Supporting Information

Computational Investigation on the Enantioselective

Copper(I)-Catalyzed Addition of Enynes to Ketones

Hanwei Li, Zhang Zhang, Mingliang Luo, Guohong Tao, Song Qin*

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

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

CONTENTS:

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

Part IV :(S, S)- BPE–CuMes system using 2.4-dimethylacetophenone

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)

Species	Ggas	ΔGgas	ΔGr(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	Ggas	ΔGgas	ΔGr(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	-809.140838		
IM2+ Pro	-3948.656539	0.01022	26.8

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     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type          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     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type          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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

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

1	6	0	-0.136348	-1.963386	-0.740907
2	6	0	-1.415262	-1.396599	-0.518786
3	6	0	-2.522937	-0.936274	-0.320658
4	6	0	0.968668	-1.256909	-1.029703
5	6	0	1.020284	0.226394	-1.159527
6	1	0	0.002190	0.635794	-1.214002
7	1	0	1.545369	0.502974	-2.086156
8	1	0	-0.065398	-3.048689	-0.665846

9	1	0	1.904931	-1.799397	-1.163690
10	6	0	5.746734	-0.659149	0.410974
11	6	0	5.453690	0.251460	-0.600034
12	6	0	1.736297	0.925061	0.010427
13	6	0	3.155570	0.389860	0.159924
14	6	0	4.169793	0.769784	-0.723700
15	6	0	3.457677	-0.533663	1.161607
16	6	0	4.742954	-1.051570	1.289037
17	1	0	4.957771	-1.770189	2.077188
18	1	0	6.751598	-1.063347	0.509885
19	1	0	6.229673	0.561995	-1.296432
20	1	0	3.957845	1.478803	-1.522995
21	1	0	2.663494	-0.854684	1.831528
22	6	0	-3.811264	-0.383238	-0.082749
23	6	0	-4.914291	-1.219956	0.147653
24	6	0	-3.999697	1.007768	-0.070696
25	6	0	-6.169354	-0.677497	0.383457
26	1	0	-4.767823	-2.297455	0.138769
27	6	0	-5.258317	1.542529	0.164584
28	1	0	-3.142826	1.654686	-0.245888
29	6	0	-6.346414	0.703682	0.392602
30	1	0	-7.016138	-1.336374	0.561654
31	1	0	-5.392209	2.621913	0.171533
32	1	0	-7.331333	1.126649	0.576384
33	6	0	1.722479	2.434587	-0.210937
34	1	0	2.241084	2.948269	0.609019
35	1	0	2.208957	2.729426	-1.147040
36	1	0	0.683530	2.781397	-0.238915
37	8	0	0.953466	0.624923	1.153271
38	1	0	1.339982	1.091541	1.903433

Zero-point correction=   0.313070 (Hartree/Particle)
 Thermal correction to Energy=   0.331481
 Thermal correction to Enthalpy=   0.332425
 Thermal correction to Gibbs Free Energy=   0.261977
 Sum of electronic and zero-point Energies=   -809.089745
 Sum of electronic and thermal Energies=   -809.071334
 Sum of electronic and thermal Enthalpies=   -809.070390
 Sum of electronic and thermal Free Energies=   -809.140838

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	Ggas	ΔGgas	ΔGr(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 reaction

B3LYP/6-31G(d,p)

Species	Ggas	ΔGgas	ΔGr(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	-809.759595			
IM2+ Pro	-3950.065144	0.015167		39.8

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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

23

| 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

25

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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

Center Number	Atomic Number	Atomic Type	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

28

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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

32

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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

34

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

36

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

Center Number	Atomic Number	Atomic Type	X	Y	Z
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 Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.337547	-1.914642	-0.231847
2	6	0	-1.632679	-1.335926	-0.187732
3	6	0	-2.764659	-0.888326	-0.146836
4	6	0	0.819120	-1.240686	-0.387779
5	6	0	0.945119	0.242695	-0.562303
6	1	0	-0.025127	0.718490	-0.389581
7	1	0	1.237676	0.462603	-1.598843
8	1	0	-0.298281	-2.998715	-0.133524
9	1	0	1.741469	-1.816136	-0.405530
10	6	0	5.980725	-0.679981	-0.366458
11	6	0	5.390910	0.188069	-1.288010
12	6	0	1.990819	0.913195	0.367084
13	6	0	3.401086	0.358556	0.105433
14	6	0	4.115130	0.700515	-1.053868
15	6	0	3.999478	-0.521925	1.015897
16	6	0	5.278279	-1.034572	0.784684
17	1	0	5.722165	-1.715050	1.506268
18	1	0	6.975393	-1.077088	-0.547538
19	1	0	5.925300	0.468714	-2.191469
20	1	0	3.675527	1.371408	-1.786650
21	1	0	3.447721	-0.812365	1.903213
22	6	0	-4.086194	-0.359133	-0.098158

23	6	0	-5.197251	-1.216420	0.042253
24	6	0	-4.310409	1.030190	-0.189408
25	6	0	-6.487862	-0.696639	0.088803
26	1	0	-5.031682	-2.286611	0.113600
27	6	0	-5.604609	1.540861	-0.141770
28	1	0	-3.459639	1.695528	-0.296101
29	6	0	-6.697835	0.681772	-0.002877
30	1	0	-7.333774	-1.369526	0.197303
31	1	0	-5.761423	2.613471	-0.212874
32	1	0	-7.706190	1.083570	0.034196
33	6	0	1.947513	2.440173	0.174763
34	1	0	2.680380	2.929392	0.826624
35	1	0	2.170716	2.738508	-0.853238
36	1	0	0.950840	2.809478	0.432618
37	8	0	1.558547	0.605402	1.695342
38	1	0	2.125747	1.094452	2.307552

Zero-point correction=	0.314326 (Hartree/Particle)
Thermal correction to Energy=	0.332644
Thermal correction to Enthalpy=	0.333588
Thermal correction to Gibbs Free Energy=	0.264189
Sum of electronic and zero-point Energies=	-809.709458
Sum of electronic and thermal Energies=	-809.691140
Sum of electronic and thermal Enthalpies=	-809.690196
Sum of electronic and thermal Free Energies=	-809.759595

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	126.1
BPE-CuMes+1			-3489.798871	0.0	0.0
TS1	-3490.31341594	0.557315	-3489.7561	0.042771	112.3
IM2	-3140.35876075	0.390983	-3139.967777		
MesH	-350.003515782	0.146255	-349.8572607		
IM2+ MesH			-3489.825038	-0.0261667	-68.9

2: the cycle of the reaction

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	-12.6
TS2	-3525.08326388	0.519005	-3524.564258		
TS2+1			-3949.313101	0.018053	47.4
IM3	-3525.10538531	0.523074	-3524.582311		
IM3+1			-3949.331154	0.0	0.0
IM31	-3950.00464093	0.684084	-3949.320556	0.010598	27.8
TS3	-3949.98578045	0.680932	-3949.304848	0.026306	69.1
Pro	-809.635539274	0.261977	-809.3735627		
IM2+Pro			-3949.341340	-0.010186	-26.7

S6: 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$_{PCM}$	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	78.6
BPE-CuMes+1			-3490.932134	0.0	0.0
TS1	-3491.41813350	0.550708	-3490.867425	0.064709	169.9
IM2	-3141.18388963	0.388291	-3140.795598		
MesH	-350.303503484	0.147042	-350.1564614		
IM2+ MesH			-3490.952059	-0.019925	-52.3

2.the cycle of the teaction

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

Species	SCF$_{PCM}$	G^*_{gas}	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	-51.3
TS2	-3526.18824283	0.515090	-3525.673152		
TS2+1			-3950.778612	0.015421	40.5
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	118.0
Pro	-810.263718401	0.263958	-809.9997604		
IM2+Pro			-3950.795358	-0.001325	-37.1

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

Part II :(S,S)- Ph- BPE–CuMes system

S21: 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)

species	Ggas	ΔGgas	ΔGr(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

S22: 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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

S23: 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.

species	Ggas	ΔGgas	ΔG_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

B3LYP/6-31G(d,p)

S24: 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:

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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

54

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

57

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	X	Y	Z
			Coordinates (Angstroms)		

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

59

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

S25: 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}	$\Delta G_r(kJ.mol^{-1})$
L_{ph}-*right-si*-TS2	-4448.81362249	0.824703	-4447.988919	0.005928	15.6
L_{ph}-*right-re*-TS2	-4448.80582377	0.827553	-4447.978270	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

S26: 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)

Species	SCF_{SMD}	G^*_{gas}	G_{sol}	ΔG_{sol}	$\Delta G_r(kJ.mol^{-1})$
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^*_{gas} =Thermal correction to Gibbs Free Energy in gas .

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

S31. 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)

species	G_{gas}	ΔG_{gas}	ΔG_r(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

S32. 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     Atomic      Atomic              Coordinates (Angstroms)
Number     Number       Type          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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	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

S33: 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).

$$M06(SMD,THF)/6\text{-}311\text{+}G \text{ (d, p)}$$

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

Part IV :(S, S)- BPE–CuMes system using 2.4-dimethylacetophenone

S41. The summarize energies of TS2s in the (S, S)-BPE-CuMes system in the gas-phase
at the M06/6-31G(d,p) level.

<div align="center">M06/6-31G(d,p)</div>

species	G_{gas}	ΔG_{gas}	$\Delta G_r(kJ.mol^{-1})$
L_{Me}-*right-si*-TS	-4525.736243	0.876901	11.2
L_{Me}-*right-re*-TS2	-4525.729685	0.880280	28.5
L_{Me}-*left-si*-TS2	-4525.732537	0.874980	21.0
L_{Me}-*left-re*-TS2	-4525.740536	0.874472	0.0

S42 Cartesian coordinates and energies of TS2s optimized stationary points of

(S, S)--BPE-CuMes reaction system in the gas-phase at the M06 /6-31G(d, p) level.

L-*right-si*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-1.015538	1.201879	1.288692
2	6	0	-2.866916	1.278985	1.414918
3	6	0	-3.554092	0.072181	0.780328
4	15	0	-2.730030	-0.501956	-0.788820
5	6	0	-3.793215	-2.019853	-1.185676
6	6	0	-4.565661	-1.656437	-2.462877
7	6	0	-4.889302	-0.174374	-2.404081
8	6	0	-3.573720	0.543754	-2.119936
9	6	0	-0.442806	0.312770	2.856796
10	6	0	-0.100618	1.422182	3.851232
11	6	0	0.488545	2.566961	3.041216
12	6	0	-0.535560	2.897282	1.947043
13	1	0	-3.150440	2.199304	0.882606
14	1	0	-3.178078	1.394341	2.462729
15	1	0	-4.620937	0.274005	0.607911
16	1	0	-3.493357	-0.796936	1.453879

17	1	0	-4.513879	-2.081830	-0.356014
18	1	0	-5.459604	-2.284188	-2.563258
19	1	0	-5.354906	0.195253	-3.327191
20	1	0	-5.609448	0.003638	-1.591754
21	1	0	0.492160	-0.162638	2.524482
22	1	0	-1.007393	1.785180	4.357736
23	1	0	0.578011	1.056667	4.632270
24	1	0	0.711750	3.454308	3.647090
25	1	0	1.433290	2.251010	2.569580
26	29	0	-0.540765	-0.117013	-0.489327
27	1	0	-3.942345	-1.854257	-3.346404
28	6	0	-3.631700	2.002220	-1.772333
29	1	0	-1.435605	3.300284	2.440907
30	6	0	-0.058013	3.894296	0.934060
31	6	0	-1.384267	-0.771333	3.296141
32	6	0	-3.043290	-3.317079	-1.257489
33	6	0	-3.152238	-4.249022	-0.223410
34	6	0	-2.496142	-5.474317	-0.291516
35	6	0	-1.721699	-5.791227	-1.402522
36	6	0	-1.589097	-4.863454	-2.432441
37	6	0	-2.237189	-3.636574	-2.354877
38	6	0	-4.782982	2.611104	-1.265591
39	6	0	-2.478575	2.783183	-1.909687
40	6	0	-2.461601	4.117082	-1.526770
41	6	0	-3.609406	4.705481	-1.001360
42	6	0	-4.771125	3.951056	-0.883293
43	6	0	-0.514503	5.212898	0.974184
44	6	0	0.875559	3.539232	-0.042348
45	6	0	1.318806	4.471023	-0.973771
46	6	0	0.857670	5.785691	-0.925197
47	6	0	-0.055853	6.155417	0.057816
48	6	0	-1.283140	-2.034017	2.697834
49	6	0	-2.164475	-3.056017	3.026831
50	6	0	-3.173643	-2.837522	3.962462
51	6	0	-3.280144	-1.590866	4.569996
52	6	0	-2.392340	-0.568416	4.242971
53	1	0	1.250626	2.516666	-0.094861
54	1	0	2.021674	4.153896	-1.743216
55	1	0	1.207651	6.516577	-1.650726
56	1	0	-0.422408	7.178934	0.105820
57	1	0	-1.246295	5.500452	1.729734
58	1	0	-5.679199	4.403491	-0.489963
59	1	0	-5.704476	2.041295	-1.163007
60	1	0	-3.594260	5.749003	-0.692974
61	1	0	-1.543561	4.693895	-1.623825
62	1	0	-1.573907	2.331709	-2.316544
63	1	0	-0.969116	-5.091390	-3.297091
64	1	0	-2.113022	-2.914292	-3.162322
65	1	0	-1.216435	-6.752258	-1.463207
66	1	0	-2.600035	-6.188016	0.523564
67	1	0	-3.764153	-4.004266	0.645881
68	1	0	-2.055442	-4.028928	2.548716

69	1	0	-0.502655	-2.186969	1.953925
70	1	0	-3.863741	-3.636165	4.225732
71	1	0	-4.055665	-1.411456	5.311865
72	1	0	-2.491209	0.394798	4.741527
73	1	0	-2.916770	0.419079	-2.997637
74	6	0	0.618246	0.259579	-2.183837
75	6	0	1.882402	0.827091	-1.862582
76	6	0	3.005114	1.208950	-1.579510
77	6	0	0.603559	-1.104593	-2.568630
78	6	0	1.622314	-2.005745	-2.316270
79	1	0	2.630962	-1.607374	-2.226822
80	1	0	1.540869	-3.016636	-2.713668
81	1	0	-0.094451	0.912906	-2.697825
82	1	0	-0.342833	-1.475943	-2.974075
83	6	0	4.346232	1.555996	-1.261487
84	6	0	5.367427	0.612035	-1.471452
85	6	0	4.690231	2.808442	-0.726665
86	6	0	6.686478	0.920496	-1.172387
87	1	0	5.102157	-0.371950	-1.854493
88	6	0	6.014081	3.111579	-0.436677
89	1	0	3.904529	3.538452	-0.538470
90	6	0	7.019204	2.173852	-0.661703
91	1	0	7.459723	0.171079	-1.331609
92	1	0	6.263083	4.088704	-0.028035
93	1	0	8.054821	2.415758	-0.433419
94	6	0	5.645181	-2.310552	0.831558
95	6	0	5.125088	-3.381183	0.104915
96	8	0	0.819940	-1.303613	0.332464
97	6	0	1.466455	-2.303835	-0.107498
98	6	0	0.734058	-3.621089	-0.181326
99	6	0	2.934080	-2.330876	0.188071
100	6	0	3.764796	-3.382296	-0.205217
101	6	0	3.487575	-1.267331	0.906032
102	6	0	4.836899	-1.249069	1.245969
103	1	0	6.709151	-2.298116	1.078322
104	1	0	3.356130	-4.212448	-0.782404
105	1	0	2.837152	-0.442157	1.196081
106	1	0	-0.281219	-3.455189	-0.554836
107	1	0	1.219216	-4.376358	-0.805936
108	1	0	0.660983	-4.032498	0.838794
109	6	0	5.999532	-4.532695	-0.296102
110	1	0	7.002105	-4.195566	-0.582835
111	1	0	6.128377	-5.244226	0.530635
112	1	0	5.572520	-5.087388	-1.138166
113	6	0	5.419738	-0.105574	2.020598
114	1	0	6.050718	0.521513	1.375941
115	1	0	4.634425	0.536747	2.433400
116	1	0	6.045198	-0.458890	2.849443

Zero-point correction=   0.964166 (Hartree/Particle)
  Thermal correction to Energy=   1.017815
  Thermal correction to Enthalpy=   1.018759

Thermal correction to Gibbs Free Energy=   0.876901
Sum of electronic and zero-point Energies=   -4525.648978
Sum of electronic and thermal Energies=   -4525.595329
Sum of electronic and thermal Enthalpies=   -4525.594385
Sum of electronic and thermal Free Energies=   -4525.736243

L-*right-re*-TS2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
			Coordinates (Angstroms)		
1	15	0	-0.922909	-0.477514	1.649273
2	6	0	-1.249837	-2.314287	1.619527
3	6	0	-0.371949	-3.127604	0.674838
4	15	0	0.094984	-2.193754	-0.845043
5	6	0	1.381541	-3.306141	-1.620741
6	6	0	0.783594	-3.662835	-2.994268
7	6	0	-0.708326	-3.887498	-2.790840
8	6	0	-1.235599	-2.631659	-2.101305
9	6	0	0.514162	-0.250358	2.881716
10	6	0	-0.136602	0.126592	4.216248
11	6	0	-1.425816	0.876087	3.904518
12	6	0	-2.210477	-0.031216	2.954025
13	1	0	-2.307002	-2.385126	1.322639
14	1	0	-1.175307	-2.716137	2.639664
15	1	0	-0.853707	-4.080562	0.412417
16	1	0	0.584891	-3.363726	1.162437
17	1	0	1.391140	-4.225927	-1.011645
18	1	0	1.293178	-4.532951	-3.427797
19	1	0	-1.241287	-4.087880	-3.729330
20	1	0	-0.847529	-4.768455	-2.145248
21	1	0	1.028216	0.631367	2.473244
22	1	0	-0.394544	-0.774068	4.792609
23	1	0	0.554643	0.710838	4.836754
24	1	0	-2.009862	1.108229	4.804387
25	1	0	-1.203072	1.834774	3.409333
26	29	0	0.278094	-0.036905	-0.529900
27	1	0	0.949075	-2.820596	-3.684750
28	6	0	-2.605653	-2.650470	-1.483610
29	1	0	-2.427452	-0.962423	3.502718
30	6	0	-3.500202	0.507422	2.416361
31	6	0	1.489947	-1.394797	2.864213
32	6	0	2.793766	-2.786184	-1.709805
33	6	0	3.108985	-1.426985	-1.671204
34	6	0	4.424657	-1.002742	-1.835785
35	6	0	5.446802	-1.928115	-2.019727
36	6	0	5.144846	-3.287242	-2.040959
37	6	0	3.828581	-3.708339	-1.892356
38	6	0	-3.273288	-3.830325	-1.150938
39	6	0	-3.219841	-1.429185	-1.173852
40	6	0	-4.450465	-1.386050	-0.530644

41	6	0	-5.099516	-2.571302	-0.190844
42	6	0	-4.511615	-3.789851	-0.510689
43	6	0	-4.707654	-0.091242	2.784407
44	6	0	-3.536652	1.605033	1.550706
45	6	0	-4.749503	2.104145	1.092405
46	6	0	-5.947140	1.501777	1.471487
47	6	0	-5.923729	0.397801	2.317000
48	6	0	2.531662	-1.384525	1.926148
49	6	0	3.393219	-2.466878	1.791307
50	6	0	3.240618	-3.585900	2.607161
51	6	0	2.229582	-3.598985	3.563147
52	6	0	1.363581	-2.515199	3.691071
53	1	0	-2.604024	2.062002	1.214953
54	1	0	-4.759948	2.959141	0.420029
55	1	0	-6.891428	1.892627	1.096999
56	1	0	-6.852249	-0.085174	2.615409
57	1	0	-4.689117	-0.956855	3.446861
58	1	0	-5.016225	-4.721142	-0.261485
59	1	0	-2.832847	-4.796008	-1.394083
60	1	0	-6.060347	-2.539095	0.318743
61	1	0	-4.896613	-0.421241	-0.285766
62	1	0	-2.714041	-0.496960	-1.431306
63	1	0	5.936266	-4.021696	-2.174424
64	1	0	3.592680	-4.773017	-1.912204
65	1	0	6.474715	-1.592618	-2.140212
66	1	0	4.648954	0.062918	-1.805117
67	1	0	2.322199	-0.704799	-1.454342
68	1	0	4.184579	-2.430634	1.042493
69	1	0	2.647794	-0.508926	1.289195
70	1	0	3.911903	-4.435873	2.507358
71	1	0	2.110409	-4.460232	4.217514
72	1	0	0.577791	-2.554750	4.443954
73	6	0	5.832044	3.755795	0.378930
74	6	0	5.544031	2.397276	0.247756
75	8	0	1.582931	1.182293	0.262094
76	6	0	1.764845	2.439071	0.178069
77	6	0	3.170028	2.930027	0.237456
78	6	0	4.210568	1.999488	0.185140
79	6	0	3.490155	4.284628	0.376028
80	6	0	4.814423	4.709125	0.449736
81	1	0	6.872817	4.080493	0.435021
82	1	0	3.961293	0.942883	0.103958
83	1	0	2.699675	5.033277	0.420543
84	6	0	0.657003	3.313224	0.716049
85	1	0	0.720238	4.360634	0.407888
86	1	0	-0.306063	2.905557	0.384157
87	1	0	0.683821	3.280366	1.816351
88	6	0	0.297369	0.855406	-2.470719
89	6	0	-1.002397	1.379851	-2.256907
90	6	0	-2.105193	1.898593	-2.164236
91	6	0	1.401046	1.734059	-2.518669
92	6	0	1.449250	3.002295	-1.977996

93	1	0	0.509463	3.530161	-1.814729
94	1	0	2.319546	3.625124	-2.166404
95	1	0	0.358846	-0.044810	-3.088767
96	1	0	2.336481	1.293443	-2.876414
97	6	0	-3.363820	2.541252	-2.066890
98	6	0	-4.558112	1.860498	-2.361703
99	6	0	-3.434347	3.898001	-1.700643
100	6	0	-5.778139	2.518185	-2.289689
101	1	0	-4.511749	0.810391	-2.645145
102	6	0	-4.658924	4.548675	-1.638825
103	1	0	-2.509874	4.427551	-1.475309
104	6	0	-5.837376	3.863490	-1.931554
105	1	0	-6.692800	1.975419	-2.519282
106	1	0	-4.695008	5.599567	-1.359740
107	1	0	-6.795094	4.376387	-1.883769
108	1	0	-1.203568	-1.804262	-2.828986
109	6	0	6.645385	1.381619	0.159947
110	1	0	6.308204	0.396416	0.503548
111	1	0	6.998448	1.263981	-0.873982
112	1	0	7.513016	1.673550	0.762475
113	6	0	5.146674	6.160980	0.630388
114	1	0	6.018232	6.451029	0.032363
115	1	0	4.308741	6.804357	0.341494
116	1	0	5.387029	6.387489	1.677306

Zero-point correction=   0.966443 (Hartree/Particle)
 Thermal correction to Energy=   1.021053
 Thermal correction to Enthalpy=   1.021997
 Thermal correction to Gibbs Free Energy=   0.880280
 Sum of electronic and zero-point Energies=   -4525.643522
 Sum of electronic and thermal Energies=   -4525.588912
 Sum of electronic and thermal Enthalpies=   -4525.587968
 Sum of electronic and thermal Free Energies=   -4525.729685

L-*left-si*-TS2:

Standard orientation:

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

1	15	0	-1.766660	1.147697	0.524520
2	6	0	-1.196825	2.851522	1.022550
3	6	0	0.136263	2.728277	1.759386
4	15	0	1.335690	1.789923	0.679804
5	6	0	2.611516	1.017664	1.831835
6	6	0	3.879915	1.877684	1.702044
7	6	0	3.524763	3.277539	1.189978
8	6	0	2.464628	3.167059	0.089497
9	6	0	-2.594439	0.593311	2.102288
10	6	0	-3.977519	1.270773	2.036004
11	6	0	-4.504165	1.082723	0.615161
12	6	0	-3.394105	1.417656	-0.396770

77

13	1	0	-1.075568	3.430160	0.093467
14	1	0	-1.943301	3.378999	1.630499
15	1	0	0.531877	3.714658	2.039196
16	1	0	0.003914	2.165806	2.692802
17	1	0	4.425456	1.926959	2.653063
18	1	0	4.414165	3.822222	0.843719
19	1	0	3.101367	3.869136	2.014360
20	1	0	-3.877158	2.340656	2.268685
21	1	0	-4.660649	0.843728	2.782638
22	1	0	-5.413226	1.667361	0.426480
23	1	0	-4.777535	0.026542	0.482083
24	29	0	0.060945	0.292008	-0.419910
25	1	0	4.554769	1.385717	0.987814
26	6	0	2.934064	2.872800	-1.310191
27	6	0	-3.406151	2.769640	-1.044889
28	6	0	-2.719763	-0.902314	2.254571
29	1	0	1.844576	4.075514	0.056759
30	6	0	2.005556	0.811162	3.189150
31	6	0	1.116489	-0.260123	3.351782
32	6	0	0.412705	-0.424324	4.538581
33	6	0	0.593695	0.471605	5.591007
34	6	0	1.488899	1.526288	5.445463
35	6	0	2.185563	1.698515	4.251733
36	6	0	2.005555	2.965245	-2.355607
37	6	0	4.231948	2.466118	-1.618499
38	6	0	4.589347	2.148700	-2.928535
39	6	0	3.657039	2.240010	-3.953649
40	6	0	2.359191	2.657806	-3.661634
41	6	0	-4.015520	3.884714	-0.466307
42	6	0	-2.700963	2.944407	-2.241890
43	6	0	-2.580843	4.199288	-2.826612
44	6	0	-3.179920	5.306568	-2.230664
45	6	0	-3.904672	5.140892	-1.055546
46	6	0	-2.733338	-1.780046	1.169320
47	6	0	-2.954075	-3.142198	1.358846
48	6	0	-3.140323	-3.649269	2.639344
49	6	0	-3.114759	-2.786265	3.732586
50	6	0	-2.914516	-1.425446	3.537281
51	1	0	-2.246372	2.072126	-2.713769
52	1	0	-2.024224	4.312357	-3.754766
53	1	0	-3.088252	6.290932	-2.683621
54	1	0	-4.387009	5.997470	-0.589178
55	1	0	-4.575692	3.775703	0.461778
56	1	0	1.617797	2.737498	-4.454294
57	1	0	0.984113	3.279854	-2.130013
58	1	0	3.935936	1.990301	-4.974354
59	1	0	5.608444	1.832403	-3.144017
60	1	0	4.984272	2.393183	-0.835176
61	1	0	1.641852	2.228324	6.262615
62	1	0	2.865331	2.544078	4.148893
63	1	0	0.046274	0.343799	6.522262
64	1	0	-0.281310	-1.257226	4.636269

65	1	0	0.971226	-0.952862	2.520366
66	1	0	-2.982878	-3.800453	0.490841
67	1	0	-2.557462	-1.410400	0.157752
68	1	0	-3.305442	-4.714056	2.787580
69	1	0	-3.258101	-3.175102	4.738683
70	1	0	-2.910022	-0.745734	4.390990
71	6	0	5.616570	-3.160504	-0.461614
72	6	0	5.145408	-1.847695	-0.531443
73	8	0	1.042270	-1.335951	0.082359
74	6	0	1.401250	-2.397506	-0.521851
75	6	0	2.868193	-2.696601	-0.516161
76	6	0	3.772017	-1.630882	-0.555983
77	6	0	3.366460	-3.997847	-0.450235
78	6	0	4.739926	-4.243487	-0.412972
79	1	0	6.692803	-3.342661	-0.451337
80	1	0	3.378684	-0.616400	-0.647913
81	1	0	2.679848	-4.843445	-0.418847
82	6	0	0.421996	-3.548705	-0.496194
83	1	0	0.652876	-4.341132	-1.216098
84	1	0	-0.581046	-3.155517	-0.702373
85	1	0	0.409800	-3.983623	0.514368
86	6	0	-0.202806	-0.072584	-2.445330
87	6	0	-1.382784	-0.862973	-2.445740
88	6	0	-2.366282	-1.586314	-2.416671
89	6	0	1.040540	-0.678010	-2.731129
90	6	0	1.291112	-2.040593	-2.676896
91	1	0	0.447923	-2.708924	-2.851362
92	1	0	2.256417	-2.405401	-3.019884
93	1	0	-0.308028	0.977446	-2.739546
94	1	0	1.880766	0.012322	-2.851424
95	6	0	-3.461143	-2.474976	-2.247933
96	6	0	-3.260169	-3.863890	-2.339164
97	6	0	-4.747907	-2.002129	-1.936930
98	6	0	-4.309097	-4.744401	-2.111155
99	1	0	-2.267613	-4.233360	-2.591529
100	6	0	-5.789817	-2.889837	-1.709420
101	1	0	-4.914671	-0.927711	-1.867814
102	6	0	-5.577055	-4.263601	-1.791904
103	1	0	-4.135867	-5.815966	-2.184083
104	1	0	-6.777944	-2.506122	-1.464925
105	1	0	-6.395381	-4.956492	-1.611905
106	1	0	-3.369311	0.662300	-1.194419
107	1	0	-2.004540	0.979236	2.948644
108	1	0	2.769897	0.024029	1.389480
109	6	0	5.262309	-5.642150	-0.269825
110	1	0	6.282928	-5.729990	-0.657407
111	1	0	5.289670	-5.950377	0.783982
112	1	0	4.631109	-6.365005	-0.798297
113	6	0	6.095765	-0.687234	-0.577391
114	1	0	5.761006	0.067800	-1.300280
115	1	0	6.166245	-0.190521	0.401207
116	1	0	7.107889	-1.001472	-0.855037

```
-------------------------------------------------------------------
```
Zero-point correction=   0.964167 (Hartree/Particle)
  Thermal correction to Energy=   1.018575
  Thermal correction to Enthalpy=   1.019519
  Thermal correction to Gibbs Free Energy=   0.874980
  Sum of electronic and zero-point Energies=   -4525.643350
  Sum of electronic and thermal Energies=   -4525.588942
  Sum of electronic and thermal Enthalpies=   -4525.587997
  Sum of electronic and thermal Free Energies=   -4525.732537

L-*left-re*-TS2:

Standard orientation:
```
---------------------------------------------------------------------
```

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
```
---------------------------------------------------------------------
```
1	15	0	0.894165	1.391139	1.288145
2	6	0	2.609803	0.933185	1.851695
3	6	0	2.737134	-0.587831	1.887894
4	15	0	2.256269	-1.275139	0.223874
5	6	0	2.263368	-3.154550	0.460027
6	6	0	3.449273	-3.647798	-0.379551
7	6	0	4.553824	-2.589974	-0.391203
8	6	0	3.930295	-1.214179	-0.646998
9	6	0	-0.051432	1.514475	2.921394
10	6	0	-0.260029	3.019335	3.169343
11	6	0	0.879924	3.790002	2.515552
12	6	0	0.981416	3.249273	1.090189
13	1	0	3.311793	1.363076	1.120311
14	1	0	2.854095	1.371111	2.829046
15	1	0	3.747508	-0.911309	2.174392
16	1	0	2.045367	-1.010107	2.631708
17	1	0	3.813807	-4.617986	-0.017699
18	1	0	5.331704	-2.819990	-1.131478
19	1	0	5.053185	-2.568815	0.587550
20	1	0	-0.352065	3.229430	4.241675
21	1	0	-1.198570	3.347881	2.701748
22	1	0	1.818207	3.626355	3.067140
23	1	0	0.696395	4.873179	2.516436
24	29	0	0.449736	-0.065377	-0.352374
25	1	0	3.092006	-3.812493	-1.405501
26	6	0	3.786063	-0.782619	-2.081769
27	6	0	2.093151	3.732902	0.210302
28	6	0	-1.283843	0.653018	2.884156
29	1	0	4.505934	-0.434142	-0.127626
30	6	0	2.218429	-3.549405	1.906972
31	6	0	0.990048	-3.476908	2.576931
32	6	0	0.901418	-3.756676	3.934942
33	6	0	2.038956	-4.120985	4.651658
34	6	0	3.260612	-4.208831	3.994468

35	6	0	3.349694	-3.923607	2.634626
36	6	0	3.585642	0.576670	-2.348216
37	6	0	3.820600	-1.666589	-3.161683
38	6	0	3.657863	-1.205832	-4.466915
39	6	0	3.458381	0.146526	-4.715906
40	6	0	3.425940	1.039102	-3.646988
41	6	0	3.371481	4.020136	0.700904
42	6	0	1.860689	3.881699	-1.162282
43	6	0	2.876278	4.292621	-2.018199
44	6	0	4.149079	4.558430	-1.520304
45	6	0	4.390046	4.425621	-0.156438
46	6	0	-2.488426	1.098133	2.334761
47	6	0	-3.577485	0.241267	2.227054
48	6	0	-3.480899	-1.081954	2.642926
49	6	0	-2.285254	-1.537307	3.187211
50	6	0	-1.202225	-0.674869	3.311525
51	1	0	0.861404	3.679019	-1.551626
52	1	0	2.666416	4.417381	-3.079175
53	1	0	4.944857	4.878620	-2.188747
54	1	0	5.376835	4.643604	0.246502
55	1	0	3.576468	3.931134	1.766857
56	1	0	3.275354	2.103645	-3.818081
57	1	0	3.546097	1.287228	-1.518488
58	1	0	3.331455	0.504717	-5.734600
59	1	0	3.691111	-1.913363	-5.292592
60	1	0	3.988253	-2.729388	-2.995911
61	1	0	4.154255	-4.500018	4.542397
62	1	0	4.317747	-3.997831	2.141294
63	1	0	1.970288	-4.340729	5.714387
64	1	0	-0.062240	-3.695695	4.438261
65	1	0	0.100650	-3.176611	2.017630
66	1	0	-4.505681	0.616335	1.797296
67	1	0	-2.592275	2.118235	1.966133
68	1	0	-4.326684	-1.756767	2.529179
69	1	0	-2.196482	-2.570998	3.518376
70	1	0	-0.265899	-1.043374	3.736675
71	8	0	-1.184436	-1.154300	-0.439710
72	6	0	-1.551582	-1.929623	-1.372728
73	6	0	-0.596597	-3.011397	-1.829931
74	6	0	-3.016025	-2.199762	-1.499422
75	6	0	-3.517338	-3.321575	-2.165557
76	6	0	-3.915497	-1.309471	-0.906427
77	6	0	0.070774	0.963697	-2.137176
78	6	0	-0.957997	1.803151	-1.640337
79	6	0	-1.817673	2.546010	-1.190796
80	6	0	-0.223777	-0.097301	-3.023631
81	6	0	-1.465960	-0.679104	-3.187114
82	1	0	-2.345654	-0.104960	-2.897732
83	1	0	-1.618477	-1.417456	-3.972482
84	1	0	1.050791	1.434357	-2.261073
85	1	0	0.645033	-0.559679	-3.501714

86	6	0	-2.831106	3.286166	-0.532301
87	6	0	-4.140862	2.777544	-0.459271
88	6	0	-2.552877	4.508341	0.106998
89	6	0	-5.122755	3.452057	0.251569
90	1	0	-4.359514	1.839662	-0.969881
91	6	0	-3.542410	5.175546	0.818002
92	1	0	-1.549482	4.928251	0.034222
93	6	0	-4.829384	4.650630	0.900949
94	1	0	-6.129440	3.039654	0.301269
95	1	0	-3.306851	6.117880	1.308517
96	1	0	-5.601154	5.174862	1.459105
97	1	0	0.027106	3.458846	0.582635
98	1	0	0.634161	1.113203	3.684000
99	1	0	1.323587	-3.486856	0.003457
100	6	0	-5.289292	-1.529724	-0.966300
101	6	0	-5.760570	-2.661322	-1.634183
102	6	0	-4.887605	-3.562799	-2.242640
103	1	0	-3.509149	-0.443092	-0.383973
104	1	0	-6.836188	-2.843038	-1.685990
105	1	0	-2.838118	-4.033515	-2.632821
106	1	0	-0.639056	-3.848895	-1.115391
107	1	0	-0.820922	-3.405074	-2.825099
108	1	0	0.424072	-2.611907	-1.838894
109	6	0	-5.423931	-4.745342	-2.994666
110	1	0	-6.351345	-5.120417	-2.546885
111	1	0	-5.655897	-4.484737	-4.036028
112	1	0	-4.700210	-5.566863	-3.019747
113	6	0	-6.253846	-0.586757	-0.305749
114	1	0	-5.866303	0.438377	-0.285909
115	1	0	-7.218644	-0.570356	-0.825780
116	1	0	-6.454015	-0.877919	0.734757

Zero-point correction=   0.964258 (Hartree/Particle)
 Thermal correction to Energy=   1.019627
 Thermal correction to Enthalpy=   1.020572
 Thermal correction to Gibbs Free Energy=   0.874472
 Sum of electronic and zero-point Energies=   -4525.650749
 Sum of electronic and thermal Energies=   -4525.595380
 Sum of electronic and thermal Enthalpies=   -4525.594436
 Sum of electronic and thermal Free Energies=   -4525.740536

S43: The summarize energies of TS2s in the *(S, S)*--BPE-CuMes system in the THF solvent at the M06/6-311+G (d, p).

$$M06(SMD,THF)/6\text{-}311+G\ (d,\ p)$$

Species	SCF$_{SMD}$	G^*_{gas}	G$_{sol}$	ΔG_{sol}(kJ mol^{-1})
L-*right-si*-TS2	-4527.40586818	0.876901	-4526.528967	13.8
L-*right-re*-TS2	-4527.39961608	0.880280	-4526.519336	39.1
L-*left-si*-TS2	-4527.39670706	0.874980	-4526.521727	32.8
L-*left-re*-TS2	-4527.40871509	0.874472	-4526.534243	0.0

Reference 77 details

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

Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.