3.074333
50	6	0	-3.766721	-1.704588	4.029653
51	6	0	-3.372491	-0.503835	4.611093
52	6	0	-2.171825	0.097904	4.242940
53	1	0	2.147170	1.888000	-0.237466
54	1	0	3.418603	3.330910	-1.766807
55	1	0	3.479514	5.799281	-1.407792
56	1	0	2.238939	6.789865	0.505060
57	1	0	0.955169	5.330464	2.039845
58	1	0	-3.642971	5.951207	-0.464359
59	1	0	-4.424469	3.733096	-1.170868
60	1	0	-1.230688	6.548075	-0.633556
61	1	0	0.376570	4.890473	-1.550693
62	1	0	-0.398090	2.662584	-2.243743

63	1	0	-2.696458	-4.710524	-3.220699
64	1	0	-2.950321	-2.265638	-3.230133
65	1	0	-3.456292	-6.044791	-1.265331
66	1	0	-4.437349	-4.884976	0.702687
67	1	0	-4.690921	-2.422348	0.692800
68	1	0	-3.227163	-3.246228	2.614470
69	1	0	-1.116798	-2.139095	1.938808
70	1	0	-4.699752	-2.177691	4.327732
71	1	0	-3.999827	-0.032590	5.364907
72	1	0	-1.880654	1.032378	4.720849
73	1	0	-2.274104	1.309054	-2.987932
74	6	0	0.816713	-0.202397	-2.229029
75	6	0	2.187683	-0.027622	-1.891935
76	6	0	3.360873	0.025249	-1.564607
77	6	0	0.381523	-1.501667	-2.587486
78	6	0	1.050318	-2.679023	-2.296690
79	1	0	2.131077	-2.634891	-2.170000
80	1	0	0.656480	-3.615343	-2.689924
81	1	0	0.331719	0.628284	-2.753019
82	1	0	-0.631452	-1.563385	-2.999032
83	6	0	4.723070	-0.021967	-1.154691
84	6	0	5.551438	-1.052952	-1.630668
85	6	0	5.254423	0.898498	-0.236954
86	6	0	6.868805	-1.153509	-1.207239
87	1	0	5.132667	-1.778051	-2.325886
88	6	0	6.575133	0.792722	0.179400
89	1	0	4.616674	1.693286	0.147611
90	6	0	7.387928	-0.230858	-0.302216
91	1	0	7.494472	-1.960084	-1.583430
92	1	0	6.972481	1.513806	0.890774
93	1	0	8.421233	-0.309277	0.028119
94	6	0	4.606825	-4.457902	0.790611
95	6	0	3.594963	-5.328410	0.398102
96	8	0	0.494766	-1.715583	0.317662
97	6	0	0.710739	-2.893004	-0.111013
98	6	0	-0.472426	-3.822842	-0.207684
99	6	0	2.052222	-3.473476	0.196010
100	6	0	2.326954	-4.840238	0.098752
101	6	0	3.074981	-2.607559	0.598968
102	6	0	4.342174	-3.092987	0.888833
103	1	0	5.130396	-2.398855	1.177804
104	1	0	5.599907	-4.840876	1.015929
105	1	0	3.793382	-6.395650	0.322039
106	1	0	1.547314	-5.532677	-0.212561
107	1	0	2.851149	-1.543108	0.659338
108	1	0	-1.340294	-3.262807	-0.568157
109	1	0	-0.316502	-4.685280	-0.861907
110	1	0	-0.707359	-4.205808	0.799290

Zero-point correction= 0.910057 (Hartree/Particle)

Thermal correction to Energy= 0.961804

Thermal correction to Enthalpy= 0.962749

Thermal correction to Gibbs Free Energy= 0.824703

Sum of electronic and zero-point Energies=	-4447.127976
Sum of electronic and thermal Energies=	-4447.076228
Sum of electronic and thermal Enthalpies=	-4447.075284
Sum of electronic and thermal Free Energies=	-4447.213330

L_{ph}-*right-re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.523661	-0.491154	1.589611
2	6	0	-0.518353	-2.349890	1.440850
3	6	0	0.472106	-2.917232	0.431380
4	15	0	0.724282	-1.810377	-1.021592
5	6	0	2.121301	-2.651327	-1.920769
6	6	0	1.595517	-2.760101	-3.359214
7	6	0	0.161159	-3.264165	-3.251767
8	6	0	-0.566896	-2.310667	-2.303523
9	6	0	0.855224	-0.067362	2.837760
10	6	0	0.154342	0.219429	4.172188
11	6	0	-1.261415	0.695333	3.873966
12	6	0	-1.854311	-0.344390	2.920206
13	1	0	-1.548691	-2.597471	1.145580
14	1	0	-0.347260	-2.797903	2.429082
15	1	0	0.171950	-3.924189	0.107154
16	1	0	1.471300	-2.999399	0.884858
17	1	0	2.159654	-3.677952	-1.517332
18	1	0	2.235781	-3.416578	-3.962531
19	1	0	-0.345083	-3.323197	-4.223278
20	1	0	0.181143	-4.283238	-2.836623
21	1	0	1.249219	0.873617	2.432698
22	1	0	0.088477	-0.692370	4.782450
23	1	0	0.728685	0.947347	4.759416
24	1	0	-1.872959	0.791200	4.780312
25	1	0	-1.245394	1.685206	3.391062
26	29	0	0.536651	0.303294	-0.486919
27	1	0	1.620849	-1.765077	-3.832417
28	6	0	-1.852050	-2.745321	-1.658668
29	1	0	-1.844444	-1.310283	3.453064
30	6	0	-3.250472	-0.091084	2.442711
31	6	0	1.980506	-1.062759	2.842068
32	6	0	3.499700	-2.058874	-1.792250
33	6	0	3.740683	-0.724878	-1.454447
34	6	0	5.048026	-0.254996	-1.348994
35	6	0	6.126950	-1.098011	-1.591990
36	6	0	5.895516	-2.426128	-1.938794
37	6	0	4.592616	-2.897727	-2.032094
38	6	0	-2.173967	-4.082586	-1.419533
39	6	0	-2.735419	-1.758731	-1.200678
40	6	0	-3.893632	-2.092677	-0.510454
41	6	0	-4.195764	-3.430692	-0.265743
42	6	0	-3.336902	-4.421489	-0.729208

43	6	0	-4.276246	-0.963373	2.815882
44	6	0	-3.569858	1.010538	1.642702
45	6	0	-4.882876	1.242903	1.250857
46	6	0	-5.897843	0.369492	1.636525
47	6	0	-5.590516	-0.739396	2.417541
48	6	0	3.068869	-0.869692	1.980650
49	6	0	4.081784	-1.817719	1.882485
50	6	0	4.035451	-2.974947	2.655489
51	6	0	2.972098	-3.169600	3.531435
52	6	0	1.955750	-2.222772	3.623328
53	1	0	-2.778783	1.683388	1.307110
54	1	0	-5.116096	2.103089	0.626413
55	1	0	-6.921123	0.555215	1.316505
56	1	0	-6.373290	-1.432573	2.719456
57	1	0	-4.034805	-1.832950	3.427552
58	1	0	-3.568457	-5.469961	-0.552822
59	1	0	-1.516345	-4.876232	-1.771208
60	1	0	-5.098081	-3.695582	0.281800
61	1	0	-4.554217	-1.300411	-0.156709
62	1	0	-2.495391	-0.708290	-1.373828
63	1	0	6.730735	-3.097482	-2.125918
64	1	0	4.409824	-3.942249	-2.287570
65	1	0	7.144043	-0.723197	-1.503074
66	1	0	5.228305	0.775516	-1.048021
67	1	0	2.900563	-0.069152	-1.217823
68	1	0	4.908410	-1.647469	1.193821
69	1	0	3.104974	0.039291	1.378499
70	1	0	4.826838	-3.717301	2.580412
71	1	0	2.931024	-4.064474	4.149198
72	1	0	1.130998	-2.399340	4.313194
73	6	0	5.258713	5.138733	0.045463
74	6	0	5.108928	3.901778	-0.580451
75	8	0	1.729483	1.638809	0.293491
76	6	0	1.606107	2.905362	0.397038
77	6	0	2.854796	3.711320	0.290618
78	6	0	3.922560	3.196790	-0.453109
79	6	0	3.012041	4.953874	0.910125
80	6	0	4.206574	5.658436	0.790994
81	1	0	4.314203	6.621058	1.286543
82	1	0	6.190030	5.692392	-0.048681
83	1	0	5.923727	3.486851	-1.171838
84	1	0	3.787297	2.232447	-0.937786
85	1	0	2.202516	5.376588	1.501264
86	6	0	0.483989	3.414252	1.268812
87	1	0	0.262046	4.475683	1.124427
88	1	0	-0.420563	2.832560	1.050345
89	1	0	0.745039	3.256929	2.328140
90	6	0	0.021550	1.382387	-2.249976
91	6	0	-1.370771	1.596892	-2.061896
92	6	0	-2.569412	1.813751	-1.992471
93	6	0	0.901932	2.484347	-2.224774
94	6	0	0.732504	3.647388	-1.499722
95	1	0	-0.274647	3.893926	-1.159932

96	1	0	1.391646	4.491584	-1.685300
97	1	0	0.271328	0.613981	-2.987896
98	1	0	1.883307	2.309258	-2.676193
99	6	0	-3.962088	2.075967	-1.917700
100	6	0	-4.901620	1.062823	-2.174289
101	6	0	-4.428897	3.360205	-1.586750
102	6	0	-6.261251	1.325219	-2.086631
103	1	0	-4.546854	0.066257	-2.431628
104	6	0	-5.791291	3.613708	-1.502747
105	1	0	-3.703218	4.148726	-1.397904
106	6	0	-6.714482	2.598483	-1.747953
107	1	0	-6.974863	0.527353	-2.281526
108	1	0	-6.136732	4.612528	-1.244597
109	1	0	-7.780848	2.801260	-1.681858
110	1	0	-0.769584	-1.376896	-2.850492

Zero-point correction= 0.911460 (Hartree/Particle)
Thermal correction to Energy= 0.962861
Thermal correction to Enthalpy= 0.963806
Thermal correction to Gibbs Free Energy= 0.827553
Sum of electronic and zero-point Energies= -4447.121535
Sum of electronic and thermal Energies= -4447.070134
Sum of electronic and thermal Enthalpies= -4447.069190
Sum of electronic and thermal Free Energies= -4447.205442

L_{ph}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.328830	1.362051	0.461082
2	6	0	-0.419316	2.927602	0.904087
3	6	0	0.863754	2.564883	1.653801
4	15	0	1.825879	1.319593	0.651664
5	6	0	2.811073	0.272860	1.875158
6	6	0	4.270048	0.740407	1.754118
7	6	0	4.322257	2.170030	1.208244
8	6	0	3.306405	2.318403	0.072565
9	6	0	-2.243043	1.038118	2.054829
10	6	0	-3.453319	1.989029	1.969193
11	6	0	-4.020549	1.870095	0.556016
12	6	0	-2.873323	1.917848	-0.470212
13	1	0	-0.180823	3.438991	-0.040921
14	1	0	-1.041687	3.615274	1.491772
15	1	0	1.470365	3.456754	1.863132
16	1	0	0.620479	2.112749	2.623778
17	1	0	4.795751	0.658320	2.713675
18	1	0	5.335638	2.453419	0.891418
19	1	0	4.039252	2.870887	2.007753
20	1	0	-3.129925	3.021236	2.168662
21	1	0	-4.204801	1.737491	2.729669

22	1	0	-4.776835	2.637346	0.347903
23	1	0	-4.524968	0.897863	0.467400
24	29	0	0.275670	0.115145	-0.456505
25	1	0	4.786533	0.057898	1.066262
26	6	0	3.709559	1.852517	-1.301648
27	6	0	-2.616577	3.214505	-1.179120
28	6	0	-2.679581	-0.394005	2.251425
29	1	0	2.962214	3.360014	-0.010367
30	6	0	2.164139	0.282238	3.228299
31	6	0	1.021464	-0.505342	3.422710
32	6	0	0.324285	-0.459681	4.624396
33	6	0	0.754391	0.374792	5.654037
34	6	0	1.891218	1.155153	5.472463
35	6	0	2.589055	1.111223	4.268198
36	6	0	2.867944	2.165226	-2.377798
37	6	0	4.848451	1.089560	-1.557562
38	6	0	5.134862	0.643696	-2.847633
39	6	0	4.293870	0.964085	-3.904906
40	6	0	3.157249	1.735636	-3.664901
41	6	0	-2.941561	4.456326	-0.628496
42	6	0	-1.942704	3.187970	-2.406312
43	6	0	-1.582726	4.365276	-3.050454
44	6	0	-1.900474	5.597020	-2.483973
45	6	0	-2.588370	5.636485	-1.275635
46	6	0	-2.813034	-1.305520	1.203048
47	6	0	-3.293271	-2.592962	1.433907
48	6	0	-3.634215	-2.993326	2.719942
49	6	0	-3.502537	-2.095306	3.776574
50	6	0	-3.036944	-0.807819	3.539611
51	1	0	-1.710962	2.222177	-2.857113
52	1	0	-1.061073	4.320854	-4.004204
53	1	0	-1.621734	6.520236	-2.986437
54	1	0	-2.850981	6.593564	-0.829812
55	1	0	-3.468462	4.504597	0.324233
56	1	0	2.488083	1.992293	-4.483703
57	1	0	1.963988	2.749116	-2.188480
58	1	0	4.517988	0.615799	-4.910085
59	1	0	6.024502	0.042029	-3.021571
60	1	0	5.531271	0.838714	-0.747107
61	1	0	2.238202	1.806882	6.271757
62	1	0	3.469902	1.739276	4.138381
63	1	0	0.210590	0.410850	6.595365
64	1	0	-0.560215	-1.081615	4.750771
65	1	0	0.674624	-1.145588	2.608280
66	1	0	-3.406290	-3.277271	0.593516
67	1	0	-2.533907	-1.027447	0.185751
68	1	0	-4.004712	-3.999878	2.900247
69	1	0	-3.768325	-2.397115	4.787660
70	1	0	-2.944653	-0.100762	4.365776
71	6	0	5.246010	-4.009638	-0.567008
72	6	0	4.897581	-2.660591	-0.628598
73	8	0	0.877281	-1.680921	0.081202
74	6	0	1.117300	-2.788039	-0.494091

75	6	0	2.544902	-3.239271	-0.530416
76	6	0	3.564523	-2.279827	-0.603272
77	6	0	2.904271	-4.587665	-0.477206
78	6	0	4.243917	-4.968655	-0.489692
79	1	0	4.503005	-6.024209	-0.438566
80	1	0	6.291766	-4.308173	-0.582879
81	1	0	5.673865	-1.899827	-0.706183
82	1	0	3.295612	-1.224954	-0.670074
83	1	0	2.134499	-5.353494	-0.412135
84	6	0	0.027646	-3.832666	-0.419312
85	1	0	0.157712	-4.659512	-1.125591
86	1	0	-0.933842	-3.341872	-0.609335
87	1	0	-0.004779	-4.242410	0.601152
88	6	0	-0.045641	-0.228879	-2.476505
89	6	0	-1.366331	-0.751193	-2.445519
90	6	0	-2.472503	-1.266491	-2.395885
91	6	0	1.030812	-1.101119	-2.757155
92	6	0	0.977966	-2.481460	-2.663069
93	1	0	0.001956	-2.954479	-2.773406
94	1	0	1.826491	-3.063539	-3.015232
95	1	0	0.071953	0.808394	-2.808815
96	1	0	2.000933	-0.618602	-2.910372
97	6	0	-3.711535	-1.930528	-2.194882
98	6	0	-3.764701	-3.335434	-2.235174
99	6	0	-4.888794	-1.221872	-1.901204
100	6	0	-4.952522	-4.003609	-1.971581
101	1	0	-2.856202	-3.886304	-2.474088
102	6	0	-6.071306	-1.898495	-1.637552
103	1	0	-4.858572	-0.133242	-1.878976
104	6	0	-6.109610	-3.290322	-1.666619
105	1	0	-4.976173	-5.090733	-2.004801
106	1	0	-6.971852	-1.334365	-1.404640
107	1	0	-7.037905	-3.816465	-1.457341
108	1	0	-3.009307	1.136781	-1.233673
109	1	0	-1.579431	1.318493	2.888674
110	1	0	2.700028	-0.740564	1.465369

Zero-point correction= 0.910081 (Hartree/Particle)
Thermal correction to Energy= 0.961603
Thermal correction to Enthalpy= 0.962547
Thermal correction to Gibbs Free Energy= 0.825657
Sum of electronic and zero-point Energies= -4447.123891
Sum of electronic and thermal Energies= -4447.072369
Sum of electronic and thermal Enthalpies= -4447.071424
Sum of electronic and thermal Free Energies= -4447.208314

L_{ph}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.179371	1.208772	-1.496323

2	6	0	-1.922175	1.247204	-2.156604
3	6	0	-2.556845	-0.128920	-1.977777
4	15	0	-2.416764	-0.635018	-0.187902
5	6	0	-3.007780	-2.431954	-0.146369
6	6	0	-4.367298	-2.392826	0.566659
7	6	0	-5.047972	-1.044808	0.323713
8	6	0	-4.023774	0.081540	0.493637
9	6	0	0.793986	0.677120	-3.026728
10	6	0	1.450765	1.959265	-3.575829
11	6	0	0.628545	3.169433	-3.146652
12	6	0	0.365718	2.991917	-1.652073
13	1	0	-2.472429	2.006831	-1.581831
14	1	0	-1.948431	1.558832	-3.209681
15	1	0	-3.601361	-0.148059	-2.319200
16	1	0	-2.012950	-0.875128	-2.575672
17	1	0	-5.001586	-3.232207	0.253418
18	1	0	-5.916451	-0.902385	0.980762
19	1	0	-5.429784	-1.010476	-0.706763
20	1	0	1.568785	1.900451	-4.664387
21	1	0	2.461269	2.062636	-3.157177
22	1	0	-0.317780	3.202558	-3.706865
23	1	0	1.150574	4.113700	-3.351715
24	29	0	-0.355797	0.030536	0.395784
25	1	0	-4.190525	-2.527103	1.642085
26	6	0	-3.815667	0.633015	1.879164
27	6	0	-0.542082	3.956725	-0.951748
28	6	0	1.719227	-0.459727	-2.693395
29	1	0	-4.277640	0.926743	-0.162808
30	6	0	-2.946029	-3.072434	-1.501762
31	6	0	-1.702635	-3.507721	-1.976970
32	6	0	-1.575031	-4.042170	-3.253254
33	6	0	-2.689479	-4.153966	-4.081324
34	6	0	-3.929427	-3.729041	-3.618059
35	6	0	-4.056449	-3.190991	-2.340605
36	6	0	-3.194505	1.880762	2.012412
37	6	0	-4.176775	-0.048304	3.042853
38	6	0	-3.915928	0.494348	4.299788
39	6	0	-3.290101	1.729366	4.416284
40	6	0	-2.935774	2.425136	3.262741
41	6	0	-1.650324	4.534411	-1.579166
42	6	0	-0.310266	4.260251	0.395075
43	6	0	-1.169856	5.098226	1.096649
44	6	0	-2.280574	5.652299	0.465587
45	6	0	-2.512512	5.371867	-0.877143
46	6	0	2.934444	-0.247819	-2.037689
47	6	0	3.731405	-1.320077	-1.657487
48	6	0	3.322308	-2.626357	-1.904823
49	6	0	2.111918	-2.849547	-2.551295
50	6	0	1.321950	-1.774648	-2.945256
51	1	0	0.560606	3.827349	0.889950
52	1	0	-0.961894	5.326725	2.140452
53	1	0	-2.953731	6.307334	1.013599
54	1	0	-3.367933	5.811393	-1.385778

55	1	0	-1.845906	4.328849	-2.630602
56	1	0	-2.451117	3.397280	3.332840
57	1	0	-2.901514	2.436049	1.118005
58	1	0	-3.084310	2.151015	5.397095
59	1	0	-4.206165	-0.056545	5.191802
60	1	0	-4.677893	-1.012209	2.981341
61	1	0	-4.807323	-3.814036	-4.254913
62	1	0	-5.036313	-2.858850	-1.999469
63	1	0	-2.591029	-4.573622	-5.079652
64	1	0	-0.600151	-4.377476	-3.603736
65	1	0	-0.823056	-3.406375	-1.337348
66	1	0	4.672785	-1.120695	-1.145589
67	1	0	3.267484	0.761861	-1.795361
68	1	0	3.938197	-3.462959	-1.582273
69	1	0	1.781197	-3.867649	-2.751854
70	1	0	0.367967	-1.959708	-3.444183
71	8	0	0.812711	-1.491217	0.825283
72	6	0	0.890357	-2.161272	1.896415
73	6	0	-0.357001	-2.846792	2.407040
74	6	0	2.211983	-2.783084	2.207382
75	6	0	2.360880	-3.875053	3.065974
76	6	0	3.351236	-2.262008	1.581592
77	6	0	0.254694	1.186782	2.028740
78	6	0	1.548029	1.528531	1.558317
79	6	0	2.654654	1.826645	1.135020
80	6	0	0.095428	0.264888	3.090162
81	6	0	1.054078	-0.638175	3.505368
82	1	0	2.095893	-0.425554	3.268182
83	1	0	0.882995	-1.237308	4.398103
84	1	0	-0.503198	1.972160	1.952556
85	1	0	-0.915636	0.201520	3.505031
86	6	0	3.918824	2.016253	0.521933
87	6	0	4.951242	1.082914	0.729906
88	6	0	4.157262	3.094167	-0.349564
89	6	0	6.159732	1.206960	0.059814
90	1	0	4.775823	0.257443	1.418968
91	6	0	5.369753	3.208208	-1.017301
92	1	0	3.375547	3.839760	-0.493805
93	6	0	6.374246	2.262910	-0.824457
94	1	0	6.942193	0.468456	0.227144
95	1	0	5.533218	4.044577	-1.693778
96	1	0	7.321053	2.353587	-1.351266
97	1	0	1.338216	2.984704	-1.133292
98	1	0	0.039347	0.315751	-3.742550
99	1	0	-2.273102	-2.941949	0.488244
100	6	0	4.601094	-2.818360	1.806433
101	6	0	4.740247	-3.911574	2.661473
102	6	0	3.615625	-4.436035	3.288095
103	1	0	3.221935	-1.416523	0.907645
104	1	0	5.475808	-2.400004	1.307504
105	1	0	5.719774	-4.351453	2.835940
106	1	0	3.712070	-5.290581	3.954658
107	1	0	1.493196	-4.305318	3.562121

108	1	0	-0.536836	-3.750792	1.803473
109	1	0	-0.297533	-3.146196	3.456981
110	1	0	-1.214105	-2.173436	2.287622

Zero-point correction= 0.909889 (Hartree/Particle)
Thermal correction to Energy= 0.961499
Thermal correction to Enthalpy= 0.962443
Thermal correction to Gibbs Free Energy= 0.825551
Sum of electronic and zero-point Energies= -4447.131355
Sum of electronic and thermal Energies= -4447.079745
Sum of electronic and thermal Enthalpies= -4447.078801
Sum of electronic and thermal Free Energies= -4447.215692

S11: The summarize energies of TS2s in the *(S, S)*-Ph-BPE-CuMes system in the gas-phase at the B3LYP/6-31G (d, p) level.

B3LYP/6-31G(d,p)

specises	***G*gas**	**Δ*G*gas**	**Δ*G*r(kJ mol^{-1})**
L$_{ph}$-*right-si*-TS2	-4448.970914	0.004584	12.0
L$_{ph}$-*right-re*-TS2	-4448.965826	0.009672	25.4
L$_{ph}$-*left-si*-TS2	-4448.967443	0.008055	21.1
L$_{ph}$-*left-re*-TS2	-4448.975498	0.0	0.0

S12: Cartesian coordinates and energies of TS2s optimized stationary points of (*S, S*)-Ph-BPE-CuMes reaction system in the gas-phase at the B3LYP /6-31G(d, p) level.

L$_{ph}$-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.006796	1.100515	1.277017
2	6	0	-1.619046	1.982611	1.537808
3	6	0	-2.806363	1.307069	0.830606
4	15	0	-2.385807	0.625812	-0.861895
5	6	0	-4.061537	-0.102695	-1.418471
6	6	0	-4.172430	0.380937	-2.874721
7	6	0	-3.853533	1.876980	-2.867150
8	6	0	-2.523533	2.086101	-2.105854
9	6	0	0.285207	-0.130466	2.715413
10	6	0	1.374035	0.502609	3.616290
11	6	0	2.221886	1.449094	2.757527
12	6	0	1.225597	2.354946	1.998754
13	1	0	-1.462542	2.983609	1.122005
14	1	0	-1.838749	2.097341	2.604169
15	1	0	-3.656551	1.995808	0.778241
16	1	0	-3.123275	0.432332	1.409931
17	1	0	-4.811366	0.450077	-0.835080
18	1	0	-5.167412	0.174196	-3.284582
19	1	0	-3.782470	2.290707	-3.879031

20	1	0	-4.669097	2.409085	-2.366363
21	1	0	0.723828	-0.984995	2.192716
22	1	0	0.917247	1.079897	4.428174
23	1	0	1.978174	-0.280645	4.086877
24	1	0	2.908659	2.050837	3.362949
25	1	0	2.831877	0.885049	2.040791
26	29	0	-0.262018	-0.170928	-0.618331
27	1	0	-3.446847	-0.147246	-3.506798
28	6	0	-2.301276	3.472878	-1.543494
29	1	0	0.656694	2.910002	2.757728
30	6	0	1.853976	3.367125	1.069017
31	6	0	-0.971417	-0.617431	3.401753
32	6	0	-4.305103	-1.577014	-1.174208
33	6	0	-4.568946	-2.034385	0.127781
34	6	0	-4.853024	-3.375455	0.378469
35	6	0	-4.885219	-4.296178	-0.671346
36	6	0	-4.629108	-3.857889	-1.969770
37	6	0	-4.341875	-2.513499	-2.217761
38	6	0	-3.325188	4.210451	-0.925721
39	6	0	-1.028540	4.059200	-1.626566
40	6	0	-0.782744	5.332878	-1.113384
41	6	0	-1.811700	6.052661	-0.503783
42	6	0	-3.083743	5.485533	-0.412011
43	6	0	1.918244	4.713604	1.456497
44	6	0	2.432188	2.998773	-0.154459
45	6	0	3.056024	3.950726	-0.962965
46	6	0	3.120942	5.288108	-0.561934
47	6	0	2.549489	5.666304	0.654291
48	6	0	-1.550049	-1.829017	2.987204
49	6	0	-2.713671	-2.312381	3.586794
50	6	0	-3.329359	-1.593389	4.613728
51	6	0	-2.768055	-0.386648	5.034392
52	6	0	-1.602459	0.094994	4.435101
53	1	0	2.405166	1.962992	-0.475984
54	1	0	3.494288	3.641230	-1.908030
55	1	0	3.613184	6.025701	-1.189595
56	1	0	2.593571	6.701986	0.980351
57	1	0	1.475161	5.018300	2.401940
58	1	0	-3.894218	6.036751	0.057041
59	1	0	-4.325901	3.796227	-0.846688
60	1	0	-1.624972	7.046051	-0.106192
61	1	0	0.214535	5.754152	-1.185302
62	1	0	-0.216838	3.507976	-2.093471
63	1	0	-4.656284	-4.560763	-2.797755
64	1	0	-4.155512	-2.198715	-3.238978
65	1	0	-5.113466	-5.340426	-0.478983
66	1	0	-5.060720	-3.698904	1.394579
67	1	0	-4.565463	-1.331249	0.956053
68	1	0	-3.133231	-3.257667	3.254019
69	1	0	-1.074313	-2.385774	2.185117
70	1	0	-4.231616	-1.971610	5.085967
71	1	0	-3.233595	0.180710	5.835784
72	1	0	-1.179224	1.031040	4.788401

73	1	0	-1.703978	1.880792	-2.802929
74	6	0	1.055701	-0.144935	-2.300897
75	6	0	2.416317	-0.147311	-1.879145
76	6	0	3.586324	-0.183063	-1.531233
77	6	0	0.504111	-1.318021	-2.873878
78	6	0	0.995917	-2.607818	-2.699723
79	1	0	2.043128	-2.722780	-2.445428
80	1	0	0.562960	-3.415770	-3.280584
81	1	0	0.696923	0.803596	-2.705753
82	1	0	-0.454648	-1.191605	-3.377364
83	6	0	4.946470	-0.273107	-1.119049
84	6	0	5.597567	-1.526430	-1.083703
85	6	0	5.677813	0.872766	-0.737874
86	6	0	6.926748	-1.623168	-0.680979
87	1	0	5.044443	-2.414855	-1.369875
88	6	0	7.007546	0.764271	-0.338841
89	1	0	5.189962	1.841887	-0.752013
90	6	0	7.640502	-0.480959	-0.308197
91	1	0	7.409452	-2.596617	-0.661184
92	1	0	7.553035	1.658427	-0.049089
93	1	0	8.678296	-0.560374	0.002463
94	6	0	3.502684	-5.763561	0.456429
95	6	0	2.363519	-6.275784	-0.165175
96	8	0	0.282253	-1.969924	-0.022564
97	6	0	0.287737	-3.092025	-0.649079
98	6	0	-1.058067	-3.678500	-1.042449
99	6	0	1.395241	-4.044865	-0.293847
100	6	0	1.320598	-5.425931	-0.538109
101	6	0	2.548619	-3.542268	0.334370
102	6	0	3.590041	-4.389671	0.703031
103	1	0	4.473411	-3.976989	1.182987
104	1	0	4.313996	-6.425935	0.745340
105	1	0	2.282303	-7.341985	-0.359673
106	1	0	0.443751	-5.849520	-1.016017
107	1	0	2.610337	-2.475307	0.516129
108	1	0	-1.703487	-2.889113	-1.424625
109	1	0	-0.991273	-4.467443	-1.793512
110	1	0	-1.542020	-4.099594	-0.150453

Zero-point correction= 0.912350 (Hartree/Particle)
Thermal correction to Energy= 0.965472
Thermal correction to Enthalpy= 0.966416
Thermal correction to Gibbs Free Energy= 0.819816
Sum of electronic and zero-point Energies= -4448.878380
Sum of electronic and thermal Energies= -4448.825258
Sum of electronic and thermal Enthalpies= -4448.824314
Sum of electronic and thermal Free Energies= -4448.970914

L_{ph}-*right-re*-TS2:

Standard orientation:

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

1	15	0	-0.888126	-0.776233	1.263167
2	6	0	-0.062297	-2.443427	1.440396
3	6	0	1.294316	-2.558083	0.730692
4	15	0	1.396509	-1.587911	-0.855715
5	6	0	3.160312	-1.926731	-1.397078
6	6	0	3.020393	-1.766018	-2.926542
7	6	0	1.862049	-2.686847	-3.353575
8	6	0	0.699229	-2.623054	-2.308905
9	6	0	-0.538072	0.299648	2.808385
10	6	0	-1.881567	0.386205	3.579498
11	6	0	-3.035926	0.078237	2.610586
12	6	0	-2.622495	-1.211185	1.870277
13	1	0	-0.773504	-3.140704	0.981926
14	1	0	0.034424	-2.715983	2.496428
15	1	0	1.547841	-3.610202	0.565337
16	1	0	2.083331	-2.120542	1.354040
17	1	0	3.331934	-2.996218	-1.205077
18	1	0	3.951285	-2.025407	-3.442179
19	1	0	1.487810	-2.428665	-4.349194
20	1	0	2.232972	-3.714093	-3.419535
21	1	0	-0.336303	1.279355	2.367725
22	1	0	-1.907788	-0.349056	4.390581
23	1	0	-1.987763	1.371708	4.045005
24	1	0	-3.984421	-0.059994	3.140933
25	1	0	-3.179705	0.898067	1.895788
26	29	0	0.089227	0.291711	-0.497140
27	1	0	2.801136	-0.717478	-3.165499
28	6	0	0.084029	-3.952749	-1.928110
29	1	0	-2.460019	-1.976311	2.642490
30	6	0	-3.592619	-1.789461	0.867974
31	6	0	0.699606	-0.108523	3.577789
32	6	0	4.288492	-1.165346	-0.734984
33	6	0	4.126514	0.108261	-0.174745
34	6	0	5.213116	0.770531	0.405121
35	6	0	6.471435	0.170071	0.445238
36	6	0	6.641771	-1.103762	-0.102158
37	6	0	5.559282	-1.762020	-0.683558
38	6	0	0.857571	-5.093267	-1.653411
39	6	0	-1.310933	-4.062243	-1.808911
40	6	0	-1.913264	-5.263942	-1.433356
41	6	0	-1.130143	-6.388483	-1.167955
42	6	0	0.258322	-6.297037	-1.279474
43	6	0	-4.217143	-3.016165	1.138396
44	6	0	-3.907046	-1.135828	-0.333280
45	6	0	-4.822956	-1.689883	-1.229311
46	6	0	-5.441843	-2.910299	-0.945284
47	6	0	-5.135235	-3.572073	0.244602
48	6	0	1.941970	0.423660	3.188775
49	6	0	3.119791	0.040963	3.830624
50	6	0	3.082220	-0.876623	4.883029
51	6	0	1.856528	-1.410307	5.281736
52	6	0	0.678205	-1.034120	4.632426

53	1	0	-3.440202	-0.185943	-0.568088
54	1	0	-5.051423	-1.163259	-2.151963
55	1	0	-6.156336	-3.338403	-1.642621
56	1	0	-5.611491	-4.519629	0.481573
57	1	0	-3.986267	-3.539774	2.063292
58	1	0	0.879604	-7.165035	-1.076411
59	1	0	1.940080	-5.048860	-1.735732
60	1	0	-1.595666	-7.326428	-0.879387
61	1	0	-2.994549	-5.313039	-1.347978
62	1	0	-1.934154	-3.194884	-2.011202
63	1	0	7.615104	-1.586018	-0.073614
64	1	0	5.699097	-2.755827	-1.103913
65	1	0	7.311929	0.687226	0.899600
66	1	0	5.067353	1.764615	0.817558
67	1	0	3.156260	0.596656	-0.185997
68	1	0	4.067319	0.458006	3.502206
69	1	0	1.977189	1.133856	2.366089
70	1	0	3.998124	-1.171541	5.386962
71	1	0	1.812890	-2.122892	6.100994
72	1	0	-0.261930	-1.466257	4.962617
73	6	0	4.543785	5.485209	-1.179735
74	6	0	4.484132	4.134981	-1.540886
75	8	0	1.226050	1.862905	-0.058559
76	6	0	1.026048	3.110324	-0.322627
77	6	0	2.233299	3.956727	-0.624049
78	6	0	3.345988	3.383883	-1.264565
79	6	0	2.305490	5.314073	-0.270158
80	6	0	3.449158	6.068427	-0.543325
81	1	0	3.481461	7.115328	-0.253380
82	1	0	5.432031	6.072694	-1.394357
83	1	0	5.328412	3.666594	-2.039751
84	1	0	3.300536	2.340456	-1.551168
85	1	0	1.472375	5.792113	0.233038
86	6	0	-0.127218	3.776759	0.419111
87	1	0	-0.407362	4.749587	0.010162
88	1	0	-1.003266	3.127697	0.389673
89	1	0	0.163867	3.918696	1.469588
90	6	0	-1.150717	1.081852	-2.067770
91	6	0	-2.320379	1.750354	-1.603093
92	6	0	-3.318367	2.345981	-1.228486
93	6	0	-0.087960	1.840763	-2.607865
94	6	0	0.167424	3.189929	-2.355143
95	1	0	-0.673313	3.826344	-2.097981
96	1	0	0.954502	3.670918	-2.924103
97	1	0	-1.329366	0.102786	-2.516812
98	1	0	0.666048	1.270774	-3.150686
99	6	0	-4.467083	3.066860	-0.792774
100	6	0	-4.445427	4.477440	-0.734618
101	6	0	-5.650403	2.397608	-0.412272
102	6	0	-5.564886	5.186812	-0.309261
103	1	0	-3.542501	5.002181	-1.030193
104	6	0	-6.765389	3.117066	0.009874
105	1	0	-5.681185	1.313415	-0.449699

106	6	0	-6.730526	4.512739	0.064739
107	1	0	-5.528608	6.272147	-0.272047
108	1	0	-7.667514	2.584285	0.298075
109	1	0	-7.602960	5.069624	0.393899
110	1	0	-0.102531	-2.000692	-2.715280

Zero-point correction= 0.912855 (Hartree/Particle)
Thermal correction to Energy= 0.965938
Thermal correction to Enthalpy= 0.966883
Thermal correction to Gibbs Free Energy= 0.818558
Sum of electronic and zero-point Energies= -4448.871530
Sum of electronic and thermal Energies= -4448.818446
Sum of electronic and thermal Enthalpies= -4448.817502
Sum of electronic and thermal Free Energies= -4448.965826

L_{ph}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.189434	0.966811	1.185956
2	6	0	-0.222511	2.400349	1.908883
3	6	0	1.233678	1.979357	2.178449
4	15	0	1.995702	1.258050	0.624058
5	6	0	3.461000	0.192655	1.209849
6	6	0	4.738926	1.011897	0.888356
7	6	0	4.401072	2.513079	0.813558
8	6	0	3.082597	2.700976	0.033641
9	6	0	-1.808394	0.144141	2.764844
10	6	0	-3.032768	1.009152	3.170628
11	6	0	-3.845615	1.326652	1.904867
12	6	0	-2.890950	1.694397	0.731440
13	1	0	-0.257952	3.213071	1.176088
14	1	0	-0.689872	2.779796	2.824126
15	1	0	1.815458	2.827728	2.557005
16	1	0	1.264651	1.204568	2.950053
17	1	0	5.528322	0.817718	1.621143
18	1	0	5.219618	3.095008	0.374063
19	1	0	4.256146	2.900455	1.829002
20	1	0	-2.676617	1.939269	3.629875
21	1	0	-3.642204	0.495768	3.922560
22	1	0	-4.572672	2.124152	2.087039
23	1	0	-4.420035	0.440369	1.618303
24	29	0	0.222854	0.054110	-0.314957
25	1	0	5.125535	0.674690	-0.078352
26	6	0	3.175056	2.760096	-1.482551
27	6	0	-2.835696	3.151102	0.321867
28	6	0	-2.145661	-1.330285	2.640512
29	1	0	2.577646	3.616022	0.365565
30	6	0	3.297327	-0.323089	2.624461
31	6	0	2.484932	-1.450963	2.836578
32	6	0	2.275311	-1.949075	4.122589

33	6	0	2.877746	-1.334982	5.223718
34	6	0	3.688114	-0.216569	5.025203
35	6	0	3.891620	0.287505	3.738195
36	6	0	2.036194	3.145838	-2.211358
37	6	0	4.339565	2.458340	-2.200158
38	6	0	4.364930	2.531981	-3.596379
39	6	0	3.226455	2.912021	-4.303882
40	6	0	2.058527	3.223908	-3.602022
41	6	0	-3.003982	4.204348	1.234144
42	6	0	-2.588861	3.476224	-1.022707
43	6	0	-2.507528	4.805568	-1.439964
44	6	0	-2.675765	5.842236	-0.520025
45	6	0	-2.927657	5.534696	0.818029
46	6	0	-2.741335	-1.880350	1.496064
47	6	0	-3.115564	-3.225215	1.460271
48	6	0	-2.887733	-4.050121	2.561999
49	6	0	-2.279003	-3.520563	3.701471
50	6	0	-1.914803	-2.174499	3.737886
51	1	0	-2.479974	2.673886	-1.748046
52	1	0	-2.324761	5.030016	-2.487225
53	1	0	-2.618487	6.877596	-0.843015
54	1	0	-3.067214	6.332327	1.542639
55	1	0	-3.201458	3.988637	2.280368
56	1	0	1.165020	3.529412	-4.139138
57	1	0	1.121971	3.392492	-1.676183
58	1	0	3.246366	2.968141	-5.388201
59	1	0	5.281630	2.291585	-4.127630
60	1	0	5.245509	2.171379	-1.677320
61	1	0	4.165347	0.267959	5.872850
62	1	0	4.523788	1.161534	3.608728
63	1	0	2.721095	-1.726412	6.224907
64	1	0	1.643515	-2.822074	4.260870
65	1	0	2.018249	-1.929493	1.978872
66	1	0	-3.584821	-3.621749	0.564624
67	1	0	-2.902537	-1.271710	0.611576
68	1	0	-3.176250	-5.096908	2.531640
69	1	0	-2.088078	-4.154346	4.563258
70	1	0	-1.444167	-1.769445	4.630823
71	6	0	4.914988	-4.200302	-2.497089
72	6	0	4.734930	-2.839392	-2.227964
73	8	0	1.119616	-1.675139	-0.429412
74	6	0	1.058896	-2.660377	-1.262140
75	6	0	2.385296	-3.223069	-1.709397
76	6	0	3.488794	-2.360901	-1.835033
77	6	0	2.577712	-4.584598	-1.988641
78	6	0	3.830622	-5.068035	-2.374829
79	1	0	3.956467	-6.128390	-2.577591
80	1	0	5.888055	-4.576338	-2.800293
81	1	0	5.570668	-2.151363	-2.327520
82	1	0	3.343529	-1.303922	-1.638267
83	1	0	1.751368	-5.281202	-1.895486
84	6	0	-0.093511	-3.637264	-1.060330
85	1	0	-0.236708	-4.322620	-1.899361

86	1	0	-1.013032	-3.071403	-0.903503
87	1	0	0.091719	-4.229716	-0.154155
88	6	0	-0.592065	0.228237	-2.292504
89	6	0	-1.926813	-0.264338	-2.232678
90	6	0	-3.081242	-0.664327	-2.213874
91	6	0	0.422279	-0.500884	-2.946969
92	6	0	0.428399	-1.880607	-3.171306
93	1	0	-0.534413	-2.380867	-3.221084
94	1	0	1.187620	-2.281494	-3.833532
95	1	0	-0.499529	1.314361	-2.341078
96	1	0	1.336013	0.057047	-3.148080
97	6	0	-4.412646	-1.166293	-2.170472
98	6	0	-4.669851	-2.541521	-2.366854
99	6	0	-5.508140	-0.308530	-1.929437
100	6	0	-5.971170	-3.034021	-2.315854
101	1	0	-3.836882	-3.208916	-2.564637
102	6	0	-6.805567	-0.811597	-1.879731
103	1	0	-5.327480	0.752799	-1.788637
104	6	0	-7.045744	-2.174718	-2.070716
105	1	0	-6.148132	-4.094813	-2.471059
106	1	0	-7.634826	-0.134694	-1.693130
107	1	0	-8.059315	-2.562678	-2.032022
108	1	0	-3.176491	1.123452	-0.155787
109	1	0	-1.016788	0.246635	3.515656
110	1	0	3.405317	-0.677935	0.551705

Zero-point correction= 0.912798 (Hartree/Particle)
Thermal correction to Energy= 0.965787
Thermal correction to Enthalpy= 0.966731
Thermal correction to Gibbs Free Energy= 0.818559
Sum of electronic and zero-point Energies= -4448.873204
Sum of electronic and thermal Energies= -4448.820215
Sum of electronic and thermal Enthalpies= -4448.819271
Sum of electronic and thermal Free Energies= -4448.967443

L_{ph}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.036177	0.810762	-1.675177
2	6	0	-1.589866	1.670606	-2.012866
3	6	0	-2.747581	0.836569	-1.433897
4	15	0	-2.445265	0.461470	0.378957
5	6	0	-3.735349	-0.880770	0.825942
6	6	0	-4.676606	-0.189793	1.841363
7	6	0	-4.803521	1.306114	1.500661
8	6	0	-3.401475	1.890134	1.209809
9	6	0	0.296486	-0.230137	-3.240964
10	6	0	1.750315	0.108100	-3.651689
11	6	0	1.911633	1.627338	-3.530715
12	6	0	1.425125	2.031992	-2.121346

13	1	0	-1.546345	2.656144	-1.536302
14	1	0	-1.739824	1.842248	-3.084792
15	1	0	-3.708505	1.343729	-1.576959
16	1	0	-2.812566	-0.123314	-1.955181
17	1	0	-5.654055	-0.682624	1.869897
18	1	0	-5.307828	1.861894	2.298956
19	1	0	-5.419079	1.421479	0.601850
20	1	0	1.955583	-0.252794	-4.665545
21	1	0	2.451599	-0.401875	-2.979765
22	1	0	1.310878	2.117805	-4.306114
23	1	0	2.949601	1.944043	-3.681483
24	29	0	-0.176457	0.087386	0.467798
25	1	0	-4.244083	-0.301646	2.841069
26	6	0	-2.665559	2.504076	2.387283
27	6	0	1.117698	3.494101	-1.890688
28	6	0	-0.000528	-1.712315	-3.166986
29	1	0	-3.481204	2.670314	0.444706
30	6	0	-4.391351	-1.550610	-0.365762
31	6	0	-3.681947	-2.548082	-1.057479
32	6	0	-4.233918	-3.188258	-2.166274
33	6	0	-5.515258	-2.849417	-2.607297
34	6	0	-6.232668	-1.863799	-1.929786
35	6	0	-5.674905	-1.218458	-0.823444
36	6	0	-1.675566	3.469373	2.138714
37	6	0	-2.929707	2.166921	3.722459
38	6	0	-2.228299	2.770077	4.770189
39	6	0	-1.246426	3.724038	4.505606
40	6	0	-0.974052	4.073138	3.180984
41	6	0	0.411954	4.275864	-2.819886
42	6	0	1.542733	4.108883	-0.700757
43	6	0	1.269208	5.454231	-0.446830
44	6	0	0.565334	6.217175	-1.380114
45	6	0	0.140303	5.621595	-2.569209
46	6	0	0.458657	-2.515239	-2.112129
47	6	0	0.228085	-3.891700	-2.112306
48	6	0	-0.461377	-4.493341	-3.167877
49	6	0	-0.929239	-3.703997	-4.220404
50	6	0	-0.702483	-2.326538	-4.214917
51	1	0	2.105093	3.524324	0.022659
52	1	0	1.618174	5.907967	0.476855
53	1	0	0.355813	7.265309	-1.187065
54	1	0	-0.402923	6.206132	-3.306754
55	1	0	0.072814	3.834780	-3.752841
56	1	0	-0.216728	4.818753	2.956465
57	1	0	-1.452634	3.755700	1.113447
58	1	0	-0.701588	4.191921	5.320090
59	1	0	-2.455079	2.491739	5.795640
60	1	0	-3.696310	1.437335	3.961243
61	1	0	-7.232193	-1.593298	-2.259402
62	1	0	-6.258697	-0.459204	-0.312550
63	1	0	-5.949827	-3.349849	-3.467860
64	1	0	-3.656330	-3.948129	-2.683537
65	1	0	-2.682777	-2.820841	-0.726293

66	1	0	0.590299	-4.488648	-1.280198
67	1	0	0.968002	-2.068800	-1.265436
68	1	0	-0.633239	-5.566189	-3.169444
69	1	0	-1.468086	-4.158327	-5.047614
70	1	0	-1.068310	-1.719676	-5.040390
71	8	0	0.377210	-1.720998	1.014742
72	6	0	0.449829	-2.266754	2.169130
73	6	0	-0.836729	-2.385901	2.975606
74	6	0	1.505028	-3.317485	2.355441
75	6	0	1.476280	-4.253948	3.401963
76	6	0	2.558622	-3.392796	1.425640
77	6	0	1.198054	1.092593	1.748845
78	6	0	2.492621	0.923277	1.181130
79	6	0	3.611597	0.801679	0.705361
80	6	0	0.854874	0.437813	2.960807
81	6	0	1.452064	-0.708908	3.461894
82	1	0	2.446812	-0.970877	3.119821
83	1	0	1.187429	-1.054977	4.455952
84	1	0	0.764919	2.085157	1.621870
85	1	0	-0.037586	0.818017	3.455986
86	6	0	4.907810	0.612947	0.149606
87	6	0	5.655246	-0.548329	0.446851
88	6	0	5.480800	1.575706	-0.710062
89	6	0	6.921363	-0.734708	-0.100797
90	1	0	5.225815	-1.294642	1.107988
91	6	0	6.747249	1.378313	-1.254045
92	1	0	4.922159	2.478465	-0.938639
93	6	0	7.475148	0.223959	-0.954015
94	1	0	7.480869	-1.634588	0.140360
95	1	0	7.170315	2.131880	-1.912962
96	1	0	8.463895	0.074259	-1.377819
97	1	0	2.203592	1.743819	-1.408018
98	1	0	-0.362699	0.207217	-4.002395
99	1	0	-3.151766	-1.648261	1.340819
100	6	0	3.547276	-4.366094	1.541093
101	6	0	3.506704	-5.293078	2.587623
102	6	0	2.466720	-5.230964	3.515538
103	1	0	2.584141	-2.667979	0.619865
104	1	0	4.351019	-4.405450	0.810464
105	1	0	4.276815	-6.054034	2.677244
106	1	0	2.421982	-5.947175	4.331659
107	1	0	0.677242	-4.231124	4.135367
108	1	0	-1.450391	-3.194565	2.553422
109	1	0	-0.675145	-2.600512	4.033096
110	1	0	-1.395623	-1.451889	2.895775

Zero-point correction= 0.912234 (Hartree/Particle)
Thermal correction to Energy= 0.965463
Thermal correction to Enthalpy= 0.966407
Thermal correction to Gibbs Free Energy= 0.817772
Sum of electronic and zero-point Energies= -4448.881036
Sum of electronic and thermal Energies= -4448.827808

Sum of electronic and thermal Enthalpies= -4448.826864
Sum of electronic and thermal Free Energies= -4448.975498

S13: The summarize energies of TS2s in the *(S, S)-Ph-BPE-MesCu* system in THF solvent at the M06/6-311+G (d, p).

M06(SMD,THF)/6-311+G(d,p)

species	**SCF_{SMD}**	G^*_{gas}	G_{sol}	ΔG_{sol}	ΔG_r(kJ.mol^{-1})
L_{ph}-*right-si*-TS2	-4448.81362249	0.824703	-4447.988919	0.005928	15.6
L_{ph}-*right-re*-TS2	-4448.80582377	0.827553	-4447.97827	0.016577	43.5
L_{ph}-*left-si*-TS2	-4448.80776652	0.825657	-4447.982109	0.005928	33.4
L_{ph}-*left-re*-TS2	-4448.82039840	0.825551	-4449.994847	0.0	0.0

S14: Cartesian coordinates and energies of TS2s optimized stationary points of (*S, S*)-Ph-BPE-MesCu reaction system in THF solvent at the M06 /6-311+G (d, p) level.

L_{ph}-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.314626	1.254866	1.276408
2	6	0	-2.014708	1.986365	1.432974
3	6	0	-3.096726	1.138346	0.768825
4	15	0	-2.530770	0.331712	-0.810929
5	6	0	-4.064615	-0.681716	-1.264879
6	6	0	-4.565485	-0.079100	-2.583776
7	6	0	-4.357821	1.422051	-2.501990
8	6	0	-2.891397	1.635228	-2.133983
9	6	0	-0.070700	0.152042	2.800871
10	6	0	0.736045	0.991436	3.793134
11	6	0	1.647567	1.888445	2.969316
12	6	0	0.736753	2.636826	1.988668
13	1	0	-1.944176	2.967997	0.941600
14	1	0	-2.259964	2.165871	2.489127
15	1	0	-4.011506	1.725967	0.606060
16	1	0	-3.363032	0.292928	1.421325
17	1	0	-4.803985	-0.444332	-0.483924
18	1	0	-5.610654	-0.358114	-2.765889

19	1	0	-4.614177	1.939041	-3.435957
20	1	0	-5.013673	1.831919	-1.719836
21	1	0	0.580517	-0.640291	2.404156
22	1	0	0.075110	1.627651	4.400627
23	1	0	1.288604	0.348380	4.489377
24	1	0	2.226577	2.592541	3.580421
25	1	0	2.370850	1.278695	2.401004
26	29	0	-0.372886	-0.143514	-0.513556
27	1	0	-3.981175	-0.472690	-3.427693
28	6	0	-2.467408	3.021899	-1.747740
29	1	0	0.054616	3.266381	2.584957
30	6	0	1.465465	3.510839	1.013101
31	6	0	-1.344015	-0.484056	3.277925
32	6	0	-3.859068	-2.168191	-1.273072
33	6	0	-4.257140	-2.928897	-0.171025
34	6	0	-4.111914	-4.312346	-0.163942
35	6	0	-3.563555	-4.962705	-1.264632
36	6	0	-3.143505	-4.215376	-2.361122
37	6	0	-3.284732	-2.832449	-2.361871
38	6	0	-3.365348	3.970316	-1.249544
39	6	0	-1.119560	3.383088	-1.856584
40	6	0	-0.678922	4.639701	-1.464908
41	6	0	-1.580491	5.567705	-0.950633
42	6	0	-2.925322	5.230701	-0.851370
43	6	0	1.500914	4.893719	1.203094
44	6	0	2.166371	2.964567	-0.064927
45	6	0	2.883612	3.781558	-0.932233
46	6	0	2.915452	5.160444	-0.731938
47	6	0	2.221308	5.714456	0.340090
48	6	0	-1.753720	-1.692312	2.700274
49	6	0	-2.945785	-2.299594	3.074333
50	6	0	-3.766721	-1.704588	4.029653
51	6	0	-3.372491	-0.503835	4.611093
52	6	0	-2.171825	0.097904	4.242940
53	1	0	2.147170	1.888000	-0.237466
54	1	0	3.418603	3.330910	-1.766807
55	1	0	3.479514	5.799281	-1.407792
56	1	0	2.238940	6.789865	0.505060
57	1	0	0.955169	5.330464	2.039845
58	1	0	-3.642971	5.951207	-0.464359
59	1	0	-4.424469	3.733096	-1.170868
60	1	0	-1.230688	6.548075	-0.633556
61	1	0	0.376570	4.890473	-1.550693
62	1	0	-0.398090	2.662584	-2.243743
63	1	0	-2.696458	-4.710524	-3.220699
64	1	0	-2.950321	-2.265638	-3.230133
65	1	0	-3.456292	-6.044791	-1.265331
66	1	0	-4.437349	-4.884976	0.702687
67	1	0	-4.690921	-2.422348	0.692800
68	1	0	-3.227163	-3.246228	2.614470
69	1	0	-1.116798	-2.139095	1.938808

70	1	0	-4.699752	-2.177691	4.327732
71	1	0	-3.999827	-0.032590	5.364907
72	1	0	-1.880654	1.032378	4.720849
73	1	0	-2.274104	1.309054	-2.987932
74	6	0	0.816713	-0.202397	-2.229029
75	6	0	2.187683	-0.027622	-1.891935
76	6	0	3.360873	0.025249	-1.564607
77	6	0	0.381523	-1.501667	-2.587486
78	6	0	1.050318	-2.679023	-2.296690
79	1	0	2.131077	-2.634891	-2.170000
80	1	0	0.656480	-3.615343	-2.689924
81	1	0	0.331719	0.628284	-2.753019
82	1	0	-0.631452	-1.563385	-2.999032
83	6	0	4.723070	-0.021967	-1.154691
84	6	0	5.551438	-1.052952	-1.630668
85	6	0	5.254423	0.898498	-0.236954
86	6	0	6.868805	-1.153509	-1.207239
87	1	0	5.132667	-1.778051	-2.325886
88	6	0	6.575133	0.792722	0.179400
89	1	0	4.616674	1.693286	0.147611
90	6	0	7.387928	-0.230859	-0.302216
91	1	0	7.494472	-1.960085	-1.583430
92	1	0	6.972481	1.513806	0.890774
93	1	0	8.421233	-0.309278	0.028119
94	6	0	4.606825	-4.457902	0.790611
95	6	0	3.594963	-5.328410	0.398102
96	8	0	0.494766	-1.715583	0.317662
97	6	0	0.710739	-2.893004	-0.111013
98	6	0	-0.472426	-3.822842	-0.207684
99	6	0	2.052222	-3.473476	0.196010
100	6	0	2.326954	-4.840238	0.098752
101	6	0	3.074981	-2.607559	0.598968
102	6	0	4.342174	-3.092987	0.888833
103	1	0	5.130396	-2.398855	1.177804
104	1	0	5.599907	-4.840876	1.015929
105	1	0	3.793382	-6.395650	0.322039
106	1	0	1.547314	-5.532677	-0.212561
107	1	0	2.851149	-1.543108	0.659338
108	1	0	-1.340294	-3.262807	-0.568157
109	1	0	-0.316502	-4.685280	-0.861907
110	1	0	-0.707359	-4.205808	0.799290

SCF Done: E(RM06) = -4448.81362249 A.U.

L_{ph}-*right-re*-TS2:

Standard orientation:

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

1	15	0	-0.523661	-0.491154	1.589611
2	6	0	-0.518353	-2.349890	1.440850
3	6	0	0.472106	-2.917232	0.431380
4	15	0	0.724282	-1.810377	-1.021592
5	6	0	2.121301	-2.651327	-1.920769
6	6	0	1.595517	-2.760101	-3.359214
7	6	0	0.161159	-3.264165	-3.251767
8	6	0	-0.566896	-2.310667	-2.303523
9	6	0	0.855224	-0.067362	2.837760
10	6	0	0.154342	0.219429	4.172188
11	6	0	-1.261415	0.695333	3.873966
12	6	0	-1.854311	-0.344390	2.920206
13	1	0	-1.548691	-2.597471	1.145580
14	1	0	-0.347260	-2.797903	2.429082
15	1	0	0.171950	-3.924189	0.107154
16	1	0	1.471300	-2.999399	0.884858
17	1	0	2.159654	-3.677952	-1.517332
18	1	0	2.235781	-3.416578	-3.962531
19	1	0	-0.345083	-3.323197	-4.223278
20	1	0	0.181143	-4.283238	-2.836623
21	1	0	1.249219	0.873617	2.432698
22	1	0	0.088477	-0.692370	4.782450
23	1	0	0.728685	0.947347	4.759416
24	1	0	-1.872959	0.791200	4.780312
25	1	0	-1.245394	1.685206	3.391062
26	29	0	0.536651	0.303294	-0.486919
27	1	0	1.620849	-1.765077	-3.832417
28	6	0	-1.852050	-2.745321	-1.658668
29	1	0	-1.844444	-1.310283	3.453064
30	6	0	-3.250472	-0.091084	2.442711
31	6	0	1.980506	-1.062759	2.842068
32	6	0	3.499700	-2.058874	-1.792250
33	6	0	3.740683	-0.724878	-1.454447
34	6	0	5.048026	-0.254996	-1.348994
35	6	0	6.126950	-1.098011	-1.591990
36	6	0	5.895516	-2.426128	-1.938794
37	6	0	4.592616	-2.897727	-2.032094
38	6	0	-2.173967	-4.082586	-1.419533
39	6	0	-2.735419	-1.758731	-1.200678
40	6	0	-3.893632	-2.092677	-0.510454
41	6	0	-4.195764	-3.430692	-0.265743
42	6	0	-3.336902	-4.421489	-0.729208
43	6	0	-4.276246	-0.963373	2.815882
44	6	0	-3.569858	1.010538	1.642702
45	6	0	-4.882876	1.242903	1.250857
46	6	0	-5.897843	0.369492	1.636525
47	6	0	-5.590516	-0.739396	2.417541
48	6	0	3.068869	-0.869692	1.980650
49	6	0	4.081784	-1.817719	1.882485
50	6	0	4.035451	-2.974947	2.655489
51	6	0	2.972098	-3.169600	3.531435
52	6	0	1.955750	-2.222772	3.623328
53	1	0	-2.778783	1.683388	1.307110

54	1	0	-5.116096	2.103089	0.626413
55	1	0	-6.921123	0.555215	1.316505
56	1	0	-6.373290	-1.432573	2.719456
57	1	0	-4.034805	-1.832950	3.427552
58	1	0	-3.568457	-5.469961	-0.552822
59	1	0	-1.516345	-4.876232	-1.771208
60	1	0	-5.098081	-3.695582	0.281800
61	1	0	-4.554217	-1.300411	-0.156709
62	1	0	-2.495391	-0.708290	-1.373828
63	1	0	6.730735	-3.097482	-2.125918
64	1	0	4.409824	-3.942249	-2.287570
65	1	0	7.144043	-0.723197	-1.503074
66	1	0	5.228305	0.775516	-1.048021
67	1	0	2.900563	-0.069152	-1.217823
68	1	0	4.908410	-1.647469	1.193821
69	1	0	3.104974	0.039291	1.378499
70	1	0	4.826838	-3.717301	2.580412
71	1	0	2.931024	-4.064474	4.149198
72	1	0	1.130998	-2.399340	4.313194
73	6	0	5.258713	5.138733	0.045463
74	6	0	5.108928	3.901778	-0.580451
75	8	0	1.729483	1.638809	0.293491
76	6	0	1.606107	2.905362	0.397038
77	6	0	2.854796	3.711320	0.290618
78	6	0	3.922560	3.196790	-0.453109
79	6	0	3.012041	4.953874	0.910125
80	6	0	4.206574	5.658436	0.790994
81	1	0	4.314203	6.621058	1.286543
82	1	0	6.190030	5.692392	-0.048681
83	1	0	5.923727	3.486851	-1.171838
84	1	0	3.787297	2.232447	-0.937786
85	1	0	2.202516	5.376588	1.501264
86	6	0	0.483989	3.414252	1.268812
87	1	0	0.262046	4.475683	1.124427
88	1	0	-0.420563	2.832560	1.050345
89	1	0	0.745039	3.256929	2.328140
90	6	0	0.021550	1.382387	-2.249976
91	6	0	-1.370771	1.596892	-2.061896
92	6	0	-2.569412	1.813751	-1.992471
93	6	0	0.901932	2.484347	-2.224774
94	6	0	0.732504	3.647388	-1.499722
95	1	0	-0.274647	3.893926	-1.159932
96	1	0	1.391646	4.491584	-1.685300
97	1	0	0.271328	0.613981	-2.987896
98	1	0	1.883307	2.309258	-2.676193
99	6	0	-3.962088	2.075967	-1.917700
100	6	0	-4.901620	1.062823	-2.174289
101	6	0	-4.428897	3.360205	-1.586750
102	6	0	-6.261251	1.325219	-2.086631
103	1	0	-4.546854	0.066257	-2.431628
104	6	0	-5.791291	3.613708	-1.502747
105	1	0	-3.703218	4.148726	-1.397904
106	6	0	-6.714482	2.598483	-1.747953

107	1	0	-6.974863	0.527353	-2.281526
108	1	0	-6.136732	4.612528	-1.244597
109	1	0	-7.780848	2.801260	-1.681858
110	1	0	-0.769584	-1.376896	-2.850492

SCF Done: E(RM06) = -4448.80582377 A.U.

L_{ph}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.328830	1.362051	0.461082
2	6	0	-0.419316	2.927602	0.904087
3	6	0	0.863754	2.564883	1.653801
4	15	0	1.825879	1.319593	0.651664
5	6	0	2.811073	0.272860	1.875158
6	6	0	4.270048	0.740407	1.754118
7	6	0	4.322257	2.170030	1.208244
8	6	0	3.306405	2.318403	0.072565
9	6	0	-2.243043	1.038118	2.054829
10	6	0	-3.453319	1.989029	1.969193
11	6	0	-4.020549	1.870095	0.556016
12	6	0	-2.873323	1.917848	-0.470212
13	1	0	-0.180823	3.438991	-0.040921
14	1	0	-1.041687	3.615274	1.491772
15	1	0	1.470365	3.456754	1.863132
16	1	0	0.620479	2.112749	2.623778
17	1	0	4.795751	0.658320	2.713675
18	1	0	5.335638	2.453419	0.891418
19	1	0	4.039252	2.870887	2.007753
20	1	0	-3.129925	3.021236	2.168662
21	1	0	-4.204801	1.737491	2.729669
22	1	0	-4.776835	2.637346	0.347903
23	1	0	-4.524968	0.897863	0.467400
24	29	0	0.275670	0.115145	-0.456505
25	1	0	4.786533	0.057898	1.066262
26	6	0	3.709559	1.852517	-1.301648
27	6	0	-2.616577	3.214505	-1.179120
28	6	0	-2.679581	-0.394005	2.251425
29	1	0	2.962214	3.360014	-0.010367
30	6	0	2.164139	0.282238	3.228299
31	6	0	1.021464	-0.505342	3.422710
32	6	0	0.324285	-0.459681	4.624396
33	6	0	0.754391	0.374792	5.654037
34	6	0	1.891218	1.155153	5.472463
35	6	0	2.589055	1.111223	4.268198
36	6	0	2.867944	2.165226	-2.377798
37	6	0	4.848451	1.089560	-1.557562
38	6	0	5.134862	0.643696	-2.847633

39	6	0	4.293870	0.964085	-3.904906
40	6	0	3.157249	1.735636	-3.664901
41	6	0	-2.941561	4.456326	-0.628496
42	6	0	-1.942704	3.187970	-2.406312
43	6	0	-1.582726	4.365276	-3.050454
44	6	0	-1.900474	5.597020	-2.483973
45	6	0	-2.588370	5.636485	-1.275635
46	6	0	-2.813034	-1.305520	1.203048
47	6	0	-3.293271	-2.592962	1.433907
48	6	0	-3.634215	-2.993326	2.719942
49	6	0	-3.502537	-2.095306	3.776574
50	6	0	-3.036944	-0.807819	3.539611
51	1	0	-1.710962	2.222177	-2.857113
52	1	0	-1.061073	4.320854	-4.004204
53	1	0	-1.621734	6.520236	-2.986437
54	1	0	-2.850981	6.593564	-0.829812
55	1	0	-3.468462	4.504597	0.324233
56	1	0	2.488083	1.992293	-4.483703
57	1	0	1.963988	2.749116	-2.188480
58	1	0	4.517988	0.615799	-4.910085
59	1	0	6.024502	0.042029	-3.021571
60	1	0	5.531271	0.838714	-0.747107
61	1	0	2.238202	1.806882	6.271757
62	1	0	3.469902	1.739276	4.138381
63	1	0	0.210590	0.410850	6.595365
64	1	0	-0.560215	-1.081615	4.750771
65	1	0	0.674624	-1.145588	2.608280
66	1	0	-3.406290	-3.277271	0.593516
67	1	0	-2.533907	-1.027447	0.185751
68	1	0	-4.004712	-3.999878	2.900247
69	1	0	-3.768325	-2.397115	4.787660
70	1	0	-2.944653	-0.100762	4.365776
71	6	0	5.246010	-4.009638	-0.567008
72	6	0	4.897581	-2.660591	-0.628598
73	8	0	0.877281	-1.680921	0.081202
74	6	0	1.117300	-2.788039	-0.494091
75	6	0	2.544902	-3.239271	-0.530416
76	6	0	3.564523	-2.279827	-0.603272
77	6	0	2.904271	-4.587665	-0.477206
78	6	0	4.243917	-4.968655	-0.489692
79	1	0	4.503005	-6.024209	-0.438566
80	1	0	6.291766	-4.308173	-0.582879
81	1	0	5.673865	-1.899827	-0.706183
82	1	0	3.295612	-1.224954	-0.670074
83	1	0	2.134499	-5.353494	-0.412135
84	6	0	0.027646	-3.832666	-0.419312
85	1	0	0.157712	-4.659512	-1.125591
86	1	0	-0.933842	-3.341872	-0.609335
87	1	0	-0.004779	-4.242410	0.601152
88	6	0	-0.045641	-0.228879	-2.476505
89	6	0	-1.366331	-0.751193	-2.445519
90	6	0	-2.472503	-1.266491	-2.395885
91	6	0	1.030812	-1.101119	-2.757155

92	6	0	0.977966	-2.481460	-2.663069
93	1	0	0.001956	-2.954479	-2.773406
94	1	0	1.826491	-3.063539	-3.015232
95	1	0	0.071953	0.808394	-2.808815
96	1	0	2.000933	-0.618602	-2.910372
97	6	0	-3.711535	-1.930528	-2.194882
98	6	0	-3.764701	-3.335434	-2.235174
99	6	0	-4.888794	-1.221872	-1.901204
100	6	0	-4.952522	-4.003609	-1.971581
101	1	0	-2.856202	-3.886304	-2.474088
102	6	0	-6.071306	-1.898495	-1.637552
103	1	0	-4.858572	-0.133242	-1.878976
104	6	0	-6.109610	-3.290322	-1.666619
105	1	0	-4.976173	-5.090733	-2.004801
106	1	0	-6.971852	-1.334365	-1.404640
107	1	0	-7.037905	-3.816465	-1.457341
108	1	0	-3.009307	1.136781	-1.233673
109	1	0	-1.579431	1.318493	2.888674
110	1	0	2.700028	-0.740564	1.465369

SCF Done: E(RM06) = -4448.80776652 A.U.

L_{ph}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.179371	1.208772	-1.496323
2	6	0	-1.922175	1.247204	-2.156604
3	6	0	-2.556845	-0.128920	-1.977777
4	15	0	-2.416764	-0.635018	-0.187902
5	6	0	-3.007780	-2.431954	-0.146369
6	6	0	-4.367298	-2.392826	0.566659
7	6	0	-5.047972	-1.044808	0.323713
8	6	0	-4.023774	0.081540	0.493637
9	6	0	0.793986	0.677120	-3.026728
10	6	0	1.450765	1.959265	-3.575829
11	6	0	0.628545	3.169433	-3.146652
12	6	0	0.365718	2.991917	-1.652073
13	1	0	-2.472429	2.006831	-1.581831
14	1	0	-1.948431	1.558832	-3.209681
15	1	0	-3.601361	-0.148059	-2.319200
16	1	0	-2.012950	-0.875128	-2.575672
17	1	0	-5.001586	-3.232207	0.253418
18	1	0	-5.916451	-0.902385	0.980762
19	1	0	-5.429784	-1.010476	-0.706763
20	1	0	1.568785	1.900451	-4.664387
21	1	0	2.461269	2.062636	-3.157177
22	1	0	-0.317780	3.202558	-3.706865

23	1	0	1.150574	4.113700	-3.351715
24	29	0	-0.355797	0.030536	0.395784
25	1	0	-4.190525	-2.527103	1.642085
26	6	0	-3.815667	0.633015	1.879164
27	6	0	-0.542082	3.956725	-0.951748
28	6	0	1.719227	-0.459727	-2.693395
29	1	0	-4.277640	0.926743	-0.162808
30	6	0	-2.946029	-3.072434	-1.501762
31	6	0	-1.702635	-3.507721	-1.976970
32	6	0	-1.575031	-4.042170	-3.253254
33	6	0	-2.689479	-4.153966	-4.081324
34	6	0	-3.929427	-3.729041	-3.618059
35	6	0	-4.056449	-3.190991	-2.340605
36	6	0	-3.194505	1.880762	2.012412
37	6	0	-4.176775	-0.048304	3.042853
38	6	0	-3.915928	0.494348	4.299788
39	6	0	-3.290101	1.729366	4.416284
40	6	0	-2.935774	2.425136	3.262741
41	6	0	-1.650324	4.534411	-1.579166
42	6	0	-0.310266	4.260251	0.395075
43	6	0	-1.169856	5.098226	1.096649
44	6	0	-2.280574	5.652299	0.465587
45	6	0	-2.512512	5.371867	-0.877143
46	6	0	2.934444	-0.247819	-2.037689
47	6	0	3.731405	-1.320077	-1.657487
48	6	0	3.322308	-2.626357	-1.904823
49	6	0	2.111918	-2.849547	-2.551295
50	6	0	1.321950	-1.774648	-2.945256
51	1	0	0.560606	3.827349	0.889950
52	1	0	-0.961894	5.326725	2.140452
53	1	0	-2.953731	6.307334	1.013599
54	1	0	-3.367933	5.811393	-1.385778
55	1	0	-1.845906	4.328849	-2.630602
56	1	0	-2.451117	3.397280	3.332840
57	1	0	-2.901514	2.436049	1.118005
58	1	0	-3.084310	2.151015	5.397095
59	1	0	-4.206165	-0.056545	5.191802
60	1	0	-4.677893	-1.012209	2.981341
61	1	0	-4.807323	-3.814036	-4.254913
62	1	0	-5.036313	-2.858850	-1.999469
63	1	0	-2.591029	-4.573622	-5.079652
64	1	0	-0.600151	-4.377476	-3.603736
65	1	0	-0.823056	-3.406375	-1.337348
66	1	0	4.672785	-1.120695	-1.145589
67	1	0	3.267484	0.761861	-1.795361
68	1	0	3.938197	-3.462959	-1.582273
69	1	0	1.781197	-3.867649	-2.751854
70	1	0	0.367967	-1.959708	-3.444183
71	8	0	0.812711	-1.491217	0.825283
72	6	0	0.890357	-2.161272	1.896415
73	6	0	-0.357001	-2.846792	2.407040
74	6	0	2.211983	-2.783084	2.207382
75	6	0	2.360880	-3.875053	3.065974

76	6	0	3.351236	-2.262008	1.581592
77	6	0	0.254694	1.186782	2.028740
78	6	0	1.548029	1.528531	1.558317
79	6	0	2.654654	1.826645	1.135020
80	6	0	0.095428	0.264888	3.090162
81	6	0	1.054078	-0.638175	3.505368
82	1	0	2.095893	-0.425554	3.268182
83	1	0	0.882995	-1.237308	4.398103
84	1	0	-0.503198	1.972160	1.952556
85	1	0	-0.915636	0.201520	3.505031
86	6	0	3.918824	2.016253	0.521933
87	6	0	4.951242	1.082914	0.729906
88	6	0	4.157262	3.094167	-0.349564
89	6	0	6.159732	1.206960	0.059814
90	1	0	4.775823	0.257443	1.418968
91	6	0	5.369753	3.208208	-1.017301
92	1	0	3.375547	3.839760	-0.493805
93	6	0	6.374246	2.262910	-0.824457
94	1	0	6.942193	0.468456	0.227144
95	1	0	5.533218	4.044577	-1.693778
96	1	0	7.321053	2.353587	-1.351266
97	1	0	1.338216	2.984704	-1.133292
98	1	0	0.039347	0.315751	-3.742550
99	1	0	-2.273102	-2.941949	0.488244
100	6	0	4.601094	-2.818360	1.806433
101	6	0	4.740247	-3.911574	2.661473
102	6	0	3.615625	-4.436035	3.288095
103	1	0	3.221935	-1.416523	0.907645
104	1	0	5.475808	-2.400004	1.307504
105	1	0	5.719774	-4.351453	2.835940
106	1	0	3.712070	-5.290581	3.954658
107	1	0	1.493196	-4.305318	3.562121
108	1	0	-0.536836	-3.750792	1.803473
109	1	0	-0.297533	-3.146196	3.456981
110	1	0	-1.214105	-2.173436	2.287622

SCF Done: E(RM06) = -4448.82039840 A.U.

S15: The summarize energies of TS2s in the *(S, S)*-Ph-BPE-CuMes system in the THF solvent at the B3LYP /6-311+G (d, p) level.

B3LYP(SMD,THF) /6-311+G (d, p)

specises	**SCF_{SMD}**	G^*_{gas}	G_{sol}	ΔG_{sol}	ΔG_r(kJ.mol^{-1})
L_{ph}-*right-si*-TS2	-4450.61851887	0.819816	-4449.798702	0.006193	16.3
L_{ph}-*right-re*-TS2	-4450.61169795	0.818558	-4449.793139	0.011756	30.9
L_{ph}-*left-si*-TS2	-4450.61460678	0.818559	-4449.796047	0.008848	23.2
L_{ph}-*left-re*-TS2	-4450.62266716	0.817772	-4449.804895	0.0	0.0

G^*_{THF} =Thermal correction to Gibbs Free Energy in gas .

S16: Cartesian coordinates and energies of TS2s optimized stationary points of (*S, S*)-Ph-BPE-CuMes reaction system in the THF solvent at the B3LYP /6-311+G (d, p) level.

L_{ph}-*right*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.006796	1.100515	1.277017
2	6	0	-1.619046	1.982611	1.537808
3	6	0	-2.806363	1.307069	0.830606
4	15	0	-2.385807	0.625812	-0.861895
5	6	0	-4.061537	-0.102695	-1.418471
6	6	0	-4.172430	0.380937	-2.874721
7	6	0	-3.853533	1.876980	-2.867150
8	6	0	-2.523533	2.086101	-2.105854
9	6	0	0.285207	-0.130466	2.715413
10	6	0	1.374035	0.502609	3.616290
11	6	0	2.221886	1.449094	2.757527
12	6	0	1.225597	2.354946	1.998754
13	1	0	-1.462542	2.983609	1.122005
14	1	0	-1.838749	2.097341	2.604169
15	1	0	-3.656551	1.995808	0.778241
16	1	0	-3.123275	0.432332	1.409931
17	1	0	-4.811366	0.450077	-0.835080
18	1	0	-5.167412	0.174196	-3.284582
19	1	0	-3.782470	2.290707	-3.879031
20	1	0	-4.669097	2.409085	-2.366363
21	1	0	0.723828	-0.984995	2.192716
22	1	0	0.917247	1.079897	4.428174
23	1	0	1.978174	-0.280645	4.086877
24	1	0	2.908659	2.050837	3.362949
25	1	0	2.831877	0.885049	2.040791
26	29	0	-0.262018	-0.170928	-0.618331
27	1	0	-3.446847	-0.147246	-3.506798
28	6	0	-2.301276	3.472878	-1.543494
29	1	0	0.656694	2.910002	2.757728
30	6	0	1.853976	3.367125	1.069017
31	6	0	-0.971417	-0.617431	3.401753
32	6	0	-4.305103	-1.577014	-1.174208
33	6	0	-4.568946	-2.034385	0.127781

34	6	0	-4.853024	-3.375455	0.378469
35	6	0	-4.885219	-4.296178	-0.671346
36	6	0	-4.629108	-3.857889	-1.969770
37	6	0	-4.341875	-2.513499	-2.217761
38	6	0	-3.325188	4.210451	-0.925721
39	6	0	-1.028540	4.059200	-1.626566
40	6	0	-0.782744	5.332878	-1.113384
41	6	0	-1.811700	6.052661	-0.503783
42	6	0	-3.083743	5.485533	-0.412011
43	6	0	1.918244	4.713604	1.456497
44	6	0	2.432188	2.998773	-0.154459
45	6	0	3.056024	3.950726	-0.962965
46	6	0	3.120942	5.288108	-0.561934
47	6	0	2.549489	5.666304	0.654291
48	6	0	-1.550049	-1.829017	2.987204
49	6	0	-2.713671	-2.312381	3.586794
50	6	0	-3.329359	-1.593389	4.613728
51	6	0	-2.768055	-0.386648	5.034392
52	6	0	-1.602459	0.094994	4.435101
53	1	0	2.405166	1.962992	-0.475984
54	1	0	3.494288	3.641230	-1.908030
55	1	0	3.613184	6.025701	-1.189595
56	1	0	2.593571	6.701986	0.980351
57	1	0	1.475161	5.018300	2.401940
58	1	0	-3.894218	6.036751	0.057041
59	1	0	-4.325901	3.796227	-0.846688
60	1	0	-1.624972	7.046051	-0.106192
61	1	0	0.214535	5.754152	-1.185302
62	1	0	-0.216838	3.507976	-2.093471
63	1	0	-4.656284	-4.560763	-2.797755
64	1	0	-4.155512	-2.198715	-3.238978
65	1	0	-5.113466	-5.340426	-0.478983
66	1	0	-5.060720	-3.698904	1.394579
67	1	0	-4.565463	-1.331249	0.956053
68	1	0	-3.133231	-3.257667	3.254019
69	1	0	-1.074313	-2.385774	2.185117
70	1	0	-4.231616	-1.971610	5.085967
71	1	0	-3.233595	0.180710	5.835784
72	1	0	-1.179224	1.031040	4.788401
73	1	0	-1.703978	1.880792	-2.802929
74	6	0	1.055701	-0.144935	-2.300897
75	6	0	2.416317	-0.147311	-1.879145
76	6	0	3.586324	-0.183063	-1.531233
77	6	0	0.504111	-1.318021	-2.873878
78	6	0	0.995917	-2.607818	-2.699723
79	1	0	2.043128	-2.722780	-2.445428
80	1	0	0.562960	-3.415770	-3.280584
81	1	0	0.696923	0.803596	-2.705753
82	1	0	-0.454648	-1.191605	-3.377364
83	6	0	4.946470	-0.273107	-1.119049
84	6	0	5.597567	-1.526430	-1.083703

85	6	0	5.677813	0.872766	-0.737874
86	6	0	6.926748	-1.623168	-0.680979
87	1	0	5.044443	-2.414855	-1.369875
88	6	0	7.007546	0.764271	-0.338841
89	1	0	5.189962	1.841887	-0.752013
90	6	0	7.640502	-0.480959	-0.308197
91	1	0	7.409452	-2.596617	-0.661184
92	1	0	7.553035	1.658427	-0.049089
93	1	0	8.678296	-0.560374	0.002463
94	6	0	3.502684	-5.763561	0.456429
95	6	0	2.363519	-6.275784	-0.165175
96	8	0	0.282253	-1.969924	-0.022564
97	6	0	0.287737	-3.092025	-0.649079
98	6	0	-1.058067	-3.678500	-1.042449
99	6	0	1.395241	-4.044865	-0.293847
100	6	0	1.320598	-5.425931	-0.538109
101	6	0	2.548619	-3.542268	0.334370
102	6	0	3.590041	-4.389671	0.703031
103	1	0	4.473411	-3.976989	1.182987
104	1	0	4.313996	-6.425935	0.745340
105	1	0	2.282303	-7.341985	-0.359673
106	1	0	0.443751	-5.849520	-1.016017
107	1	0	2.610337	-2.475307	0.516129
108	1	0	-1.703487	-2.889113	-1.424625
109	1	0	-0.991273	-4.467443	-1.793512
110	1	0	-1.542020	-4.099594	-0.150453

SCF Done: E(RB3LYP) = -4450.61851887 A.U.

L_{ph}-*right*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.888126	-0.776233	1.263167
2	6	0	-0.062297	-2.443427	1.440396
3	6	0	1.294316	-2.558083	0.730692
4	15	0	1.396509	-1.587911	-0.855715
5	6	0	3.160312	-1.926731	-1.397078
6	6	0	3.020393	-1.766018	-2.926542
7	6	0	1.862049	-2.686847	-3.353575
8	6	0	0.699229	-2.623054	-2.308905
9	6	0	-0.538072	0.299648	2.808385
10	6	0	-1.881567	0.386205	3.579498
11	6	0	-3.035926	0.078237	2.610586
12	6	0	-2.622495	-1.211185	1.870277
13	1	0	-0.773504	-3.140704	0.981926
14	1	0	0.034424	-2.715983	2.496428
15	1	0	1.547841	-3.610202	0.565337
16	1	0	2.083331	-2.120542	1.354040

17	1	0	3.331934	-2.996218	-1.205077
18	1	0	3.951285	-2.025407	-3.442179
19	1	0	1.487810	-2.428665	-4.349194
20	1	0	2.232972	-3.714093	-3.419535
21	1	0	-0.336303	1.279355	2.367725
22	1	0	-1.907788	-0.349056	4.390581
23	1	0	-1.987763	1.371708	4.045005
24	1	0	-3.984421	-0.059994	3.140933
25	1	0	-3.179705	0.898067	1.895788
26	29	0	0.089227	0.291711	-0.497140
27	1	0	2.801136	-0.717478	-3.165499
28	6	0	0.084029	-3.952749	-1.928110
29	1	0	-2.460019	-1.976311	2.642490
30	6	0	-3.592619	-1.789461	0.867974
31	6	0	0.699606	-0.108523	3.577789
32	6	0	4.288492	-1.165346	-0.734984
33	6	0	4.126514	0.108261	-0.174745
34	6	0	5.213116	0.770531	0.405121
35	6	0	6.471435	0.170070	0.445238
36	6	0	6.641771	-1.103763	-0.102158
37	6	0	5.559282	-1.762021	-0.683558
38	6	0	0.857571	-5.093267	-1.653411
39	6	0	-1.310933	-4.062243	-1.808911
40	6	0	-1.913264	-5.263942	-1.433356
41	6	0	-1.130144	-6.388483	-1.167955
42	6	0	0.258321	-6.297037	-1.279474
43	6	0	-4.217143	-3.016165	1.138396
44	6	0	-3.907046	-1.135828	-0.333280
45	6	0	-4.822956	-1.689883	-1.229311
46	6	0	-5.441843	-2.910299	-0.945284
47	6	0	-5.135235	-3.572073	0.244602
48	6	0	1.941970	0.423660	3.188775
49	6	0	3.119791	0.040963	3.830624
50	6	0	3.082220	-0.876623	4.883029
51	6	0	1.856528	-1.410307	5.281736
52	6	0	0.678205	-1.034120	4.632426
53	1	0	-3.440202	-0.185943	-0.568088
54	1	0	-5.051423	-1.163259	-2.151963
55	1	0	-6.156336	-3.338403	-1.642621
56	1	0	-5.611491	-4.519629	0.481573
57	1	0	-3.986267	-3.539774	2.063292
58	1	0	0.879603	-7.165035	-1.076411
59	1	0	1.940080	-5.048860	-1.735732
60	1	0	-1.595667	-7.326428	-0.879387
61	1	0	-2.994549	-5.313039	-1.347978
62	1	0	-1.934154	-3.194884	-2.011202
63	1	0	7.615104	-1.586019	-0.073614
64	1	0	5.699097	-2.755828	-1.103913
65	1	0	7.311929	0.687225	0.899600
66	1	0	5.067353	1.764615	0.817558
67	1	0	3.156260	0.596656	-0.185997
68	1	0	4.067319	0.458006	3.502206
69	1	0	1.977189	1.133856	2.366089

70	1	0	3.998124	-1.171541	5.386962
71	1	0	1.812890	-2.122892	6.100994
72	1	0	-0.261930	-1.466257	4.962617
73	6	0	4.543785	5.485209	-1.179735
74	6	0	4.484132	4.134981	-1.540886
75	8	0	1.226050	1.862905	-0.058559
76	6	0	1.026048	3.110324	-0.322627
77	6	0	2.233299	3.956727	-0.624049
78	6	0	3.345988	3.383883	-1.264565
79	6	0	2.305490	5.314073	-0.270158
80	6	0	3.449159	6.068427	-0.543325
81	1	0	3.481462	7.115328	-0.253380
82	1	0	5.432032	6.072694	-1.394357
83	1	0	5.328412	3.666594	-2.039751
84	1	0	3.300536	2.340456	-1.551168
85	1	0	1.472375	5.792113	0.233038
86	6	0	-0.127218	3.776759	0.419111
87	1	0	-0.407362	4.749587	0.010162
88	1	0	-1.003266	3.127697	0.389673
89	1	0	0.163867	3.918696	1.469588
90	6	0	-1.150717	1.081852	-2.067770
91	6	0	-2.320379	1.750354	-1.603093
92	6	0	-3.318367	2.345981	-1.228486
93	6	0	-0.087960	1.840763	-2.607865
94	6	0	0.167424	3.189929	-2.355143
95	1	0	-0.673313	3.826344	-2.097981
96	1	0	0.954502	3.670918	-2.924103
97	1	0	-1.329366	0.102786	-2.516812
98	1	0	0.666048	1.270774	-3.150686
99	6	0	-4.467083	3.066860	-0.792774
100	6	0	-4.445427	4.477440	-0.734618
101	6	0	-5.650403	2.397608	-0.412272
102	6	0	-5.564886	5.186812	-0.309261
103	1	0	-3.542501	5.002181	-1.030193
104	6	0	-6.765389	3.117067	0.009874
105	1	0	-5.681185	1.313415	-0.449699
106	6	0	-6.730526	4.512740	0.064739
107	1	0	-5.528607	6.272147	-0.272047
108	1	0	-7.667514	2.584286	0.298075
109	1	0	-7.602960	5.069625	0.393899
110	1	0	-0.102531	-2.000692	-2.715280

SCF Done: E(RB3LYP) = -4450.61169795 A.U.

L_{ph}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.189434	0.966811	1.185956

2	6	0	-0.222511	2.400349	1.908883
3	6	0	1.233678	1.979357	2.178449
4	15	0	1.995702	1.258050	0.624058
5	6	0	3.461000	0.192655	1.209849
6	6	0	4.738926	1.011897	0.888356
7	6	0	4.401072	2.513079	0.813558
8	6	0	3.082597	2.700976	0.033641
9	6	0	-1.808394	0.144141	2.764844
10	6	0	-3.032768	1.009152	3.170628
11	6	0	-3.845615	1.326652	1.904867
12	6	0	-2.890950	1.694397	0.731440
13	1	0	-0.257952	3.213071	1.176088
14	1	0	-0.689872	2.779796	2.824126
15	1	0	1.815458	2.827728	2.557005
16	1	0	1.264651	1.204568	2.950053
17	1	0	5.528322	0.817718	1.621143
18	1	0	5.219618	3.095008	0.374063
19	1	0	4.256146	2.900455	1.829002
20	1	0	-2.676617	1.939269	3.629875
21	1	0	-3.642204	0.495768	3.922560
22	1	0	-4.572672	2.124152	2.087039
23	1	0	-4.420035	0.440369	1.618303
24	29	0	0.222854	0.054110	-0.314957
25	1	0	5.125535	0.674690	-0.078352
26	6	0	3.175056	2.760096	-1.482551
27	6	0	-2.835696	3.151102	0.321867
28	6	0	-2.145661	-1.330285	2.640512
29	1	0	2.577646	3.616022	0.365565
30	6	0	3.297327	-0.323089	2.624461
31	6	0	2.484932	-1.450963	2.836578
32	6	0	2.275311	-1.949075	4.122589
33	6	0	2.877746	-1.334982	5.223718
34	6	0	3.688114	-0.216569	5.025203
35	6	0	3.891620	0.287505	3.738195
36	6	0	2.036194	3.145838	-2.211358
37	6	0	4.339565	2.458340	-2.200158
38	6	0	4.364930	2.531981	-3.596379
39	6	0	3.226455	2.912021	-4.303882
40	6	0	2.058527	3.223908	-3.602022
41	6	0	-3.003982	4.204348	1.234144
42	6	0	-2.588861	3.476224	-1.022707
43	6	0	-2.507528	4.805568	-1.439964
44	6	0	-2.675765	5.842236	-0.520025
45	6	0	-2.927657	5.534696	0.818029
46	6	0	-2.741335	-1.880350	1.496064
47	6	0	-3.115564	-3.225215	1.460271
48	6	0	-2.887733	-4.050121	2.561999
49	6	0	-2.279003	-3.520563	3.701471
50	6	0	-1.914803	-2.174499	3.737886
51	1	0	-2.479974	2.673886	-1.748046
52	1	0	-2.324761	5.030016	-2.487225

53	1	0	-2.618487	6.877596	-0.843015
54	1	0	-3.067214	6.332327	1.542639
55	1	0	-3.201458	3.988637	2.280368
56	1	0	1.165020	3.529412	-4.139138
57	1	0	1.121971	3.392492	-1.676183
58	1	0	3.246366	2.968141	-5.388201
59	1	0	5.281630	2.291585	-4.127630
60	1	0	5.245509	2.171379	-1.677320
61	1	0	4.165347	0.267959	5.872850
62	1	0	4.523788	1.161534	3.608728
63	1	0	2.721095	-1.726412	6.224907
64	1	0	1.643515	-2.822074	4.260870
65	1	0	2.018249	-1.929493	1.978872
66	1	0	-3.584821	-3.621749	0.564624
67	1	0	-2.902537	-1.271710	0.611576
68	1	0	-3.176250	-5.096908	2.531640
69	1	0	-2.088078	-4.154346	4.563258
70	1	0	-1.444167	-1.769445	4.630823
71	6	0	4.914988	-4.200302	-2.497089
72	6	0	4.734930	-2.839392	-2.227964
73	8	0	1.119616	-1.675139	-0.429412
74	6	0	1.058896	-2.660377	-1.262140
75	6	0	2.385296	-3.223069	-1.709397
76	6	0	3.488794	-2.360901	-1.835033
77	6	0	2.577712	-4.584598	-1.988641
78	6	0	3.830622	-5.068035	-2.374829
79	1	0	3.956467	-6.128390	-2.577591
80	1	0	5.888055	-4.576338	-2.800293
81	1	0	5.570668	-2.151363	-2.327520
82	1	0	3.343529	-1.303922	-1.638267
83	1	0	1.751368	-5.281202	-1.895486
84	6	0	-0.093511	-3.637264	-1.060330
85	1	0	-0.236708	-4.322620	-1.899361
86	1	0	-1.013032	-3.071403	-0.903503
87	1	0	0.091719	-4.229716	-0.154155
88	6	0	-0.592065	0.228237	-2.292504
89	6	0	-1.926813	-0.264338	-2.232678
90	6	0	-3.081242	-0.664327	-2.213874
91	6	0	0.422279	-0.500884	-2.946969
92	6	0	0.428399	-1.880607	-3.171306
93	1	0	-0.534413	-2.380867	-3.221084
94	1	0	1.187620	-2.281494	-3.833532
95	1	0	-0.499529	1.314361	-2.341078
96	1	0	1.336013	0.057047	-3.148080
97	6	0	-4.412646	-1.166293	-2.170472
98	6	0	-4.669851	-2.541521	-2.366854
99	6	0	-5.508140	-0.308530	-1.929437
100	6	0	-5.971170	-3.034021	-2.315854
101	1	0	-3.836882	-3.208916	-2.564637
102	6	0	-6.805567	-0.811597	-1.879731
103	1	0	-5.327480	0.752799	-1.788637

104	6	0	-7.045744	-2.174718	-2.070716
105	1	0	-6.148132	-4.094813	-2.471059
106	1	0	-7.634826	-0.134694	-1.693130
107	1	0	-8.059315	-2.562678	-2.032022
108	1	0	-3.176491	1.123452	-0.155787
109	1	0	-1.016788	0.246635	3.515656
110	1	0	3.405317	-0.677935	0.551705

SCF Done: E(RB3LYP) = -4450.61460678 A.U.

L_{ph}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.036177	0.810762	-1.675177
2	6	0	-1.589866	1.670606	-2.012866
3	6	0	-2.747581	0.836569	-1.433897
4	15	0	-2.445265	0.461470	0.378957
5	6	0	-3.735349	-0.880770	0.825942
6	6	0	-4.676606	-0.189793	1.841363
7	6	0	-4.803521	1.306114	1.500661
8	6	0	-3.401475	1.890134	1.209809
9	6	0	0.296486	-0.230137	-3.240964
10	6	0	1.750315	0.108100	-3.651689
11	6	0	1.911633	1.627338	-3.530715
12	6	0	1.425125	2.031992	-2.121346
13	1	0	-1.546345	2.656144	-1.536302
14	1	0	-1.739824	1.842248	-3.084792
15	1	0	-3.708505	1.343729	-1.576959
16	1	0	-2.812566	-0.123314	-1.955181
17	1	0	-5.654055	-0.682624	1.869897
18	1	0	-5.307828	1.861894	2.298956
19	1	0	-5.419079	1.421479	0.601850
20	1	0	1.955583	-0.252794	-4.665545
21	1	0	2.451599	-0.401875	-2.979765
22	1	0	1.310878	2.117805	-4.306114
23	1	0	2.949601	1.944043	-3.681483
24	29	0	-0.176457	0.087386	0.467798
25	1	0	-4.244083	-0.301646	2.841069
26	6	0	-2.665559	2.504076	2.387283
27	6	0	1.117698	3.494101	-1.890688
28	6	0	-0.000528	-1.712315	-3.166986
29	1	0	-3.481204	2.670314	0.444706
30	6	0	-4.391351	-1.550610	-0.365762
31	6	0	-3.681947	-2.548082	-1.057479
32	6	0	-4.233918	-3.188258	-2.166274
33	6	0	-5.515258	-2.849417	-2.607297
34	6	0	-6.232668	-1.863799	-1.929786

35	6	0	-5.674905	-1.218458	-0.823444
36	6	0	-1.675566	3.469373	2.138714
37	6	0	-2.929707	2.166921	3.722459
38	6	0	-2.228299	2.770077	4.770189
39	6	0	-1.246426	3.724038	4.505606
40	6	0	-0.974052	4.073138	3.180984
41	6	0	0.411954	4.275864	-2.819886
42	6	0	1.542733	4.108883	-0.700757
43	6	0	1.269208	5.454231	-0.446830
44	6	0	0.565334	6.217175	-1.380114
45	6	0	0.140303	5.621595	-2.569209
46	6	0	0.458657	-2.515239	-2.112129
47	6	0	0.228085	-3.891700	-2.112306
48	6	0	-0.461377	-4.493341	-3.167877
49	6	0	-0.929239	-3.703997	-4.220404
50	6	0	-0.702483	-2.326538	-4.214917
51	1	0	2.105093	3.524324	0.022659
52	1	0	1.618174	5.907967	0.476855
53	1	0	0.355813	7.265309	-1.187065
54	1	0	-0.402923	6.206132	-3.306754
55	1	0	0.072814	3.834780	-3.752841
56	1	0	-0.216728	4.818753	2.956465
57	1	0	-1.452634	3.755700	1.113447
58	1	0	-0.701588	4.191921	5.320090
59	1	0	-2.455079	2.491739	5.795640
60	1	0	-3.696310	1.437335	3.961243
61	1	0	-7.232193	-1.593298	-2.259402
62	1	0	-6.258697	-0.459204	-0.312550
63	1	0	-5.949827	-3.349849	-3.467860
64	1	0	-3.656330	-3.948129	-2.683537
65	1	0	-2.682777	-2.820841	-0.726293
66	1	0	0.590299	-4.488648	-1.280198
67	1	0	0.968002	-2.068800	-1.265436
68	1	0	-0.633239	-5.566189	-3.169444
69	1	0	-1.468086	-4.158327	-5.047614
70	1	0	-1.068310	-1.719676	-5.040390
71	8	0	0.377210	-1.720998	1.014742
72	6	0	0.449829	-2.266754	2.169130
73	6	0	-0.836729	-2.385901	2.975606
74	6	0	1.505028	-3.317485	2.355441
75	6	0	1.476280	-4.253948	3.401963
76	6	0	2.558622	-3.392796	1.425640
77	6	0	1.198054	1.092593	1.748845
78	6	0	2.492621	0.923277	1.181130
79	6	0	3.611597	0.801679	0.705361
80	6	0	0.854874	0.437813	2.960807
81	6	0	1.452064	-0.708908	3.461894
82	1	0	2.446812	-0.970877	3.119821
83	1	0	1.187429	-1.054977	4.455952
84	1	0	0.764919	2.085157	1.621870
85	1	0	-0.037586	0.818017	3.455986

86	6	0	4.907810	0.612947	0.149606
87	6	0	5.655246	-0.548329	0.446851
88	6	0	5.480800	1.575706	-0.710062
89	6	0	6.921363	-0.734708	-0.100797
90	1	0	5.225815	-1.294642	1.107988
91	6	0	6.747249	1.378313	-1.254045
92	1	0	4.922159	2.478465	-0.938639
93	6	0	7.475148	0.223959	-0.954015
94	1	0	7.480869	-1.634588	0.140360
95	1	0	7.170315	2.131880	-1.912962
96	1	0	8.463895	0.074259	-1.377819
97	1	0	2.203592	1.743819	-1.408018
98	1	0	-0.362699	0.207217	-4.002395
99	1	0	-3.151766	-1.648261	1.340819
100	6	0	3.547276	-4.366094	1.541093
101	6	0	3.506704	-5.293078	2.587623
102	6	0	2.466720	-5.230964	3.515538
103	1	0	2.584141	-2.667979	0.619865
104	1	0	4.351019	-4.405450	0.810464
105	1	0	4.276815	-6.054034	2.677244
106	1	0	2.421982	-5.947175	4.331659
107	1	0	0.677242	-4.231124	4.135367
108	1	0	-1.450391	-3.194565	2.553422
109	1	0	-0.675145	-2.600512	4.033096
110	1	0	-1.395623	-1.451889	2.895775

SCF Done: E(RB3LYP) = -4450.62266716 A.U.

Part III :(S, S)- Me- BPE–CuMes system

S17. The summarize energies of TS2s in the *(S, S)*-Me-BPE-CuMes system in the gas-phase at the M06/6-31G(d,p) level.

M06/6-31G(d,p)

specises	***Ggas***	ΔG_{gas}	ΔGr*(*kJ.mol^{-1}*)*
L_{Me}-*right-si*-TS	-3681.045207	0.0	0.0
L_{Me}-*right-re*-TS2	-3681.037947	0.00726	19.1
L_{Me}-*left-si*-TS2	-3681.037452	0.007755	20.4
L_{Me}-*left-re*-TS2	-3681.04352	0.001681	4.4

S18. Cartesian coordinates and energies of TS2s optimized stationary points of *(S, S)*-Me-BPE-CuMes reaction system in the gas-phase at the M06 /6-31G(d, p) level.

L_{Me}-*right-si*-TS2:

Standard orientation:

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

1	15	0	0.862972	-1.655879	0.975156
2	6	0	2.572502	-2.181489	1.489068
3	6	0	3.597817	-1.056575	1.372513
4	15	0	3.305033	0.100988	-0.067591
5	6	0	4.671762	1.348464	0.254979
6	6	0	5.569006	1.275531	-0.983310
7	6	0	5.639801	-0.183299	-1.411953
8	6	0	4.196775	-0.672152	-1.520416
9	6	0	-0.110581	-1.200341	2.500806
10	6	0	-0.903071	-2.457985	2.860870
11	6	0	-1.278354	-3.133327	1.544991
12	6	0	0.026505	-3.308165	0.766113
13	1	0	2.822577	-2.992650	0.788439
14	1	0	2.573082	-2.624947	2.494915
15	1	0	4.625451	-1.448623	1.353861
16	1	0	3.530965	-0.395529	2.251082
17	1	0	5.240545	0.968208	1.118392
18	1	0	6.556121	1.714278	-0.787541
19	1	0	6.184831	-0.323421	-2.355382
20	1	0	6.170961	-0.772559	-0.646079
21	1	0	-0.805416	-0.436612	2.117347
22	1	0	-0.268348	-3.137067	3.456160
23	1	0	-1.778111	-2.214511	3.477874
24	1	0	-1.791405	-4.094403	1.684976
25	1	0	-1.962195	-2.482762	0.973692
26	29	0	1.095594	0.159555	-0.306123
27	1	0	5.111069	1.869237	-1.791888
28	1	0	0.644519	-4.043429	1.309902
29	1	0	3.734861	-0.184519	-2.395499
30	6	0	0.151097	0.173682	-2.156893
31	6	0	-1.122391	-0.414105	-1.929018
32	6	0	-2.228042	-0.882194	-1.710947
33	6	0	0.230243	1.572701	-2.363771
34	6	0	-0.758094	2.480687	-2.031014
35	1	0	-1.781664	2.115616	-1.962004
36	1	0	-0.645229	3.524546	-2.317529
37	1	0	0.877882	-0.447587	-2.691604
38	1	0	1.207677	1.946023	-2.686155
39	6	0	-3.526247	-1.378289	-1.415401
40	6	0	-4.596088	-0.482924	-1.238063
41	6	0	-3.776043	-2.754971	-1.279585
42	6	0	-5.863736	-0.950698	-0.922309
43	1	0	-4.407575	0.584310	-1.341891
44	6	0	-5.049005	-3.213720	-0.969115
45	1	0	-2.957221	-3.458205	-1.421901
46	6	0	-6.098527	-2.316884	-0.785939
47	1	0	-6.676607	-0.239803	-0.785373
48	1	0	-5.223813	-4.283022	-0.868954
49	1	0	-7.093839	-2.680710	-0.541646
50	6	0	-4.606338	3.527047	1.097753
51	6	0	-3.700550	4.560217	0.885656
52	8	0	-0.143675	1.430434	0.542977
53	6	0	-0.510873	2.592698	0.195507

54	6	0	0.527528	3.686944	0.177047
55	6	0	-1.929951	2.955576	0.480102
56	6	0	-2.373215	4.277763	0.577412
57	6	0	-2.852557	1.922153	0.689388
58	6	0	-4.175911	2.204961	0.994727
59	1	0	-4.878197	1.387340	1.150056
60	1	0	-5.643544	3.749231	1.339085
61	1	0	-4.026166	5.595557	0.962783
62	1	0	-1.677608	5.099721	0.422363
63	1	0	-2.508239	0.893004	0.587032
64	1	0	1.441343	3.297782	-0.280192
65	1	0	0.217615	4.584882	-0.364171
66	1	0	0.762317	3.971490	1.214308
67	6	0	-0.113654	-3.736684	-0.681816
68	1	0	-0.644350	-2.973050	-1.264428
69	1	0	0.868335	-3.885798	-1.150601
70	1	0	-0.662637	-4.684709	-0.761682
71	6	0	0.708847	-0.584527	3.617189
72	1	0	1.467488	-1.280959	4.001027
73	1	0	1.218757	0.326800	3.277438
74	1	0	0.067382	-0.306097	4.462401
75	6	0	4.027026	-2.172630	-1.656645
76	1	0	4.464148	-2.705241	-0.801193
77	1	0	2.967236	-2.450962	-1.728181
78	1	0	4.529262	-2.540985	-2.559734
79	6	0	4.150076	2.737721	0.563577
80	1	0	4.970943	3.433447	0.778706
81	1	0	3.588530	3.135264	-0.292797
82	1	0	3.470824	2.733142	1.425849

Zero-point correction= 0.697599 (Hartree/Particle)
Thermal correction to Energy= 0.736981
Thermal correction to Enthalpy= 0.737925
Thermal correction to Gibbs Free Energy= 0.627114
Sum of electronic and zero-point Energies= -3680.974722
Sum of electronic and thermal Energies= -3680.935340
Sum of electronic and thermal Enthalpies= -3680.934396
Sum of electronic and thermal Free Energies= -3681.045207

L_{Me}-*right-re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.063039	-1.813473	1.347439
2	6	0	1.136806	-3.240835	1.279918
3	6	0	2.521200	-2.839826	0.776224
4	15	0	2.452092	-1.559901	-0.576239
5	6	0	4.244756	-1.048163	-0.706012
6	6	0	4.645241	-1.406728	-2.140832
7	6	0	3.953312	-2.717137	-2.496735
8	6	0	2.472577	-2.521182	-2.175721

9	6	0	0.087862	-1.092583	3.067019
10	6	0	-0.947204	-1.844458	3.904143
11	6	0	-2.159716	-2.060005	3.007237
12	6	0	-1.659101	-2.711901	1.716386
13	1	0	0.671369	-3.951138	0.580135
14	1	0	1.193607	-3.750010	2.252435
15	1	0	3.112009	-3.715782	0.471703
16	1	0	3.080550	-2.343442	1.583017
17	1	0	4.816408	-1.687052	-0.013615
18	1	0	5.736145	-1.453424	-2.252185
19	1	0	4.105496	-3.007237	-3.545286
20	1	0	4.359024	-3.534259	-1.876862
21	1	0	-0.252104	-0.053018	2.938044
22	1	0	-0.535401	-2.819749	4.214760
23	1	0	-1.191022	-1.296336	4.824333
24	1	0	-2.944306	-2.664136	3.481003
25	1	0	-2.611213	-1.084051	2.761628
26	29	0	0.595413	-0.378067	-0.215563
27	1	0	4.289341	-0.613544	-2.819610
28	1	0	-1.393220	-3.758729	1.939273
29	6	0	2.347159	6.169137	0.587089
30	6	0	3.036810	4.959259	0.582277
31	8	0	0.963034	1.383395	0.605955
32	6	0	0.251138	2.419270	0.411644
33	6	0	0.943685	3.741320	0.480423
34	6	0	2.341598	3.758802	0.531494
35	6	0	0.260502	4.962223	0.488319
36	6	0	0.956310	6.164094	0.540391
37	1	0	0.407706	7.103773	0.543828
38	1	0	2.890255	7.110865	0.626871
39	1	0	4.124348	4.953263	0.622070
40	1	0	2.862080	2.803850	0.535217
41	1	0	-0.826166	4.979808	0.438488
42	6	0	-1.194079	2.342863	0.853539
43	1	0	-1.821022	3.167415	0.502823
44	1	0	-1.637751	1.401087	0.509523
45	1	0	-1.207290	2.348702	1.953992
46	6	0	-0.468050	0.035522	-1.980888
47	6	0	-1.872116	0.074866	-1.777355
48	6	0	-3.076744	0.122803	-1.596214
49	6	0	0.254311	1.237333	-2.153828
50	6	0	-0.142617	2.508187	-1.759692
51	1	0	-1.212415	2.705686	-1.683055
52	1	0	0.470087	3.351452	-2.067748
53	1	0	-0.105036	-0.829258	-2.546530
54	1	0	1.283287	1.110862	-2.507102
55	6	0	-4.469864	0.176126	-1.328797
56	6	0	-5.066429	1.366015	-0.878046
57	6	0	-5.277401	-0.962703	-1.489634
58	6	0	-6.424531	1.409766	-0.597137
59	1	0	-4.441893	2.248819	-0.754102
60	6	0	-6.634929	-0.909422	-1.207464
61	1	0	-4.817713	-1.885851	-1.838037

62	6	0	-7.215598	0.274786	-0.759484
63	1	0	-6.870880	2.338518	-0.247772
64	1	0	-7.246429	-1.799805	-1.337914
65	1	0	-8.279702	0.313470	-0.538631
66	1	0	2.057081	-1.812751	-2.912686
67	6	0	1.493893	-1.071503	3.635136
68	1	0	1.906276	-2.085308	3.736265
69	1	0	2.171660	-0.481310	3.004880
70	1	0	1.499350	-0.619282	4.634731
71	6	0	-2.642721	-2.655575	0.564255
72	1	0	-2.894087	-1.614548	0.324059
73	1	0	-2.222741	-3.097311	-0.350168
74	1	0	-3.571494	-3.188432	0.805566
75	6	0	1.624804	-3.778616	-2.176363
76	1	0	0.574752	-3.556253	-1.942294
77	1	0	1.649643	-4.266173	-3.158587
78	1	0	1.989948	-4.509131	-1.441598
79	6	0	4.441577	0.413343	-0.344324
80	1	0	4.130334	0.615620	0.688638
81	1	0	5.490925	0.715156	-0.453914
82	1	0	3.828520	1.055924	-0.991710

Zero-point correction= 0.698234 (Hartree/Particle)
Thermal correction to Energy= 0.737290
Thermal correction to Enthalpy= 0.738234
Thermal correction to Gibbs Free Energy= 0.628035
Sum of electronic and zero-point Energies= -3680.967748
Sum of electronic and thermal Energies= -3680.928692
Sum of electronic and thermal Enthalpies= -3680.927748
Sum of electronic and thermal Free Energies= -3681.037947

L_{Me}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.107045	-1.584106	-0.640971
2	6	0	-0.208837	-3.182053	-0.993529
3	6	0	1.244474	-2.893090	-1.366627
4	15	0	2.028650	-1.805622	-0.079949
5	6	0	3.824529	-1.639186	-0.554922
6	6	0	4.464204	-1.689964	0.836722
7	6	0	3.915912	-2.926122	1.550971
8	6	0	2.386421	-2.983017	1.345416
9	6	0	-1.876872	-1.206614	-2.298404
10	6	0	-3.192388	-1.990772	-2.276004
11	6	0	-3.810697	-1.804102	-0.892394
12	6	0	-2.727938	-2.080955	0.168475
13	1	0	-0.234868	-3.794858	-0.081614
14	1	0	-0.707032	-3.763124	-1.781811
15	1	0	1.808259	-3.825480	-1.503047
16	1	0	1.290245	-2.335372	-2.314967

17	1	0	5.561008	-1.700936	0.772328
18	1	0	4.161105	-2.908829	2.621111
19	1	0	4.388080	-3.827460	1.140108
20	1	0	-2.998321	-3.059962	-2.452421
21	1	0	-3.869338	-1.655835	-3.074695
22	1	0	-4.674736	-2.465425	-0.740181
23	1	0	-4.185693	-0.776265	-0.785658
24	29	0	0.478496	-0.210561	0.225187
25	1	0	4.184180	-0.785000	1.400513
26	1	0	2.081879	-3.995362	1.038834
27	6	0	5.252319	3.374683	-0.300712
28	6	0	4.731040	2.092400	-0.139306
29	8	0	0.663962	1.445946	-0.826335
30	6	0	1.026823	2.637732	-0.601702
31	6	0	2.485908	2.938088	-0.486277
32	6	0	3.363975	1.879632	-0.237865
33	6	0	3.017171	4.220562	-0.648361
34	6	0	4.388860	4.435194	-0.557066
35	1	0	4.786425	5.439369	-0.689580
36	1	0	6.324009	3.545698	-0.228001
37	1	0	5.395204	1.251885	0.061407
38	1	0	2.925444	0.891870	-0.118787
39	1	0	2.357408	5.061935	-0.850572
40	6	0	0.111768	3.720204	-1.124222
41	1	0	0.224311	4.682409	-0.615167
42	1	0	-0.919834	3.372322	-1.008002
43	1	0	0.305810	3.872100	-2.196167
44	6	0	-0.206598	0.700368	1.971531
45	6	0	-1.560037	0.991374	1.648463
46	6	0	-2.728781	1.208172	1.372897
47	6	0	0.735981	1.747539	2.087749
48	6	0	0.590083	3.011323	1.550288
49	1	0	-0.423236	3.358365	1.349306
50	1	0	1.324538	3.780017	1.780304
51	1	0	-0.069440	-0.147285	2.649641
52	1	0	1.701571	1.466067	2.518757
53	6	0	-4.085924	1.370283	0.985065
54	6	0	-4.447517	2.270138	-0.032758
55	6	0	-5.096009	0.595564	1.583510
56	6	0	-5.767957	2.372266	-0.448496
57	1	0	-3.672805	2.879477	-0.493881
58	6	0	-6.412814	0.701001	1.158755
59	1	0	-4.825029	-0.093053	2.381593
60	6	0	-6.755911	1.586102	0.139503
61	1	0	-6.028169	3.070091	-1.241529
62	1	0	-7.179848	0.089568	1.629478
63	1	0	-7.788467	1.665942	-0.192051
64	1	0	-2.844979	-1.391851	1.014925
65	1	0	-1.194656	-1.582201	-3.076050
66	1	0	3.969341	-0.650451	-1.009317
67	6	0	-2.772035	-3.508717	0.691934
68	1	0	-1.965664	-3.716529	1.406940
69	1	0	-3.720842	-3.684333	1.214166

70	1	0	-2.705166	-4.246992	-0.118393
71	6	0	-2.079570	0.292860	-2.481820
72	1	0	-2.538782	0.500219	-3.457081
73	1	0	-2.742142	0.706392	-1.708694
74	1	0	-1.130430	0.836533	-2.408693
75	6	0	1.617493	-2.587973	2.597717
76	1	0	0.531897	-2.577303	2.429360
77	1	0	1.825972	-3.281013	3.422613
78	1	0	1.905782	-1.578100	2.923601
79	6	0	4.370317	-2.703553	-1.495433
80	1	0	4.191383	-3.721777	-1.126972
81	1	0	3.923554	-2.632291	-2.493306
82	1	0	5.455581	-2.584754	-1.612888

Zero-point correction= 0.698800 (Hartree/Particle)
Thermal correction to Energy= 0.737779
Thermal correction to Enthalpy= 0.738723
Thermal correction to Gibbs Free Energy= 0.629620
Sum of electronic and zero-point Energies= -3680.968272
Sum of electronic and thermal Energies= -3680.929293
Sum of electronic and thermal Enthalpies= -3680.928349
Sum of electronic and thermal Free Energies= -3681.037452

L_{Me}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.694122	-2.051269	-0.515014
2	6	0	2.428143	-2.587729	-0.938253
3	6	0	3.194684	-1.387195	-1.497196
4	15	0	3.111031	0.004103	-0.264102
5	6	0	3.992983	1.459754	-1.019423
6	6	0	4.791438	1.955305	0.192446
7	6	0	5.508889	0.749362	0.800084
8	6	0	4.495768	-0.403479	0.939705
9	6	0	-0.249824	-2.357345	-2.102275
10	6	0	-1.267895	-3.448210	-1.742186
11	6	0	-0.629208	-4.385473	-0.725153
12	6	0	-0.058698	-3.497051	0.378825
13	1	0	2.908689	-2.927343	-0.008154
14	1	0	2.436513	-3.434472	-1.638344
15	1	0	4.232826	-1.649754	-1.742662
16	1	0	2.713694	-1.033664	-2.422807
17	1	0	5.489396	2.755037	-0.089690
18	1	0	5.953460	0.996232	1.773591
19	1	0	6.338840	0.448340	0.147263
20	1	0	-1.623179	-3.969691	-2.640351
21	1	0	-2.147837	-2.968935	-1.281651
22	1	0	0.187205	-4.959932	-1.194801
23	1	0	-1.344620	-5.117928	-0.324379
24	29	0	0.956402	-0.006139	0.346293

25	1	0	4.099478	2.382435	0.936195
26	1	0	4.952090	-1.357029	0.635020
27	8	0	-0.062558	1.466931	-0.475115
28	6	0	-0.207093	2.661069	-0.083426
29	6	0	1.025530	3.526714	0.035370
30	6	0	-1.512065	3.319627	-0.383867
31	6	0	-1.695957	4.704822	-0.350077
32	6	0	-2.599038	2.508169	-0.732819
33	6	0	0.020449	0.087735	2.196968
34	6	0	-1.274005	-0.376411	1.842157
35	6	0	-2.380416	-0.757001	1.494551
36	6	0	0.228824	1.461753	2.470717
37	6	0	-0.626668	2.486278	2.114683
38	1	0	-1.673906	2.242000	1.943694
39	1	0	-0.425711	3.499866	2.457073
40	1	0	0.653030	-0.620131	2.741628
41	1	0	1.211730	1.714084	2.880834
42	6	0	-3.649172	-1.159738	1.003143
43	6	0	-4.610945	-0.195911	0.649108
44	6	0	-3.971183	-2.518714	0.838624
45	6	0	-5.838516	-0.582875	0.131337
46	1	0	-4.369947	0.857593	0.784567
47	6	0	-5.203161	-2.896006	0.321830
48	1	0	-3.239340	-3.272591	1.127908
49	6	0	-6.141857	-1.932145	-0.038220
50	1	0	-6.568478	0.177919	-0.139592
51	1	0	-5.434083	-3.952422	0.200774
52	1	0	-7.105858	-2.231234	-0.442907
53	1	0	-0.897046	-3.036110	0.926803
54	1	0	0.471053	-2.761769	-2.831883
55	1	0	3.225809	2.194322	-1.299050
56	6	0	-3.832430	3.064902	-1.036052
57	6	0	-4.005331	4.448028	-1.002666
58	6	0	-2.932667	5.263197	-0.659051
59	1	0	-2.448108	1.430368	-0.747027
60	1	0	-4.664450	2.414550	-1.303317
61	1	0	-4.971372	4.886838	-1.242386
62	1	0	-3.056687	6.343787	-0.631188
63	1	0	-0.870273	5.361459	-0.083866
64	1	0	1.325213	3.859555	-0.970444
65	1	0	0.888085	4.413076	0.660262
66	1	0	1.841285	2.925999	0.452287
67	6	0	-0.891959	-1.094305	-2.648804
68	1	0	-1.562131	-0.651614	-1.899843
69	1	0	-0.146903	-0.328989	-2.896508
70	1	0	-1.480135	-1.311682	-3.549706
71	6	0	0.858861	-4.180445	1.373161
72	1	0	1.693904	-4.686783	0.871130
73	1	0	1.277736	-3.462032	2.090672
74	1	0	0.315185	-4.939820	1.948080
75	6	0	3.954179	-0.542734	2.355061
76	1	0	3.185300	-1.323706	2.416753
77	1	0	4.754451	-0.792783	3.063041

78	1	0	3.486499	0.393972	2.689560
79	6	0	4.871609	1.164926	-2.225838
80	1	0	4.283485	0.823834	-3.084828
81	1	0	5.408637	2.071179	-2.535425
82	1	0	5.624387	0.394822	-2.015929

Zero-point correction= 0.698350 (Hartree/Particle)
Thermal correction to Energy= 0.737317
Thermal correction to Enthalpy= 0.738261
Thermal correction to Gibbs Free Energy= 0.628998
Sum of electronic and zero-point Energies= -3680.974174
Sum of electronic and thermal Energies= -3680.935207
Sum of electronic and thermal Enthalpies= -3680.934263
Sum of electronic and thermal Free Energies= -3681.043526

S19: The summarize energies of TS2s in the *(S, S)*-Me-BPE-CuMes system in the gas-phase at the B3LYP/6-31G (d, p) level.

B3LYP/6-31G (d, p)

specises	G_{gas}	ΔG_{gas}	ΔGr(kJ.mol^{-1})
L_{Me}-*right-si*-TS2	-3682.228895	0.0	0.0
L_{Me}-*right-re*-TS2	-3682.224056	0.004839	12.7
L_{Me}-*left-si*-TS2	-3682.220327	0.008568	22.5
L_{Me}-*left-re*-TS2	-3682.227498	0.001397	3.7

S20:Cartesian coordinates and energies of TS2s optimized stationary points of *(S, S)*-Me-BPE-CuMes reaction system in the gas-phase at the B3LYP/6-31G (d, p) level.

L_{Me}-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.976156	-1.508677	1.356984
2	6	0	2.744719	-2.099797	1.545140
3	6	0	3.789151	-1.056460	1.115984
4	15	0	3.280701	-0.010800	-0.363480
5	6	0	4.727000	1.221273	-0.381993
6	6	0	5.471898	0.968053	-1.710405
7	6	0	5.394476	-0.529656	-2.026022
8	6	0	3.919349	-0.944326	-1.876596
9	6	0	0.434813	-0.795786	3.016789
10	6	0	-0.243304	-1.958310	3.767626
11	6	0	-0.974194	-2.812411	2.722846
12	6	0	0.030856	-3.124790	1.595733
13	1	0	2.811766	-2.980904	0.897204
14	1	0	2.944702	-2.446367	2.565754
15	1	0	4.762816	-1.530250	0.942118

16	1	0	3.935160	-0.328616	1.923234
17	1	0	5.387820	0.925854	0.443995
18	1	0	6.505357	1.329782	-1.655636
19	1	0	5.772569	-0.761021	-3.029444
20	1	0	6.012965	-1.096222	-1.315800
21	1	0	-0.332378	-0.066839	2.729047
22	1	0	0.516627	-2.568492	4.276525
23	1	0	-0.921376	-1.583196	4.543774
24	1	0	-1.381408	-3.736167	3.150618
25	1	0	-1.822036	-2.249249	2.310869
26	29	0	1.003158	0.122642	-0.221657
27	1	0	4.981108	1.533298	-2.514542
28	1	0	0.757304	-3.851533	1.987069
29	1	0	3.358552	-0.498576	-2.710027
30	6	0	-0.030778	-0.000088	-2.089367
31	6	0	-1.312987	-0.586166	-1.891739
32	6	0	-2.425903	-1.067672	-1.752156
33	6	0	0.076407	1.384140	-2.373422
34	6	0	-0.870511	2.354316	-2.060902
35	1	0	-1.897540	2.037053	-1.920493
36	1	0	-0.739016	3.358483	-2.451252
37	1	0	0.696856	-0.646442	-2.584053
38	1	0	1.046397	1.711635	-2.749159
39	6	0	-3.733285	-1.600734	-1.575039
40	6	0	-4.795317	-0.771702	-1.150271
41	6	0	-4.005117	-2.964399	-1.820286
42	6	0	-6.074160	-1.293483	-0.976273
43	1	0	-4.598601	0.278381	-0.958498
44	6	0	-5.287778	-3.476071	-1.642144
45	1	0	-3.198736	-3.609957	-2.154310
46	6	0	-6.329425	-2.645986	-1.219737
47	1	0	-6.878374	-0.639425	-0.649822
48	1	0	-5.476482	-4.528392	-1.837367
49	1	0	-7.329424	-3.047821	-1.084326
50	6	0	-4.494913	3.856385	1.216924
51	6	0	-3.592073	4.823320	0.773956
52	8	0	-0.124726	1.530989	0.550132
53	6	0	-0.487307	2.676780	0.102969
54	6	0	0.589442	3.743297	-0.044159
55	6	0	-1.876172	3.122704	0.467040
56	6	0	-2.296061	4.461023	0.401820
57	6	0	-2.795944	2.158372	0.916394
58	6	0	-4.088830	2.519616	1.285245
59	1	0	-4.782555	1.757372	1.630678
60	1	0	-5.503199	4.139377	1.506103
61	1	0	-3.894265	5.865808	0.719042
62	1	0	-1.612855	5.232930	0.063538
63	1	0	-2.469942	1.125342	0.961742
64	1	0	1.478283	3.295048	-0.487422
65	1	0	0.286384	4.594911	-0.655696
66	1	0	0.859402	4.117706	0.953610
67	6	0	-0.595658	-3.685462	0.318492
68	1	0	-1.280353	-2.965009	-0.136120

69	1	0	0.167538	-3.930868	-0.428424
70	1	0	-1.152655	-4.604856	0.535141
71	6	0	1.513531	-0.054031	3.808051
72	1	0	2.341682	-0.713735	4.091372
73	1	0	1.919580	0.785857	3.235353
74	1	0	1.092255	0.354477	4.733817
75	6	0	3.670392	-2.454003	-1.892812
76	1	0	4.204063	-2.960984	-1.081631
77	1	0	2.605143	-2.689354	-1.800919
78	1	0	4.023616	-2.888129	-2.835258
79	6	0	4.316956	2.680378	-0.178898
80	1	0	5.198777	3.332003	-0.165571
81	1	0	3.664229	3.019728	-0.989447
82	1	0	3.777988	2.825019	0.762300

Zero-point correction= 0.699385 (Hartree/Particle)
Thermal correction to Energy= 0.740169
Thermal correction to Enthalpy= 0.741113
Thermal correction to Gibbs Free Energy= 0.622673
Sum of electronic and zero-point Energies= -3682.152183
Sum of electronic and thermal Energies= -3682.111400
Sum of electronic and thermal Enthalpies= -3682.110455
Sum of electronic and thermal Free Energies= -3682.228895

L_{Me}-*right-re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.125657	-1.909040	1.340651
2	6	0	1.080912	-3.341858	1.204377
3	6	0	2.466257	-2.938239	0.672239
4	15	0	2.400144	-1.630481	-0.673739
5	6	0	4.234333	-1.192891	-0.833802
6	6	0	4.616895	-1.565334	-2.282858
7	6	0	3.835048	-2.826067	-2.672157
8	6	0	2.360259	-2.570982	-2.308196
9	6	0	0.007543	-1.261779	3.108784
10	6	0	-1.037002	-2.053516	3.919138
11	6	0	-2.250422	-2.271232	3.005759
12	6	0	-1.732316	-2.847260	1.672148
13	1	0	0.604849	-4.041189	0.507558
14	1	0	1.172978	-3.868903	2.161262
15	1	0	3.029666	-3.820756	0.346534
16	1	0	3.047774	-2.472300	1.476378
17	1	0	4.774486	-1.866070	-0.154385
18	1	0	5.700418	-1.700361	-2.379805
19	1	0	3.945848	-3.069683	-3.736011
20	1	0	4.212780	-3.690351	-2.107630
21	1	0	-0.336858	-0.224041	3.021402
22	1	0	-0.618838	-3.025382	4.217978

23	1	0	-1.302625	-1.525116	4.842842
24	1	0	-2.996654	-2.936992	3.455062
25	1	0	-2.749861	-1.310915	2.820078
26	29	0	0.553517	-0.373750	-0.172150
27	1	0	4.338668	-0.742501	-2.955493
28	1	0	-1.443726	-3.892931	1.849328
29	6	0	2.969692	5.975389	0.668126
30	6	0	3.493792	4.684855	0.768123
31	8	0	0.988840	1.368249	0.637598
32	6	0	0.401875	2.497419	0.457614
33	6	0	1.267972	3.728823	0.515948
34	6	0	2.652097	3.576125	0.693858
35	6	0	0.752660	5.033338	0.421322
36	6	0	1.593585	6.142682	0.494204
37	1	0	1.172793	7.141628	0.415014
38	1	0	3.623857	6.840910	0.726338
39	1	0	4.562204	4.542112	0.909846
40	1	0	3.043533	2.569740	0.782651
41	1	0	-0.311259	5.188509	0.273755
42	6	0	-1.013575	2.616249	1.017447
43	1	0	-1.540136	3.522363	0.712020
44	1	0	-1.604080	1.750483	0.712507
45	1	0	-0.944012	2.619582	2.114194
46	6	0	-0.647316	0.145565	-1.892583
47	6	0	-2.042750	0.253672	-1.637598
48	6	0	-3.246293	0.345525	-1.454829
49	6	0	0.143525	1.296888	-2.102346
50	6	0	-0.130645	2.598174	-1.673181
51	1	0	-1.169824	2.877545	-1.528956
52	1	0	0.516216	3.389900	-2.033407
53	1	0	-0.358986	-0.740948	-2.460384
54	1	0	1.129581	1.107593	-2.526533
55	6	0	-4.647881	0.464082	-1.240438
56	6	0	-5.210306	1.678140	-0.789085
57	6	0	-5.512792	-0.627145	-1.475214
58	6	0	-6.581830	1.790243	-0.579688
59	1	0	-4.556010	2.525062	-0.608408
60	6	0	-6.883301	-0.505131	-1.262626
61	1	0	-5.093600	-1.564116	-1.828270
62	6	0	-7.426441	0.701609	-0.813831
63	1	0	-6.994832	2.733502	-0.232529
64	1	0	-7.532124	-1.356470	-1.450248
65	1	0	-8.496234	0.793419	-0.650331
66	1	0	1.962909	-1.833836	-3.019774
67	6	0	1.415677	-1.239009	3.706335
68	1	0	1.842257	-2.245391	3.787520
69	1	0	2.091480	-0.622294	3.105755
70	1	0	1.392718	-0.813509	4.716131
71	6	0	-2.741064	-2.799596	0.524369
72	1	0	-3.015241	-1.771082	0.277201
73	1	0	-2.334630	-3.255477	-0.384952

74	1	0	-3.652974	-3.346771	0.791510
75	6	0	1.458818	-3.806304	-2.355053
76	1	0	0.421882	-3.559060	-2.104876
77	1	0	1.460447	-4.241925	-3.360673
78	1	0	1.800466	-4.583982	-1.663434
79	6	0	4.554889	0.254611	-0.455392
80	1	0	4.302784	0.460646	0.589099
81	1	0	5.622716	0.463515	-0.592045
82	1	0	3.987818	0.959135	-1.071424

Zero-point correction= 0.699954 (Hartree/Particle)
Thermal correction to Energy= 0.740543
Thermal correction to Enthalpy= 0.741487
Thermal correction to Gibbs Free Energy= 0.623731
Sum of electronic and zero-point Energies= -3682.147833
Sum of electronic and thermal Energies= -3682.107244
Sum of electronic and thermal Enthalpies= -3682.106300
Sum of electronic and thermal Free Energies= -3682.224056

L_{Me}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.978970	-1.962415	0.571798
2	6	0	-0.037863	-3.539730	0.579286
3	6	0	-1.500572	-3.226889	0.946077
4	15	0	-2.184543	-1.883201	-0.168315
5	6	0	-3.830461	-1.356433	0.598997
6	6	0	-4.870754	-1.674201	-0.503365
7	6	0	-4.459945	-2.987119	-1.190694
8	6	0	-2.967455	-2.873215	-1.575098
9	6	0	1.586781	-1.885911	2.353544
10	6	0	2.892756	-2.709232	2.342471
11	6	0	3.651467	-2.367271	1.049578
12	6	0	2.664765	-2.434699	-0.146961
13	1	0	0.005906	-3.974492	-0.425392
14	1	0	0.380472	-4.282537	1.268118
15	1	0	-2.112150	-4.135675	0.907161
16	1	0	-1.546304	-2.851470	1.974022
17	1	0	-5.881326	-1.733109	-0.082480
18	1	0	-5.083124	-3.199702	-2.068147
19	1	0	-4.599941	-3.822506	-0.493548
20	1	0	2.656380	-3.781166	2.358466
21	1	0	3.499160	-2.506539	3.233932
22	1	0	4.499877	-3.043269	0.890940
23	1	0	4.065929	-1.356317	1.122405
24	29	0	-0.401827	-0.389798	-0.276746
25	1	0	-4.884851	-0.864317	-1.242675
26	1	0	-2.499495	-3.864620	-1.604199

27	6	0	-4.636317	4.797328	0.488355
28	6	0	-4.647346	3.462789	0.070392
29	8	0	-1.201113	1.153397	0.611334
30	6	0	-1.012998	2.422862	0.485411
31	6	0	-2.253786	3.279468	0.490340
32	6	0	-3.473170	2.715745	0.077009
33	6	0	-2.256291	4.620716	0.905268
34	6	0	-3.435145	5.369769	0.906516
35	1	0	-3.411888	6.404539	1.238301
36	1	0	-5.552336	5.381432	0.487318
37	1	0	-5.576888	3.005237	-0.259205
38	1	0	-3.473673	1.681194	-0.247719
39	1	0	-1.336718	5.089646	1.238760
40	6	0	0.234532	2.985047	1.161524
41	1	0	0.483391	4.003203	0.853327
42	1	0	1.082362	2.335826	0.936242
43	1	0	0.080280	2.983697	2.249512
44	6	0	0.527833	0.512884	-1.979476
45	6	0	1.862021	0.839077	-1.601095
46	6	0	3.013886	1.107330	-1.297197
47	6	0	-0.448678	1.518368	-2.136191
48	6	0	-0.422284	2.793687	-1.561120
49	1	0	0.552773	3.218000	-1.340704
50	1	0	-1.167882	3.508322	-1.891645
51	1	0	0.434740	-0.350956	-2.639974
52	1	0	-1.365967	1.200573	-2.631282
53	6	0	4.346058	1.428109	-0.911847
54	6	0	4.622281	2.599761	-0.173406
55	6	0	5.425389	0.584323	-1.254803
56	6	0	5.925291	2.907614	0.207557
57	1	0	3.802041	3.258841	0.092683
58	6	0	6.725074	0.900158	-0.867372
59	1	0	5.229439	-0.313702	-1.832586
60	6	0	6.983626	2.061336	-0.134564
61	1	0	6.116378	3.814133	0.775369
62	1	0	7.541535	0.237818	-1.142250
63	1	0	7.998744	2.305522	0.164430
64	1	0	2.901674	-1.641510	-0.860988
65	1	0	0.831774	-2.361642	2.991488
66	1	0	-3.749850	-0.276426	0.749834
67	6	0	2.708956	-3.777311	-0.888953
68	1	0	1.984730	-3.817446	-1.709300
69	1	0	3.702992	-3.925345	-1.326005
70	1	0	2.512688	-4.625845	-0.224925
71	6	0	1.784372	-0.436885	2.820988
72	1	0	2.156624	-0.415759	3.851989
73	1	0	2.505295	0.097742	2.193892
74	1	0	0.845298	0.121808	2.779537
75	6	0	-2.746691	-2.188223	-2.931437
76	1	0	-1.680643	-2.104516	-3.164502
77	1	0	-3.226703	-2.757608	-3.735956
78	1	0	-3.161374	-1.174600	-2.945493
79	6	0	-4.182142	-1.993279	1.950672

80	1	0	-4.287988	-3.081631	1.888616
81	1	0	-3.429438	-1.770117	2.712579
82	1	0	-5.135579	-1.589330	2.310321

Zero-point correction= 0.700506 (Hartree/Particle)
Thermal correction to Energy= 0.740915
Thermal correction to Enthalpy= 0.741859
Thermal correction to Gibbs Free Energy= 0.623498
Sum of electronic and zero-point Energies= -3682.143319
Sum of electronic and thermal Energies= -3682.102909
Sum of electronic and thermal Enthalpies= -3682.101965
Sum of electronic and thermal Free Energies= -3682.220327

L_{Me}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.675213	-1.953949	0.847348
2	6	0	-2.379479	-2.720511	0.740378
3	6	0	-3.455743	-1.640683	0.964072
4	15	0	-3.180521	-0.178259	-0.188476
5	6	0	-4.396847	1.153652	0.411345
6	6	0	-5.549907	1.173694	-0.629578
7	6	0	-5.674044	-0.220271	-1.265968
8	6	0	-4.255891	-0.689583	-1.652706
9	6	0	-0.312571	-1.985395	2.702223
10	6	0	0.976303	-2.827756	2.827066
11	6	0	0.901793	-3.967464	1.802584
12	6	0	0.536823	-3.334725	0.445494
13	1	0	-2.486172	-3.147924	-0.263450
14	1	0	-2.504135	-3.540796	1.457006
15	1	0	-4.459499	-2.062542	0.837796
16	1	0	-3.391454	-1.269282	1.992193
17	1	0	-6.490621	1.487398	-0.162359
18	1	0	-6.344412	-0.210947	-2.134503
19	1	0	-6.110134	-0.917340	-0.539628
20	1	0	1.103922	-3.196024	3.851870
21	1	0	1.845615	-2.195038	2.604322
22	1	0	0.125125	-4.686464	2.100107
23	1	0	1.844720	-4.523741	1.737735
24	29	0	-0.892133	-0.000253	-0.265106
25	1	0	-5.329321	1.910951	-1.409589
26	1	0	-4.218548	-1.782763	-1.733554
27	8	0	-0.002612	1.546857	0.541299
28	6	0	0.129900	2.741673	0.100917
29	6	0	-1.142413	3.547504	-0.133030
30	6	0	1.367472	3.480750	0.525302
31	6	0	1.511088	4.872566	0.404210

32	6	0	2.428898	2.749441	1.088031
33	6	0	0.171955	0.040944	-2.103400
34	6	0	1.487002	-0.419348	-1.813204
35	6	0	2.617460	-0.819667	-1.584500
36	6	0	-0.068714	1.405245	-2.404943
37	6	0	0.727464	2.480504	-2.027530
38	1	0	1.768183	2.291050	-1.789740
39	1	0	0.510060	3.463410	-2.433721
40	1	0	-0.451592	-0.676893	-2.639453
41	1	0	-1.037075	1.616644	-2.858184
42	6	0	3.941656	-1.250002	-1.293708
43	6	0	4.895105	-0.343948	-0.778200
44	6	0	4.339327	-2.587170	-1.512462
45	6	0	6.190647	-0.765494	-0.492902
46	1	0	4.600597	0.686799	-0.606783
47	6	0	5.637488	-2.998864	-1.222132
48	1	0	3.619003	-3.290878	-1.918626
49	6	0	6.570644	-2.092859	-0.711550
50	1	0	6.909883	-0.053013	-0.097840
51	1	0	5.924176	-4.032094	-1.399459
52	1	0	7.583246	-2.416681	-0.489077
53	1	0	1.415876	-2.798003	0.068268
54	1	0	-1.132956	-2.545210	3.173009
55	1	0	-3.841174	2.094683	0.360994
56	6	0	3.593115	3.386557	1.508630
57	6	0	3.724823	4.772869	1.380880
58	6	0	2.677832	5.510979	0.827778
59	1	0	2.314314	1.675579	1.183355
60	1	0	4.400007	2.801929	1.943071
61	1	0	4.632475	5.271044	1.709990
62	1	0	2.766320	6.589408	0.726338
63	1	0	0.711686	5.470035	-0.021368
64	1	0	-1.549683	3.860602	0.838762
65	1	0	-0.995482	4.440070	-0.743550
66	1	0	-1.881884	2.910798	-0.622313
67	6	0	-0.214203	-0.601467	3.350560
68	1	0	0.511551	0.032011	2.832589
69	1	0	-1.172811	-0.073612	3.321072
70	1	0	0.086090	-0.690713	4.401540
71	6	0	0.087663	-4.322467	-0.632899
72	1	0	-0.782876	-4.906756	-0.315460
73	1	0	-0.166574	-3.810886	-1.567306
74	1	0	0.893166	-5.030972	-0.857317
75	6	0	-3.761678	-0.086108	-2.974861
76	1	0	-2.759041	-0.444336	-3.224051
77	1	0	-4.432800	-0.359980	-3.797209
78	1	0	-3.715616	1.007524	-2.935594
79	6	0	-4.889264	0.989177	1.855393
80	1	0	-4.058384	0.940279	2.566512
81	1	0	-5.508292	1.848701	2.136448
82	1	0	-5.498926	0.088917	1.984024

Zero-point correction= 0.700212 (Hartree/Particle)
Thermal correction to Energy= 0.740736
Thermal correction to Enthalpy= 0.741680
Thermal correction to Gibbs Free Energy= 0.623955
Sum of electronic and zero-point Energies= -3682.151241
Sum of electronic and thermal Energies= -3682.110718
Sum of electronic and thermal Enthalpies= -3682.109773
Sum of electronic and thermal Free Energies= -3682.227498

S21: The summarize energies of TS2s in the *(S, S)*-Me-BPE-CuMes system in the THF solvent at the M06/6-311+G (d, p).

M06(SMD,THF)/6-311+G (d, p)

species	**SCF_{SMD}**	G^*_{gas}	G_{sol}	ΔG_{sol}	ΔG_{sol}(kJ mol^{-1})
L_{Me}-*right-si*-TS2	-3682.25605895	0.627114	-3681.628944	0.0	0.0
L_{Me}-*right-re*-TS2	-3682.25164931	0.628035	-3681.623614	0.005063	13.3
L_{Me}-*left-si*-TS2	-3682.25196755	0.629620	-3681.622347	0.006597	17.3
L_{Me}-*left-re*-TS2	-3682.25767507	0.628998	-3681.628677	0.000267	0.7

S22:Cartesian coordinates and energies of TS2s optimized stationary points of *(S, S)*-Me-BPE-CuMes reaction system in THF solvent at the M06 /6-311+G(d, p) level.

L_{Me}-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.862972	-1.655879	0.975156
2	6	0	2.572502	-2.181489	1.489068
3	6	0	3.597817	-1.056575	1.372513
4	15	0	3.305033	0.100988	-0.067591
5	6	0	4.671762	1.348464	0.254979
6	6	0	5.569006	1.275531	-0.983310
7	6	0	5.639801	-0.183299	-1.411953
8	6	0	4.196775	-0.672152	-1.520416
9	6	0	-0.110581	-1.200341	2.500806
10	6	0	-0.903071	-2.457985	2.860870
11	6	0	-1.278354	-3.133327	1.544991
12	6	0	0.026505	-3.308165	0.766113
13	1	0	2.822577	-2.992650	0.788439
14	1	0	2.573082	-2.624947	2.494915
15	1	0	4.625451	-1.448623	1.353861
16	1	0	3.530965	-0.395529	2.251082
17	1	0	5.240545	0.968208	1.118392

18	1	0	6.556121	1.714278	-0.787541
19	1	0	6.184831	-0.323421	-2.355382
20	1	0	6.170961	-0.772559	-0.646079
21	1	0	-0.805416	-0.436612	2.117347
22	1	0	-0.268348	-3.137067	3.456160
23	1	0	-1.778111	-2.214511	3.477874
24	1	0	-1.791405	-4.094403	1.684976
25	1	0	-1.962195	-2.482762	0.973692
26	29	0	1.095594	0.159555	-0.306123
27	1	0	5.111069	1.869237	-1.791888
28	1	0	0.644519	-4.043429	1.309902
29	1	0	3.734861	-0.184519	-2.395499
30	6	0	0.151097	0.173682	-2.156893
31	6	0	-1.122391	-0.414105	-1.929018
32	6	0	-2.228042	-0.882194	-1.710947
33	6	0	0.230243	1.572701	-2.363771
34	6	0	-0.758094	2.480687	-2.031014
35	1	0	-1.781664	2.115616	-1.962004
36	1	0	-0.645229	3.524546	-2.317529
37	1	0	0.877882	-0.447587	-2.691604
38	1	0	1.207677	1.946023	-2.686155
39	6	0	-3.526247	-1.378289	-1.415401
40	6	0	-4.596088	-0.482924	-1.238063
41	6	0	-3.776043	-2.754971	-1.279585
42	6	0	-5.863736	-0.950698	-0.922309
43	1	0	-4.407575	0.584310	-1.341891
44	6	0	-5.049005	-3.213720	-0.969115
45	1	0	-2.957221	-3.458205	-1.421901
46	6	0	-6.098527	-2.316884	-0.785939
47	1	0	-6.676607	-0.239803	-0.785373
48	1	0	-5.223813	-4.283022	-0.868954
49	1	0	-7.093839	-2.680710	-0.541646
50	6	0	-4.606338	3.527047	1.097753
51	6	0	-3.700550	4.560217	0.885656
52	8	0	-0.143675	1.430434	0.542977
53	6	0	-0.510873	2.592698	0.195507
54	6	0	0.527528	3.686944	0.177047
55	6	0	-1.929951	2.955576	0.480102
56	6	0	-2.373215	4.277763	0.577412
57	6	0	-2.852557	1.922153	0.689388
58	6	0	-4.175911	2.204961	0.994727
59	1	0	-4.878197	1.387340	1.150056
60	1	0	-5.643544	3.749231	1.339085
61	1	0	-4.026166	5.595557	0.962783
62	1	0	-1.677608	5.099721	0.422363
63	1	0	-2.508239	0.893004	0.587032
64	1	0	1.441343	3.297782	-0.280192
65	1	0	0.217615	4.584882	-0.364171
66	1	0	0.762317	3.971490	1.214308
67	6	0	-0.113654	-3.736684	-0.681816
68	1	0	-0.644350	-2.973050	-1.264428

69	1	0	0.868335	-3.885798	-1.150601
70	1	0	-0.662637	-4.684709	-0.761682
71	6	0	0.708847	-0.584527	3.617189
72	1	0	1.467488	-1.280959	4.001027
73	1	0	1.218757	0.326800	3.277438
74	1	0	0.067382	-0.306097	4.462401
75	6	0	4.027026	-2.172630	-1.656645
76	1	0	4.464148	-2.705241	-0.801193
77	1	0	2.967236	-2.450962	-1.728181
78	1	0	4.529262	-2.540985	-2.559734
79	6	0	4.150076	2.737721	0.563577
80	1	0	4.970943	3.433447	0.778706
81	1	0	3.588530	3.135264	-0.292797
82	1	0	3.470824	2.733142	1.425849

SCF Done: E(RM06) = -3682.25605895 A.U.

L_{Me}-*right*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.063039	-1.813473	1.347439
2	6	0	1.136806	-3.240835	1.279918
3	6	0	2.521200	-2.839826	0.776224
4	15	0	2.452092	-1.559901	-0.576239
5	6	0	4.244756	-1.048163	-0.706012
6	6	0	4.645241	-1.406728	-2.140832
7	6	0	3.953312	-2.717137	-2.496735
8	6	0	2.472577	-2.521182	-2.175721
9	6	0	0.087862	-1.092583	3.067019
10	6	0	-0.947204	-1.844458	3.904143
11	6	0	-2.159716	-2.060005	3.007237
12	6	0	-1.659101	-2.711901	1.716386
13	1	0	0.671369	-3.951138	0.580135
14	1	0	1.193607	-3.750010	2.252435
15	1	0	3.112009	-3.715782	0.471703
16	1	0	3.080550	-2.343442	1.583017
17	1	0	4.816408	-1.687052	-0.013615
18	1	0	5.736145	-1.453424	-2.252185
19	1	0	4.105496	-3.007237	-3.545286
20	1	0	4.359024	-3.534259	-1.876862
21	1	0	-0.252104	-0.053018	2.938044
22	1	0	-0.535401	-2.819749	4.214760
23	1	0	-1.191022	-1.296336	4.824333
24	1	0	-2.944306	-2.664136	3.481003
25	1	0	-2.611213	-1.084051	2.761628
26	29	0	0.595413	-0.378067	-0.215563
27	1	0	4.289341	-0.613544	-2.819610

28	1	0	-1.393220	-3.758729	1.939273
29	6	0	2.347159	6.169137	0.587089
30	6	0	3.036810	4.959259	0.582277
31	8	0	0.963034	1.383395	0.605955
32	6	0	0.251138	2.419270	0.411644
33	6	0	0.943685	3.741320	0.480423
34	6	0	2.341598	3.758802	0.531494
35	6	0	0.260502	4.962223	0.488319
36	6	0	0.956310	6.164094	0.540391
37	1	0	0.407706	7.103773	0.543828
38	1	0	2.890255	7.110865	0.626871
39	1	0	4.124348	4.953263	0.622070
40	1	0	2.862080	2.803850	0.535217
41	1	0	-0.826166	4.979808	0.438488
42	6	0	-1.194079	2.342863	0.853539
43	1	0	-1.821022	3.167415	0.502823
44	1	0	-1.637751	1.401087	0.509523
45	1	0	-1.207290	2.348702	1.953992
46	6	0	-0.468050	0.035522	-1.980888
47	6	0	-1.872116	0.074866	-1.777355
48	6	0	-3.076744	0.122803	-1.596214
49	6	0	0.254311	1.237333	-2.153828
50	6	0	-0.142617	2.508187	-1.759692
51	1	0	-1.212415	2.705686	-1.683055
52	1	0	0.470087	3.351452	-2.067748
53	1	0	-0.105036	-0.829258	-2.546530
54	1	0	1.283287	1.110862	-2.507102
55	6	0	-4.469864	0.176126	-1.328797
56	6	0	-5.066429	1.366015	-0.878046
57	6	0	-5.277401	-0.962703	-1.489634
58	6	0	-6.424531	1.409766	-0.597137
59	1	0	-4.441893	2.248819	-0.754102
60	6	0	-6.634929	-0.909422	-1.207464
61	1	0	-4.817713	-1.885851	-1.838037
62	6	0	-7.215598	0.274786	-0.759484
63	1	0	-6.870880	2.338518	-0.247772
64	1	0	-7.246429	-1.799805	-1.337914
65	1	0	-8.279702	0.313470	-0.538631
66	1	0	2.057081	-1.812751	-2.912686
67	6	0	1.493893	-1.071503	3.635136
68	1	0	1.906276	-2.085308	3.736265
69	1	0	2.171660	-0.481310	3.004880
70	1	0	1.499350	-0.619282	4.634731
71	6	0	-2.642721	-2.655575	0.564255
72	1	0	-2.894087	-1.614548	0.324059
73	1	0	-2.222741	-3.097311	-0.350168
74	1	0	-3.571494	-3.188432	0.805566
75	6	0	1.624804	-3.778616	-2.176363
76	1	0	0.574752	-3.556253	-1.942294
77	1	0	1.649643	-4.266173	-3.158587
78	1	0	1.989948	-4.509131	-1.441598

79	6	0	4.441577	0.413343	-0.344324
80	1	0	4.130334	0.615620	0.688638
81	1	0	5.490925	0.715156	-0.453914
82	1	0	3.828520	1.055924	-0.991710

SCF Done: E(RM06) = -3682.25164931 A.U.

L_{Me}-*right*-*re*-TS2:

Standard orientation:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.107045	-1.584106	-0.640971
2	6	0	-0.208837	-3.182053	-0.993529
3	6	0	1.244474	-2.893090	-1.366627
4	15	0	2.028650	-1.805622	-0.079949
5	6	0	3.824529	-1.639186	-0.554922
6	6	0	4.464204	-1.689964	0.836722
7	6	0	3.915912	-2.926122	1.550971
8	6	0	2.386421	-2.983017	1.345416
9	6	0	-1.876872	-1.206614	-2.298404
10	6	0	-3.192388	-1.990772	-2.276004
11	6	0	-3.810697	-1.804102	-0.892394
12	6	0	-2.727938	-2.080955	0.168475
13	1	0	-0.234868	-3.794858	-0.081614
14	1	0	-0.707032	-3.763124	-1.781811
15	1	0	1.808259	-3.825480	-1.503047
16	1	0	1.290245	-2.335372	-2.314967
17	1	0	5.561008	-1.700936	0.772328
18	1	0	4.161105	-2.908829	2.621111
19	1	0	4.388080	-3.827460	1.140108
20	1	0	-2.998321	-3.059962	-2.452421
21	1	0	-3.869338	-1.655835	-3.074695
22	1	0	-4.674736	-2.465425	-0.740181
23	1	0	-4.185693	-0.776265	-0.785658
24	29	0	0.478496	-0.210561	0.225187
25	1	0	4.184180	-0.785000	1.400513
26	1	0	2.081879	-3.995362	1.038834
27	6	0	5.252319	3.374683	-0.300712
28	6	0	4.731040	2.092400	-0.139306
29	8	0	0.663962	1.445946	-0.826335
30	6	0	1.026823	2.637732	-0.601702
31	6	0	2.485908	2.938088	-0.486277
32	6	0	3.363975	1.879632	-0.237865
33	6	0	3.017171	4.220562	-0.648361
34	6	0	4.388860	4.435194	-0.557066
35	1	0	4.786425	5.439369	-0.689580
36	1	0	6.324009	3.545698	-0.228001
37	1	0	5.395204	1.251885	0.061407

38	1	0	2.925444	0.891870	-0.118787
39	1	0	2.357408	5.061935	-0.850572
40	6	0	0.111768	3.720204	-1.124222
41	1	0	0.224311	4.682409	-0.615167
42	1	0	-0.919834	3.372322	-1.008002
43	1	0	0.305810	3.872100	-2.196167
44	6	0	-0.206598	0.700368	1.971531
45	6	0	-1.560037	0.991374	1.648463
46	6	0	-2.728781	1.208172	1.372897
47	6	0	0.735981	1.747539	2.087749
48	6	0	0.590083	3.011323	1.550288
49	1	0	-0.423236	3.358365	1.349306
50	1	0	1.324538	3.780017	1.780304
51	1	0	-0.069440	-0.147285	2.649641
52	1	0	1.701571	1.466067	2.518757
53	6	0	-4.085924	1.370283	0.985065
54	6	0	-4.447517	2.270138	-0.032758
55	6	0	-5.096009	0.595564	1.583510
56	6	0	-5.767957	2.372266	-0.448496
57	1	0	-3.672805	2.879477	-0.493881
58	6	0	-6.412814	0.701001	1.158755
59	1	0	-4.825029	-0.093053	2.381593
60	6	0	-6.755911	1.586102	0.139503
61	1	0	-6.028169	3.070091	-1.241529
62	1	0	-7.179848	0.089568	1.629478
63	1	0	-7.788467	1.665942	-0.192051
64	1	0	-2.844979	-1.391851	1.014925
65	1	0	-1.194656	-1.582201	-3.076050
66	1	0	3.969341	-0.650451	-1.009317
67	6	0	-2.772035	-3.508717	0.691934
68	1	0	-1.965664	-3.716529	1.406940
69	1	0	-3.720842	-3.684333	1.214166
70	1	0	-2.705166	-4.246992	-0.118393
71	6	0	-2.079570	0.292860	-2.481820
72	1	0	-2.538782	0.500219	-3.457081
73	1	0	-2.742142	0.706392	-1.708694
74	1	0	-1.130430	0.836533	-2.408693
75	6	0	1.617493	-2.587973	2.597717
76	1	0	0.531897	-2.577303	2.429360
77	1	0	1.825972	-3.281013	3.422613
78	1	0	1.905782	-1.578100	2.923601
79	6	0	4.370317	-2.703553	-1.495433
80	1	0	4.191383	-3.721777	-1.126972
81	1	0	3.923554	-2.632291	-2.493306
82	1	0	5.455581	-2.584754	-1.612888

SCF Done: E(RM06) = -3682.25196755 A.U.

L_{Me}-*left-re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.694122	-2.051269	-0.515014
2	6	0	2.428143	-2.587729	-0.938253
3	6	0	3.194684	-1.387195	-1.497196
4	15	0	3.111031	0.004103	-0.264102
5	6	0	3.992983	1.459754	-1.019423
6	6	0	4.791438	1.955305	0.192446
7	6	0	5.508889	0.749362	0.800084
8	6	0	4.495768	-0.403479	0.939705
9	6	0	-0.249824	-2.357345	-2.102275
10	6	0	-1.267895	-3.448210	-1.742186
11	6	0	-0.629208	-4.385473	-0.725153
12	6	0	-0.058698	-3.497051	0.378825
13	1	0	2.908689	-2.927343	-0.008154
14	1	0	2.436513	-3.434472	-1.638344
15	1	0	4.232826	-1.649754	-1.742662
16	1	0	2.713694	-1.033664	-2.422807
17	1	0	5.489396	2.755037	-0.089690
18	1	0	5.953460	0.996232	1.773591
19	1	0	6.338840	0.448340	0.147263
20	1	0	-1.623179	-3.969691	-2.640351
21	1	0	-2.147837	-2.968935	-1.281651
22	1	0	0.187205	-4.959932	-1.194801
23	1	0	-1.344620	-5.117928	-0.324379
24	29	0	0.956402	-0.006139	0.346293
25	1	0	4.099478	2.382435	0.936195
26	1	0	4.952090	-1.357029	0.635020
27	8	0	-0.062558	1.466931	-0.475115
28	6	0	-0.207093	2.661069	-0.083426
29	6	0	1.025530	3.526714	0.035370
30	6	0	-1.512065	3.319627	-0.383867
31	6	0	-1.695957	4.704822	-0.350077
32	6	0	-2.599038	2.508169	-0.732819
33	6	0	0.020449	0.087735	2.196968
34	6	0	-1.274005	-0.376411	1.842157
35	6	0	-2.380416	-0.757001	1.494551
36	6	0	0.228824	1.461753	2.470717
37	6	0	-0.626668	2.486278	2.114683
38	1	0	-1.673906	2.242000	1.943694
39	1	0	-0.425711	3.499866	2.457073
40	1	0	0.653030	-0.620131	2.741628
41	1	0	1.211730	1.714084	2.880834
42	6	0	-3.649172	-1.159738	1.003143
43	6	0	-4.610945	-0.195911	0.649108
44	6	0	-3.971183	-2.518714	0.838624
45	6	0	-5.838516	-0.582875	0.131337
46	1	0	-4.369947	0.857593	0.784567
47	6	0	-5.203161	-2.896006	0.321830
48	1	0	-3.239340	-3.272591	1.127908

49	6	0	-6.141857	-1.932145	-0.038220
50	1	0	-6.568478	0.177919	-0.139592
51	1	0	-5.434083	-3.952422	0.200774
52	1	0	-7.105858	-2.231234	-0.442907
53	1	0	-0.897046	-3.036110	0.926803
54	1	0	0.471053	-2.761769	-2.831883
55	1	0	3.225809	2.194322	-1.299050
56	6	0	-3.832430	3.064902	-1.036052
57	6	0	-4.005331	4.448028	-1.002666
58	6	0	-2.932667	5.263197	-0.659051
59	1	0	-2.448108	1.430368	-0.747027
60	1	0	-4.664450	2.414550	-1.303317
61	1	0	-4.971372	4.886838	-1.242386
62	1	0	-3.056687	6.343787	-0.631188
63	1	0	-0.870273	5.361459	-0.083866
64	1	0	1.325213	3.859555	-0.970444
65	1	0	0.888085	4.413076	0.660262
66	1	0	1.841285	2.925999	0.452287
67	6	0	-0.891959	-1.094305	-2.648804
68	1	0	-1.562131	-0.651614	-1.899843
69	1	0	-0.146903	-0.328989	-2.896508
70	1	0	-1.480135	-1.311682	-3.549706
71	6	0	0.858861	-4.180445	1.373161
72	1	0	1.693904	-4.686783	0.871130
73	1	0	1.277736	-3.462032	2.090672
74	1	0	0.315185	-4.939820	1.948080
75	6	0	3.954179	-0.542734	2.355061
76	1	0	3.185300	-1.323706	2.416753
77	1	0	4.754451	-0.792783	3.063041
78	1	0	3.486499	0.393972	2.689560
79	6	0	4.871609	1.164926	-2.225838
80	1	0	4.283485	0.823834	-3.084828
81	1	0	5.408637	2.071179	-2.535425
82	1	0	5.624387	0.394822	-2.015929

SCF Done: E(RM06) = -3682.25767507 A.U.

S23. The summarize energies of TS2s in the *(S, S)*-Me-BPE-CuMes system in the THF solvent at the B3LYP /6-311+G (d, p) level.

B3LYP(SMD,THF) /6-311+G (d, p)

species	**SCF_{SMD}**	G^*_{gas}	G_{sol}	ΔG_{sol}	ΔG_r(kJ.mol^{-1})
L_{Me}-*right-si*-TS2	-3683.47958176	0.622673	-3682.856908	0.0	0.0
L_{Me}-*right-re*-TS2	-3683.47825505	0.623731	-3682.854524	0.007565	19.9
L_{Me}-*left-si*-TS2	-3683.47284197	0.623498	-3682.849343	0.006764	17.8
L_{Me}-*left-re*-TS2	-3683.48006283	0.623955	-3682.856107	0.000801	2.1

G^*_{THF} =Thermal correction to Gibbs Free Energy in gas .

S24: Cartesian coordinates and energies of TS2s optimized stationary points of (*S, S*)-Me-BPE-CuMes reaction system in the THF solvent at the B3LYP /6-311+G (d, p) level.

L_{Me}-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.976156	-1.508677	1.356984
2	6	0	2.744719	-2.099797	1.545140
3	6	0	3.789151	-1.056460	1.115984
4	15	0	3.280701	-0.010800	-0.363480
5	6	0	4.727000	1.221273	-0.381993
6	6	0	5.471898	0.968053	-1.710405
7	6	0	5.394476	-0.529656	-2.026022
8	6	0	3.919349	-0.944326	-1.876596
9	6	0	0.434813	-0.795786	3.016789
10	6	0	-0.243304	-1.958310	3.767626
11	6	0	-0.974194	-2.812411	2.722846
12	6	0	0.030856	-3.124790	1.595733
13	1	0	2.811766	-2.980904	0.897204
14	1	0	2.944702	-2.446367	2.565754
15	1	0	4.762816	-1.530250	0.942118
16	1	0	3.935160	-0.328616	1.923234
17	1	0	5.387820	0.925854	0.443995
18	1	0	6.505357	1.329782	-1.655636
19	1	0	5.772569	-0.761021	-3.029444
20	1	0	6.012965	-1.096222	-1.315800
21	1	0	-0.332378	-0.066839	2.729047
22	1	0	0.516627	-2.568492	4.276525
23	1	0	-0.921376	-1.583196	4.543774
24	1	0	-1.381408	-3.736167	3.150618
25	1	0	-1.822036	-2.249249	2.310869
26	29	0	1.003158	0.122642	-0.221657
27	1	0	4.981108	1.533298	-2.514542
28	1	0	0.757304	-3.851533	1.987069
29	1	0	3.358552	-0.498576	-2.710027
30	6	0	-0.030778	-0.000088	-2.089367
31	6	0	-1.312987	-0.586166	-1.891739
32	6	0	-2.425903	-1.067672	-1.752156
33	6	0	0.076407	1.384140	-2.373422
34	6	0	-0.870511	2.354316	-2.060902
35	1	0	-1.897540	2.037053	-1.920493
36	1	0	-0.739016	3.358483	-2.451252
37	1	0	0.696856	-0.646442	-2.584053
38	1	0	1.046397	1.711635	-2.749159
39	6	0	-3.733285	-1.600734	-1.575039
40	6	0	-4.795317	-0.771702	-1.150271

41	6	0	-4.005117	-2.964399	-1.820286
42	6	0	-6.074160	-1.293483	-0.976273
43	1	0	-4.598601	0.278381	-0.958498
44	6	0	-5.287778	-3.476071	-1.642144
45	1	0	-3.198736	-3.609957	-2.154310
46	6	0	-6.329425	-2.645986	-1.219737
47	1	0	-6.878374	-0.639425	-0.649822
48	1	0	-5.476482	-4.528392	-1.837367
49	1	0	-7.329424	-3.047821	-1.084326
50	6	0	-4.494913	3.856385	1.216924
51	6	0	-3.592073	4.823320	0.773956
52	8	0	-0.124726	1.530989	0.550132
53	6	0	-0.487307	2.676780	0.102969
54	6	0	0.589442	3.743297	-0.044159
55	6	0	-1.876172	3.122704	0.467040
56	6	0	-2.296061	4.461023	0.401820
57	6	0	-2.795944	2.158372	0.916394
58	6	0	-4.088830	2.519616	1.285245
59	1	0	-4.782555	1.757372	1.630678
60	1	0	-5.503199	4.139377	1.506103
61	1	0	-3.894265	5.865808	0.719042
62	1	0	-1.612855	5.232930	0.063538
63	1	0	-2.469942	1.125342	0.961742
64	1	0	1.478283	3.295048	-0.487422
65	1	0	0.286384	4.594911	-0.655696
66	1	0	0.859402	4.117706	0.953610
67	6	0	-0.595658	-3.685462	0.318492
68	1	0	-1.280353	-2.965009	-0.136120
69	1	0	0.167538	-3.930868	-0.428424
70	1	0	-1.152655	-4.604856	0.535141
71	6	0	1.513531	-0.054031	3.808051
72	1	0	2.341682	-0.713735	4.091372
73	1	0	1.919580	0.785857	3.235353
74	1	0	1.092255	0.354477	4.733817
75	6	0	3.670392	-2.454003	-1.892812
76	1	0	4.204063	-2.960984	-1.081631
77	1	0	2.605143	-2.689354	-1.800919
78	1	0	4.023616	-2.888129	-2.835258
79	6	0	4.316956	2.680378	-0.178898
80	1	0	5.198777	3.332003	-0.165571
81	1	0	3.664229	3.019728	-0.989447
82	1	0	3.777988	2.825019	0.762300

SCF Done: E(RB3LYP) = -3683.47958176 A.U.

L_{Me}-*right*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.125657	-1.909040	1.340651

2	6	0	1.080912	-3.341858	1.204377
3	6	0	2.466257	-2.938239	0.672239
4	15	0	2.400144	-1.630481	-0.673739
5	6	0	4.234333	-1.192891	-0.833802
6	6	0	4.616895	-1.565334	-2.282858
7	6	0	3.835048	-2.826067	-2.672157
8	6	0	2.360259	-2.570982	-2.308196
9	6	0	0.007543	-1.261779	3.108784
10	6	0	-1.037002	-2.053516	3.919138
11	6	0	-2.250422	-2.271232	3.005759
12	6	0	-1.732316	-2.847260	1.672148
13	1	0	0.604849	-4.041189	0.507558
14	1	0	1.172978	-3.868903	2.161262
15	1	0	3.029666	-3.820756	0.346534
16	1	0	3.047774	-2.472300	1.476378
17	1	0	4.774486	-1.866070	-0.154385
18	1	0	5.700418	-1.700361	-2.379805
19	1	0	3.945848	-3.069683	-3.736011
20	1	0	4.212780	-3.690351	-2.107630
21	1	0	-0.336858	-0.224041	3.021402
22	1	0	-0.618838	-3.025382	4.217978
23	1	0	-1.302625	-1.525116	4.842842
24	1	0	-2.996654	-2.936992	3.455062
25	1	0	-2.749861	-1.310915	2.820078
26	29	0	0.553517	-0.373750	-0.172150
27	1	0	4.338668	-0.742501	-2.955493
28	1	0	-1.443726	-3.892931	1.849328
29	6	0	2.969692	5.975389	0.668126
30	6	0	3.493792	4.684855	0.768123
31	8	0	0.988840	1.368249	0.637598
32	6	0	0.401875	2.497419	0.457614
33	6	0	1.267972	3.728823	0.515948
34	6	0	2.652097	3.576125	0.693858
35	6	0	0.752660	5.033338	0.421322
36	6	0	1.593585	6.142682	0.494204
37	1	0	1.172793	7.141628	0.415014
38	1	0	3.623857	6.840910	0.726338
39	1	0	4.562204	4.542112	0.909846
40	1	0	3.043533	2.569740	0.782651
41	1	0	-0.311259	5.188509	0.273755
42	6	0	-1.013575	2.616249	1.017447
43	1	0	-1.540136	3.522363	0.712020
44	1	0	-1.604080	1.750483	0.712507
45	1	0	-0.944012	2.619582	2.114194
46	6	0	-0.647316	0.145565	-1.892583
47	6	0	-2.042750	0.253672	-1.637598
48	6	0	-3.246293	0.345525	-1.454829
49	6	0	0.143525	1.296888	-2.102346
50	6	0	-0.130645	2.598174	-1.673181
51	1	0	-1.169824	2.877545	-1.528956
52	1	0	0.516216	3.389900	-2.033407
53	1	0	-0.358986	-0.740948	-2.460384
54	1	0	1.129581	1.107593	-2.526533

55	6	0	-4.647881	0.464082	-1.240438
56	6	0	-5.210306	1.678140	-0.789085
57	6	0	-5.512792	-0.627145	-1.475214
58	6	0	-6.581830	1.790243	-0.579688
59	1	0	-4.556010	2.525062	-0.608408
60	6	0	-6.883301	-0.505131	-1.262626
61	1	0	-5.093600	-1.564116	-1.828270
62	6	0	-7.426441	0.701609	-0.813831
63	1	0	-6.994832	2.733502	-0.232529
64	1	0	-7.532124	-1.356470	-1.450248
65	1	0	-8.496234	0.793419	-0.650331
66	1	0	1.962909	-1.833836	-3.019774
67	6	0	1.415677	-1.239009	3.706335
68	1	0	1.842257	-2.245391	3.787520
69	1	0	2.091480	-0.622294	3.105755
70	1	0	1.392718	-0.813509	4.716131
71	6	0	-2.741064	-2.799596	0.524369
72	1	0	-3.015241	-1.771082	0.277201
73	1	0	-2.334630	-3.255477	-0.384952
74	1	0	-3.652974	-3.346771	0.791510
75	6	0	1.458818	-3.806304	-2.355053
76	1	0	0.421882	-3.559060	-2.104876
77	1	0	1.460447	-4.241925	-3.360673
78	1	0	1.800466	-4.583982	-1.663434
79	6	0	4.554889	0.254611	-0.455392
80	1	0	4.302784	0.460646	0.589099
81	1	0	5.622716	0.463515	-0.592045
82	1	0	3.987818	0.959135	-1.071424

SCF Done: E(RB3LYP) = -3683.47825505 A.U.

L_{Me}-*left*-*si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.978970	-1.962415	0.571798
2	6	0	-0.037863	-3.539730	0.579286
3	6	0	-1.500572	-3.226889	0.946077
4	15	0	-2.184543	-1.883201	-0.168315
5	6	0	-3.830461	-1.356433	0.598997
6	6	0	-4.870754	-1.674201	-0.503365
7	6	0	-4.459945	-2.987119	-1.190694
8	6	0	-2.967455	-2.873215	-1.575098
9	6	0	1.586781	-1.885911	2.353544
10	6	0	2.892756	-2.709232	2.342471
11	6	0	3.651467	-2.367271	1.049578
12	6	0	2.664765	-2.434699	-0.146961
13	1	0	0.005906	-3.974492	-0.425392
14	1	0	0.380472	-4.282537	1.268118
15	1	0	-2.112150	-4.135675	0.907161

16	1	0	-1.546304	-2.851470	1.974022
17	1	0	-5.881326	-1.733109	-0.082480
18	1	0	-5.083124	-3.199702	-2.068147
19	1	0	-4.599941	-3.822506	-0.493548
20	1	0	2.656380	-3.781166	2.358466
21	1	0	3.499160	-2.506539	3.233932
22	1	0	4.499877	-3.043269	0.890940
23	1	0	4.065929	-1.356317	1.122405
24	29	0	-0.401827	-0.389798	-0.276746
25	1	0	-4.884851	-0.864317	-1.242675
26	1	0	-2.499495	-3.864620	-1.604199
27	6	0	-4.636317	4.797328	0.488355
28	6	0	-4.647346	3.462789	0.070392
29	8	0	-1.201113	1.153397	0.611334
30	6	0	-1.012998	2.422862	0.485411
31	6	0	-2.253786	3.279468	0.490340
32	6	0	-3.473170	2.715745	0.077009
33	6	0	-2.256291	4.620716	0.905268
34	6	0	-3.435145	5.369769	0.906516
35	1	0	-3.411889	6.404539	1.238301
36	1	0	-5.552336	5.381432	0.487318
37	1	0	-5.576888	3.005237	-0.259205
38	1	0	-3.473673	1.681194	-0.247719
39	1	0	-1.336718	5.089646	1.238760
40	6	0	0.234532	2.985047	1.161524
41	1	0	0.483391	4.003203	0.853327
42	1	0	1.082362	2.335826	0.936242
43	1	0	0.080280	2.983697	2.249512
44	6	0	0.527833	0.512884	-1.979476
45	6	0	1.862021	0.839077	-1.601095
46	6	0	3.013886	1.107330	-1.297197
47	6	0	-0.448678	1.518368	-2.136191
48	6	0	-0.422284	2.793687	-1.561120
49	1	0	0.552773	3.218000	-1.340704
50	1	0	-1.167882	3.508322	-1.891645
51	1	0	0.434740	-0.350956	-2.639974
52	1	0	-1.365967	1.200573	-2.631282
53	6	0	4.346058	1.428109	-0.911847
54	6	0	4.622281	2.599761	-0.173406
55	6	0	5.425389	0.584323	-1.254803
56	6	0	5.925291	2.907614	0.207557
57	1	0	3.802041	3.258841	0.092683
58	6	0	6.725074	0.900158	-0.867372
59	1	0	5.229439	-0.313702	-1.832586
60	6	0	6.983626	2.061336	-0.134564
61	1	0	6.116378	3.814133	0.775369
62	1	0	7.541535	0.237818	-1.142250
63	1	0	7.998744	2.305523	0.164430
64	1	0	2.901674	-1.641510	-0.860988
65	1	0	0.831774	-2.361642	2.991488
66	1	0	-3.749850	-0.276426	0.749834
67	6	0	2.708956	-3.777311	-0.888953
68	1	0	1.984730	-3.817446	-1.709300

69	1	0	3.702992	-3.925345	-1.326005
70	1	0	2.512688	-4.625845	-0.224925
71	6	0	1.784372	-0.436885	2.820988
72	1	0	2.156624	-0.415759	3.851989
73	1	0	2.505295	0.097742	2.193892
74	1	0	0.845298	0.121808	2.779537
75	6	0	-2.746691	-2.188223	-2.931437
76	1	0	-1.680643	-2.104516	-3.164502
77	1	0	-3.226703	-2.757608	-3.735956
78	1	0	-3.161374	-1.174600	-2.945493
79	6	0	-4.182142	-1.993279	1.950672
80	1	0	-4.287988	-3.081631	1.888616
81	1	0	-3.429438	-1.770117	2.712579
82	1	0	-5.135579	-1.589330	2.310321

SCF Done: E(RB3LYP) = -3683.47284197 A.U.

L_{Me}-*left*-*re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.675213	-1.953949	0.847348
2	6	0	-2.379479	-2.720511	0.740378
3	6	0	-3.455743	-1.640683	0.964072
4	15	0	-3.180521	-0.178259	-0.188476
5	6	0	-4.396847	1.153652	0.411345
6	6	0	-5.549907	1.173694	-0.629578
7	6	0	-5.674044	-0.220271	-1.265968
8	6	0	-4.255891	-0.689583	-1.652706
9	6	0	-0.312571	-1.985395	2.702223
10	6	0	0.976303	-2.827756	2.827066
11	6	0	0.901793	-3.967464	1.802584
12	6	0	0.536823	-3.334725	0.445494
13	1	0	-2.486172	-3.147924	-0.263450
14	1	0	-2.504135	-3.540796	1.457006
15	1	0	-4.459499	-2.062542	0.837796
16	1	0	-3.391454	-1.269282	1.992193
17	1	0	-6.490621	1.487398	-0.162359
18	1	0	-6.344412	-0.210947	-2.134503
19	1	0	-6.110134	-0.917340	-0.539628
20	1	0	1.103922	-3.196024	3.851870
21	1	0	1.845615	-2.195038	2.604322
22	1	0	0.125125	-4.686464	2.100107
23	1	0	1.844720	-4.523741	1.737735
24	29	0	-0.892133	-0.000253	-0.265106
25	1	0	-5.329321	1.910951	-1.409589
26	1	0	-4.218548	-1.782763	-1.733554
27	8	0	-0.002612	1.546857	0.541299
28	6	0	0.129900	2.741673	0.100917
29	6	0	-1.142413	3.547504	-0.133030

30	6	0	1.367472	3.480750	0.525302
31	6	0	1.511088	4.872566	0.404210
32	6	0	2.428898	2.749441	1.088031
33	6	0	0.171955	0.040944	-2.103400
34	6	0	1.487002	-0.419348	-1.813204
35	6	0	2.617460	-0.819667	-1.584500
36	6	0	-0.068714	1.405245	-2.404943
37	6	0	0.727464	2.480504	-2.027530
38	1	0	1.768183	2.291050	-1.789740
39	1	0	0.510060	3.463410	-2.433721
40	1	0	-0.451592	-0.676893	-2.639453
41	1	0	-1.037075	1.616644	-2.858184
42	6	0	3.941656	-1.250002	-1.293708
43	6	0	4.895105	-0.343948	-0.778200
44	6	0	4.339327	-2.587170	-1.512462
45	6	0	6.190647	-0.765494	-0.492902
46	1	0	4.600597	0.686799	-0.606783
47	6	0	5.637488	-2.998864	-1.222132
48	1	0	3.619003	-3.290878	-1.918626
49	6	0	6.570644	-2.092859	-0.711550
50	1	0	6.909883	-0.053013	-0.097840
51	1	0	5.924176	-4.032094	-1.399459
52	1	0	7.583246	-2.416681	-0.489077
53	1	0	1.415876	-2.798003	0.068268
54	1	0	-1.132956	-2.545210	3.173009
55	1	0	-3.841174	2.094683	0.360994
56	6	0	3.593115	3.386557	1.508630
57	6	0	3.724823	4.772869	1.380880
58	6	0	2.677832	5.510979	0.827778
59	1	0	2.314314	1.675579	1.183355
60	1	0	4.400007	2.801929	1.943071
61	1	0	4.632475	5.271044	1.709990
62	1	0	2.766320	6.589408	0.726338
63	1	0	0.711686	5.470035	-0.021368
64	1	0	-1.549683	3.860602	0.838762
65	1	0	-0.995482	4.440070	-0.743550
66	1	0	-1.881884	2.910798	-0.622313
67	6	0	-0.214203	-0.601467	3.350560
68	1	0	0.511551	0.032011	2.832589
69	1	0	-1.172811	-0.073612	3.321072
70	1	0	0.086090	-0.690713	4.401540
71	6	0	0.087663	-4.322467	-0.632899
72	1	0	-0.782876	-4.906756	-0.315460
73	1	0	-0.166574	-3.810886	-1.567306
74	1	0	0.893166	-5.030972	-0.857317
75	6	0	-3.761678	-0.086108	-2.974861
76	1	0	-2.759041	-0.444336	-3.224051
77	1	0	-4.432800	-0.359980	-3.797209
78	1	0	-3.715616	1.007524	-2.935594
79	6	0	-4.889264	0.989177	1.855393
80	1	0	-4.058384	0.940279	2.566512
81	1	0	-5.508292	1.848701	2.136448
82	1	0	-5.498926	0.088917	1.984024

SCF Done: E(RB3LYP) = -3683.48006283 A.U.

S25. Reference 77 details

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