Supplemental material for "The hydrogen abstraction of carbon/phosphorus-containing radicals in the photoassisted polymerization &"

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Abbreviation list

Abbreviation	
TS	transient state
BAPO	Phenyl bis (2,4,6-trimethylbenzoyl)-phosphine oxide
TPO	diphenyl-(2,4,6-trimethylbenzoyl) phosphine oxide
TPO-L	ethyl-2,4,6-trimethyl benzoyl phenyl phosphinate
APA	aroyl-phosphinoyl
TMB	2,4,6-trimethylbenzaldehyde
B	benzaldehyde
EL	3,6-nonadiene
APAR	aroyl-phosphinoyl radical
TMBR	2,4,6-trimethylbenzoyl radical
BR	benzoyl radical
ELR	3,6-nonadiene radical

Part I : Data from B3LYP 6-311++g(d,p)

BAPO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.131704	0.850834	-0.425364
2	8	0	0.033052	0.280903	-1.813436
3	6	0	2.217422	-3.509466	-0.670683
4	6	0	1.336194	-2.504584	-0.269840
5	6	0	1.859465	-1.393712	0.421416
6	6	0	3.237971	-1.305215	0.715681
7	6	0	4.076277	-2.326025	0.268576
8	6	0	3.589274	-3.433080	-0.429135
9	6	0	0.966966	-0.291069	0.893891
10	8	0	0.818188	0.015876	2.054828
11	6	0	3.826926	-0.145691	1.487202
12	6	0	-0.141775	-2.661201	-0.539440
13	6	0	4.525182	-4.508019	-0.923399
14	6	0	1.707482	2.794617	-1.559396

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15	6	0	2.504349	3.936788	-1.589066
16	6	0	2.756241	4.642710	-0.413859
17	6	0	2.214302	4.205138	0.794802
18	6	0	1.417801	3.063591	0.835827
19	6	0	1.158977	2.357227	-0.346836
20	1	0	1.815974	-4.377196	-1.184983
21	1	0	5.139252	-2.256410	0.478745
22	1	0	4.915815	-0.213852	1.499082
23	1	0	3.473646	-0.138211	2.520932
24	1	0	3.556978	0.818188	1.047677
25	1	0	-0.357085	-3.665855	-0.907472
26	1	0	-0.738565	-2.508293	0.364395
27	1	0	-0.475510	-1.941648	-1.290905
28	1	0	4.019410	-5.473015	-1.000853
29	1	0	5.385318	-4.624485	-0.259946
30	1	0	4.910338	-4.258761	-1.918329
31	1	0	1.504797	2.233801	-2.464439
32	1	0	2.927540	4.273374	-2.528795
33	1	0	3.376002	5.532261	-0.438375
34	1	0	2.409794	4.754602	1.708713
35	1	0	0.998209	2.728721	1.774526
36	1	0	-6.811111	-1.743689	-1.168905
37	6	0	-6.129703	-2.140428	-0.412829
38	6	0	-4.963931	-1.211836	-0.179477
39	1	0	-6.697366	-2.307395	0.505408
40	1	0	-5.782303	-3.117646	-0.766129
41	6	0	-4.476326	-0.401109	-1.205817
42	6	0	-4.338908	-1.145582	1.066154
43	6	0	-3.364748	0.424409	-1.034959
44	1	0	-4.978313	-0.403291	-2.168517
45	6	0	-3.241503	-0.315673	1.303223
46	1	0	-4.722880	-1.745886	1.885441
47	6	0	-2.731966	0.442204	0.225770
48	6	0	-2.925624	1.322537	-2.168191
49	6	0	-2.666373	-0.240834	2.700029
50	6	0	-1.529977	1.300531	0.473549
51	1	0	-3.641162	1.271957	-2.990745
52	1	0	-1.942902	1.030518	-2.545776
53	1	0	-2.866819	2.367199	-1.846832
54	1	0	-3.028498	-1.076341	3.301853
55	1	0	-1.575608	-0.256798	2.714924
56	1	0	-2.973400	0.686796	3.191202
57	8	0	-1.491377	2.192156	1.284786

Zero-point correction= 0.459077 (Hartree/Particle)
Thermal correction to Energy= 0.490833
Thermal correction to Enthalpy= 0.491777
Thermal correction to Gibbs Free Energy= 0.392047
Sum of electronic and zero-point Energies= -1573.967529
Sum of electronic and thermal Energies= -1573.935773
Sum of electronic and thermal Enthalpies= -1573.934829
Sum of electronic and thermal Free Energies= -1574.034559

Excited State 1: Triplet-A 2.5373 eV 488.64 nm f=0.0000
Excited State 3: Singlet-A 3.0223 eV 410.23 nm f=0.0176

TPO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.803490	-0.103257	-0.580352
2	8	0	-0.325368	-0.357148	-1.981764
3	6	0	3.837783	-1.439766	-0.505308
4	6	0	2.473317	-1.374496	-0.222704
5	6	0	1.979675	-0.235595	0.446211
6	6	0	2.849350	0.811590	0.828430
7	6	0	4.198102	0.708990	0.489826
8	6	0	4.713166	-0.404611	-0.176453
9	6	0	0.535197	-0.116603	0.799047
10	8	0	0.133135	0.099971	1.924139
11	6	0	2.371200	2.037797	1.573784
12	6	0	1.587880	-2.538844	-0.602203
13	6	0	6.173291	-0.477057	-0.547835
14	6	0	-1.446746	2.384752	-1.554222
15	6	0	-1.965338	3.678348	-1.527537
16	6	0	-2.540037	4.176288	-0.360247
17	6	0	-2.597352	3.379587	0.783896
18	6	0	-2.083098	2.085858	0.763802
19	6	0	-1.506296	1.582477	-0.408773
20	1	0	4.225051	-2.326996	-0.996808
21	1	0	4.867008	1.519414	0.762969
22	1	0	3.158387	2.793177	1.597898
23	1	0	2.098534	1.793439	2.602901
24	1	0	1.489876	2.486482	1.108696
25	1	0	2.193290	-3.420560	-0.820386
26	1	0	0.894346	-2.807797	0.199303
27	1	0	0.998648	-2.296755	-1.490405
28	1	0	6.524958	-1.510566	-0.584443
29	1	0	6.794543	0.071293	0.164037
30	1	0	6.343246	-0.038247	-1.537288
31	1	0	-0.997233	1.981249	-2.454078
32	1	0	-1.919315	4.294578	-2.418467
33	1	0	-2.943198	5.182747	-0.339789
34	1	0	-3.043514	3.766013	1.693396
35	1	0	-2.124610	1.479958	1.659498
36	6	0	-4.021601	-3.220934	0.564005
37	6	0	-3.594233	-3.055078	-0.751968
38	6	0	-3.467190	-2.441857	1.578972
39	6	0	-2.615898	-2.110640	-1.055274
40	1	0	-4.018072	-3.663228	-1.543249
41	6	0	-2.492349	-1.491560	1.283107
42	1	0	-3.790827	-2.575665	2.605138
43	6	0	-2.065410	-1.318095	-0.040163
44	1	0	-4.781166	-3.957988	0.799933
45	1	0	-2.266782	-1.981539	-2.073212
46	1	0	-2.053436	-0.906046	2.080273

Zero-point correction= 0.368401
(Hartree/Particle)
Thermal correction to Energy= 0.392573
Thermal correction to Enthalpy= 0.393517

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 Thermal correction to Gibbs Free Energy=          0.311866
 Sum of electronic and zero-point Energies=          -1342.733643
 Sum of electronic and thermal Energies=             -1342.709471
 Sum of electronic and thermal Enthalpies=           -1342.708527
 Sum of electronic and thermal Free Energies=        -1342.790177
 SCF Done:  E(RB+HF-LYP) =  -1343.10204353

Excited State   1:   Triplet-A      2.6707 eV  464.24 nm  f=0.0000
Excited State   3:   Singlet-A      3.1743 eV  390.59 nm  f=0.0084
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TPO-L

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.946200	0.652123	0.623100
2	8	0	-0.440543	0.752349	2.018354
3	6	0	3.897652	0.692888	0.585479
4	6	0	2.564533	1.004913	0.317468
5	6	0	1.786309	0.067535	-0.392861
6	6	0	2.347529	-1.153215	-0.831264
7	6	0	3.675491	-1.427339	-0.506327
8	6	0	4.467707	-0.520740	0.200577
9	6	0	0.362682	0.354667	-0.733872
10	8	0	-0.074124	0.325806	-1.869170
11	6	0	1.558864	-2.173293	-1.622267
12	6	0	2.019983	2.345343	0.752780
13	6	0	5.895385	-0.853693	0.555686
14	6	0	-2.653587	-1.250055	1.615602
15	6	0	-3.596672	-2.274075	1.575713
16	6	0	-4.047324	-2.762202	0.350379
17	6	0	-3.551623	-2.227120	-0.838087
18	6	0	-2.611073	-1.199683	-0.806649
19	6	0	-2.160976	-0.699743	0.423959
20	1	0	4.506463	1.422642	1.110377
21	1	0	4.105174	-2.373163	-0.822139
22	1	0	2.113132	-3.111140	-1.685793
23	1	0	1.363790	-1.821563	-2.637945
24	1	0	0.589060	-2.388373	-1.166326
25	1	0	2.836820	3.015873	1.025740
26	1	0	1.444672	2.831787	-0.039639
27	1	0	1.362108	2.231695	1.617897
28	1	0	6.508218	0.047312	0.631590
29	1	0	6.348364	-1.514436	-0.187071
30	1	0	5.944366	-1.365447	1.523220
31	1	0	-2.283717	-0.872891	2.561851
32	1	0	-3.973571	-2.694331	2.501309
33	1	0	-4.778226	-3.562702	0.320591
34	1	0	-3.894506	-2.611619	-1.792110
35	1	0	-2.220743	-0.799774	-1.733803
36	8	0	-1.643622	2.036217	0.142398
37	6	0	-3.008585	3.689907	-0.921428
38	6	0	-2.560094	2.242399	-0.960852
39	1	0	-2.156014	4.363152	-1.032296

40	1	0	-3.708758	3.880390	-1.739969
41	1	0	-3.507879	3.915107	0.023151
42	1	0	-3.410202	1.564242	-0.845964
43	1	0	-2.046462	2.007472	-1.896036

Zero-point correction= 0.348644
(Hartree/Particle)
Thermal correction to Energy= 0.372130
Thermal correction to Enthalpy= 0.373074
Thermal correction to Gibbs Free Energy= 0.293304
Sum of electronic and zero-point Energies= -1265.555980
Sum of electronic and thermal Energies= -1265.532495
Sum of electronic and thermal Enthalpies= -1265.531551
Sum of electronic and thermal Free Energies= -1265.611321
SCF Done: E(RB+HF-LYP) = -1265.90462459

Excited State 1: Triplet-A 2.6221 eV 472.84 nm f=0.0000 <S**2>=2.000
Excited State 3: Singlet-A 3.1502 eV 393.58 nm f=0.0043 <S**2>=0.000

APAR(from BAPO)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.062162	0.000359	0.993493
2	8	0	-0.671407	-1.319634	1.620666
3	6	0	3.284338	-1.342762	-0.562743
4	6	0	1.933407	-0.995510	-0.612136
5	6	0	1.566493	0.310274	-0.236328
6	6	0	2.535897	1.248853	0.177526
7	6	0	3.867626	0.840814	0.234608
8	6	0	4.263277	-0.448473	-0.129623
9	6	0	0.139664	0.746588	-0.297352
10	8	0	-0.281627	1.649199	-0.984029
11	6	0	2.169693	2.663946	0.562727
12	6	0	0.921524	-2.010074	-1.090078
13	6	0	5.709670	-0.866956	-0.037439
14	6	0	-3.538601	-1.140160	0.560518
15	6	0	-4.855204	-1.181061	0.112689
16	6	0	-5.395605	-0.094790	-0.575709
17	6	0	-4.616773	1.037593	-0.814663
18	6	0	-3.299618	1.092610	-0.368205
19	6	0	-2.749575	-0.006356	0.311269
20	1	0	4.617748	1.553175	0.564457
21	1	0	3.576391	-2.341247	-0.873180
22	1	0	3.036975	3.182101	0.974448
23	1	0	1.376173	2.689766	1.315429
24	1	0	1.810474	3.229193	-0.300445
25	1	0	1.419161	-2.825420	-1.617992
26	1	0	0.374789	-2.435115	-0.243599
27	1	0	0.191013	-1.570312	-1.774400
28	1	0	5.940589	-1.243863	0.964969
29	1	0	6.381388	-0.028003	-0.233556
30	1	0	5.940642	-1.663496	-0.747997

31	1	0	-3.110582	-1.977906	1.098339
32	1	0	-5.459324	-2.061580	0.300409
33	1	0	-6.422326	-0.129173	-0.922421
34	1	0	-5.036233	1.882619	-1.348804
35	1	0	-2.697452	1.970148	-0.561518

Zero-point correction= 0.276092 (Hartree/Particle)
Thermal correction to Energy= 0.295415
Thermal correction to Enthalpy= 0.296359
Thermal correction to Gibbs Free Energy= 0.225443
Sum of electronic and zero-point Energies= -1111.081260
Sum of electronic and thermal Energies= -1111.061938
Sum of electronic and thermal Enthalpies= -1111.060994
Sum of electronic and thermal Free Energies= -1111.131909

APA (from BAPO)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.181572	1.637169	0.107056
2	8	0	0.764812	2.354410	-1.141669
3	6	0	-3.494301	0.446416	-0.524342
4	6	0	-2.337924	1.011949	0.013729
5	6	0	-1.368804	0.152165	0.571997
6	6	0	-1.574693	-1.246007	0.606278
7	6	0	-2.735305	-1.758076	0.027755
8	6	0	-3.704716	-0.932571	-0.545775
9	6	0	-0.116432	0.699012	1.166411
10	8	0	0.255597	0.487400	2.301085
11	6	0	-0.582431	-2.197690	1.235671
12	6	0	-2.191548	2.515829	0.039802
13	6	0	-4.937857	-1.519818	-1.185799
14	6	0	2.712873	0.007391	-1.512681
15	6	0	3.666768	-0.968299	-1.796934
16	6	0	4.350294	-1.600208	-0.759808
17	6	0	4.083149	-1.257873	0.566675
18	6	0	3.130749	-0.285216	0.858708
19	6	0	2.441703	0.347779	-0.183425
20	1	0	1.733918	2.437115	1.140299
21	1	0	-4.252932	1.105983	-0.934050
22	1	0	-2.889346	-2.832844	0.032885
23	1	0	-0.842628	-3.229010	0.991929
24	1	0	-0.573381	-2.094553	2.323202
25	1	0	0.438293	-2.018009	0.889346
26	1	0	-3.124126	2.992948	-0.266108
27	1	0	-1.952383	2.878763	1.044352
28	1	0	-1.397583	2.845919	-0.634792
29	1	0	-5.768262	-0.810549	-1.177828
30	1	0	-5.258813	-2.429518	-0.672936
31	1	0	-4.742393	-1.784896	-2.230713
32	1	0	2.182089	0.517261	-2.308637
33	1	0	3.878028	-1.230651	-2.827405
34	1	0	5.093870	-2.357141	-0.983193

35	1	0	4.618909	-1.746166	1.372820
36	1	0	2.920723	-0.025364	1.890081

Zero-point correction= 0.286557 (Hartree/Particle)
Thermal correction to Energy= 0.305809
Thermal correction to Enthalpy= 0.306753
Thermal correction to Gibbs Free Energy= 0.236623
Sum of electronic and zero-point Energies= -1111.699760
Sum of electronic and thermal Energies= -1111.680508
Sum of electronic and thermal Enthalpies= -1111.679563
Sum of electronic and thermal Free Energies= -1111.749694

TMBR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.432102	1.068732	-0.009322
2	6	0	-0.061271	1.314104	-0.000907
3	6	0	0.825652	0.212776	0.003025
4	6	0	0.330791	-1.116633	-0.002945
5	6	0	-1.050474	-1.304358	-0.011042
6	6	0	-1.945591	-0.231121	-0.011225
7	6	0	2.267000	0.501009	0.012704
8	8	0	3.210889	-0.225602	0.006863
9	6	0	1.243141	-2.315886	-0.004032
10	6	0	0.446646	2.736425	-0.003721
11	6	0	-3.433946	-0.470305	0.014014
12	1	0	-2.118231	1.909765	-0.015761
13	1	0	-1.439893	-2.317851	-0.019083
14	1	0	0.659132	-3.237750	-0.007071
15	1	0	1.897871	-2.321031	0.870904
16	1	0	1.901027	-2.317117	-0.876604
17	1	0	-0.387053	3.439987	0.035691
18	1	0	1.100492	2.928837	0.849965
19	1	0	1.030824	2.948389	-0.902785
20	1	0	-3.694665	-1.419870	-0.458097
21	1	0	-3.975379	0.328613	-0.497346
22	1	0	-3.800313	-0.505614	1.045998

Zero-point correction= 0.178854 (Hartree/Particle)
Thermal correction to Energy= 0.190638
Thermal correction to Enthalpy= 0.191582
Thermal correction to Gibbs Free Energy= 0.138958
Sum of electronic and zero-point Energies= -462.819494
Sum of electronic and thermal Energies= -462.807710
Sum of electronic and thermal Enthalpies= -462.806766
Sum of electronic and thermal Free Energies= -462.859390

TMB

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.452393	1.060414	-0.009701
2	6	0	-0.081176	1.304370	-0.002911
3	6	0	0.815239	0.204369	0.001025
4	6	0	0.307330	-1.120923	-0.004206
5	6	0	-1.075215	-1.305990	-0.011214
6	6	0	-1.971240	-0.236342	-0.010468
7	6	0	2.266458	0.475246	0.007264
8	8	0	3.156593	-0.354474	0.011806
9	6	0	1.193507	-2.341567	-0.005706
10	6	0	0.385926	2.746657	-0.003643
11	6	0	-3.460034	-0.472410	0.016618
12	1	0	2.539363	1.546268	0.008982
13	1	0	-2.136280	1.903592	-0.016260
14	1	0	-1.463366	-2.319788	-0.019039
15	1	0	0.582214	-3.246395	-0.013295
16	1	0	1.848237	-2.363488	0.867934
17	1	0	1.857748	-2.355024	-0.872285
18	1	0	-0.475992	3.415619	-0.008916
19	1	0	0.983146	2.987908	0.879844
20	1	0	0.991557	2.984612	-0.882273
21	1	0	-3.721080	-1.430134	-0.438512
22	1	0	-3.999426	0.317475	-0.511052
23	1	0	-3.829272	-0.487802	1.048085

Zero-point correction= 0.191657 (Hartree/Particle)
Thermal correction to Energy= 0.203121
Thermal correction to Enthalpy= 0.204065
Thermal correction to Gibbs Free Energy= 0.153799
Sum of electronic and zero-point Energies= -463.454637
Sum of electronic and thermal Energies= -463.443173
Sum of electronic and thermal Enthalpies= -463.442229
Sum of electronic and thermal Free Energies= -463.492495

ELR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.664818	0.887574	-0.136635
2	1	0	5.630238	0.744727	-0.630465
3	1	0	4.175826	1.755542	-0.586783
4	1	0	4.858662	1.122055	0.914332
5	6	0	3.787139	-0.370405	-0.270614
6	1	0	4.340053	-1.223758	0.146740
7	1	0	3.624054	-0.596716	-1.329585
8	6	0	2.467507	-0.246041	0.426910
9	1	0	2.500188	-0.050852	1.498437
10	6	0	1.247542	-0.351465	-0.178457
11	1	0	1.226449	-0.544718	-1.251309
12	6	0	0.000000	-0.234339	0.473093

13	6	0	-1.247542	-0.351465	-0.178457
14	1	0	-1.226449	-0.544718	-1.251309
15	6	0	-2.467507	-0.246041	0.426910
16	1	0	-2.500188	-0.050852	1.498436
17	6	0	-3.787139	-0.370405	-0.270614
18	1	0	-3.624054	-0.596716	-1.329585
19	1	0	-4.340052	-1.223758	0.146739
20	6	0	-4.664818	0.887574	-0.136634
21	1	0	-5.630238	0.744726	-0.630464
22	1	0	-4.858662	1.122055	0.914332
23	1	0	-4.175826	1.755542	-0.586783
24	1	0	0.000000	-0.042477	1.544251

Zero-point correction= 0.212482 (Hartree/Particle)
Thermal correction to Energy= 0.223953
Thermal correction to Enthalpy= 0.224897
Thermal correction to Gibbs Free Energy= 0.173871
Sum of electronic and zero-point Energies= -351.828465
Sum of electronic and thermal Energies= -351.816994
Sum of electronic and thermal Enthalpies= -351.816050
Sum of electronic and thermal Free Energies= -351.867075

EL

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.048958	0.059700	1.204002
2	1	0	5.041258	0.477101	1.397118
3	1	0	3.330437	0.578639	1.844128
4	1	0	4.065278	-0.991726	1.507157
5	6	0	3.667854	0.203692	-0.278405
6	1	0	4.438541	-0.285003	-0.888842
7	1	0	3.671837	1.261314	-0.562086
8	6	0	2.327847	-0.397747	-0.600115
9	1	0	2.222267	-1.463585	-0.392835
10	6	0	1.283142	0.263938	-1.096760
11	1	0	1.383430	1.330877	-1.297955
12	6	0	-0.060674	-0.344002	-1.414876
13	1	0	-0.240508	-0.248053	-2.496110
14	6	0	-1.197112	0.322128	-0.679073
15	1	0	-1.308991	1.394037	-0.844571
16	6	0	-2.050684	-0.295012	0.137289
17	1	0	-1.931770	-1.366109	0.306795
18	6	0	-3.182646	0.364424	0.875294
19	1	0	-3.231070	1.423263	0.600388
20	1	0	-4.132130	-0.083951	0.554586
21	6	0	-3.063597	0.226649	2.401841
22	1	0	-3.917883	0.687370	2.905934
23	1	0	-3.027674	-0.825223	2.701745
24	1	0	-2.152250	0.707391	2.767445
25	1	0	-0.048228	-1.415160	-1.191743

Zero-point correction= 0.225787 (Hartree/Particle)
Thermal correction to Energy= 0.237385
Thermal correction to Enthalpy= 0.238329
Thermal correction to Gibbs Free Energy= 0.187174
Sum of electronic and zero-point Energies= -352.438040
Sum of electronic and thermal Energies= -352.426442
Sum of electronic and thermal Enthalpies= -352.425497
Sum of electronic and thermal Free Energies= -352.476652

B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.729535	1.063648	0.000005
2	6	0	-0.354916	1.286968	-0.000004
3	6	0	0.534008	0.206633	-0.000008
4	6	0	0.038300	-1.104591	-0.000006
5	6	0	-1.332438	-1.326057	0.000000
6	6	0	-2.216565	-0.242619	0.000006
7	1	0	-2.417789	1.900960	0.000008
8	1	0	0.034559	2.300467	-0.000005
9	1	0	0.742996	-1.927881	-0.000011
10	1	0	-1.718914	-2.338870	0.000001
11	1	0	-3.286412	-0.419397	0.000010
12	6	0	1.992144	0.463642	-0.000016
13	8	0	2.848569	-0.392487	0.000014
14	1	0	2.271023	1.538872	0.000028

Zero-point correction= 0.109359 (Hartree/Particle)
Thermal correction to Energy= 0.115692
Thermal correction to Enthalpy= 0.116636
Thermal correction to Gibbs Free Energy= 0.078770
Sum of electronic and zero-point Energies= -345.559828
Sum of electronic and thermal Energies= -345.553495
Sum of electronic and thermal Enthalpies= -345.552551
Sum of electronic and thermal Free Energies= -345.590417

BR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.706751	-1.055224	-0.000004
2	6	0	-0.336632	-1.301557	-0.000003
3	6	0	0.563836	-0.231592	0.000009

4	6	0	0.090264	1.090390	0.000005
5	6	0	-1.277842	1.329972	0.000000
6	6	0	-2.174936	0.258201	-0.000003
7	1	0	-2.407288	-1.882040	-0.000010
8	1	0	0.048581	-2.314667	0.000001
9	1	0	0.801475	1.908044	0.000007
10	1	0	-1.650191	2.348160	0.000002
11	1	0	-3.242118	0.450109	-0.000007
12	6	0	2.016978	-0.511122	0.000021
13	8	0	2.925004	0.251998	-0.000018

Zero-point correction=	0.097125 (Hartree/Particle)
Thermal correction to Energy=	0.103491
Thermal correction to Enthalpy=	0.104436
Thermal correction to Gibbs Free Energy=	0.065795
Sum of electronic and zero-point Energies=	-344.919155
Sum of electronic and thermal Energies=	-344.912788
Sum of electronic and thermal Enthalpies=	-344.911844
Sum of electronic and thermal Free Energies=	-344.950484

TS: TMBR+EL

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.880246	-2.776535	-0.575384
2	1	0	6.431260	-3.515684	-1.164067
3	1	0	6.273058	-1.785445	-0.817916
4	1	0	6.090244	-2.967894	0.481292
5	6	0	4.371149	-2.854974	-0.862343
6	1	0	4.030430	-3.879111	-0.657749
7	1	0	4.185985	-2.673706	-1.926575
8	6	0	3.564389	-1.891610	-0.039810
9	1	0	3.642002	-2.002324	1.041981
10	6	0	2.786910	-0.914280	-0.533035
11	1	0	2.718227	-0.806714	-1.616118
12	6	0	1.969321	0.011222	0.268578
13	6	0	1.646542	1.320919	-0.320835
14	1	0	1.564915	1.353682	-1.408223
15	6	0	1.415073	2.451171	0.365436
16	1	0	1.508075	2.431995	1.451766
17	6	0	1.053325	3.775942	-0.242731
18	1	0	0.952618	3.665740	-1.327787
19	1	0	0.068458	4.089010	0.129729
20	6	0	2.071195	4.884222	0.075669
21	1	0	1.759576	5.839897	-0.355676
22	1	0	2.176051	5.024248	1.155843
23	1	0	3.057769	4.634627	-0.323971
24	1	0	2.283816	0.069687	1.313680
25	1	0	0.837904	-0.607997	0.492248
26	6	0	-3.071675	-1.455146	-1.245135
27	6	0	-1.784913	-1.413060	-0.710273
28	6	0	-1.630951	-1.269663	0.686858
29	6	0	-2.771227	-1.161887	1.526363
30	6	0	-4.033082	-1.182352	0.934136

31	6	0	-4.207524	-1.335112	-0.443375
32	6	0	-0.267740	-1.215574	1.264081
33	8	0	0.048917	-1.421693	2.402420
34	6	0	-2.676020	-1.019188	3.025385
35	6	0	-0.603980	-1.532331	-1.645202
36	6	0	-5.589914	-1.399146	-1.042313
37	1	0	-3.189523	-1.580681	-2.317025
38	1	0	-4.907846	-1.082722	1.569794
39	1	0	-3.664167	-0.825534	3.447021
40	1	0	-2.007258	-0.206320	3.316784
41	1	0	-2.273170	-1.924672	3.484817
42	1	0	-0.929876	-1.900011	-2.620057
43	1	0	-0.129415	-0.559413	-1.800056
44	1	0	0.161538	-2.209726	-1.264102
45	1	0	-5.988272	-2.418271	-0.986385
46	1	0	-5.583923	-1.106173	-2.094252
47	1	0	-6.286015	-0.748173	-0.508237

Zero-point correction=	0.400733 (Hartree/Particle)
Thermal correction to Energy=	0.425136
Thermal correction to Enthalpy=	0.426081
Thermal correction to Gibbs Free Energy=	0.341921
Sum of electronic and zero-point Energies=	-815.239812
Sum of electronic and thermal Energies=	-815.215408
Sum of electronic and thermal Enthalpies=	-815.214464
Sum of electronic and thermal Free Energies=	-815.298623

TS: APAR+EL

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.729204	1.064784	-0.616084
2	1	0	7.586436	0.726682	-1.204679
3	1	0	6.689884	2.156123	-0.667507
4	1	0	6.909517	0.786084	0.426498
5	6	0	5.424030	0.440917	-1.138996
6	1	0	5.523900	-0.652527	-1.114840
7	1	0	5.271878	0.716233	-2.187485
8	6	0	4.221634	0.834538	-0.334239
9	1	0	4.254226	0.590037	0.727572
10	6	0	3.135810	1.463119	-0.818990
11	1	0	3.100102	1.702938	-1.880949
12	6	0	1.955496	1.819498	-0.034812
13	6	0	1.130715	2.941928	-0.475461
14	1	0	1.115894	3.137677	-1.547050
15	6	0	0.385952	3.717926	0.332706
16	1	0	0.404466	3.523966	1.405384
17	6	0	-0.456577	4.874932	-0.117315
18	1	0	-0.423105	4.951658	-1.208730
19	1	0	-1.504423	4.682533	0.149189
20	6	0	-0.028640	6.210102	0.516108
21	1	0	-0.685758	7.022719	0.194413
22	1	0	-0.069667	6.159804	1.608309
23	1	0	0.995348	6.467295	0.232623
24	1	0	2.081568	1.741067	1.046020

25	1	0	1.120238	0.712789	-0.192254
26	15	0	0.268984	-0.713005	-0.464218
27	8	0	-0.030373	-0.942420	-1.925126
28	6	0	-4.448216	-1.641107	-0.795448
29	6	0	-3.107017	-1.657520	-0.411467
30	6	0	-2.595719	-0.552806	0.304335
31	6	0	-3.437260	0.535937	0.638490
32	6	0	-4.760448	0.513617	0.200255
33	6	0	-5.286236	-0.561342	-0.518795
34	6	0	-1.177897	-0.523517	0.762842
35	8	0	-0.837289	-0.218980	1.892465
36	6	0	-2.958180	1.724321	1.440100
37	6	0	-2.274938	-2.876031	-0.737400
38	6	0	-6.716180	-0.545663	-0.998094
39	6	0	1.895309	-2.932898	-0.644583
40	6	0	2.753756	-3.927737	-0.182466
41	6	0	3.075759	-4.001443	1.172097
42	6	0	2.537147	-3.075802	2.066665
43	6	0	1.680157	-2.075916	1.613797
44	6	0	1.348593	-2.005035	0.252482
45	1	0	-5.402002	1.357219	0.436454
46	1	0	-4.847624	-2.500445	-1.325186
47	1	0	-3.694627	2.528805	1.393201
48	1	0	-2.005296	2.111084	1.071586
49	1	0	-2.805870	1.457302	2.488160
50	1	0	-2.921334	-3.708107	-1.022554
51	1	0	-1.595996	-2.668461	-1.568751
52	1	0	-1.672541	-3.203349	0.113868
53	1	0	-6.789977	-0.059910	-1.977390
54	1	0	-7.362135	0.005522	-0.310629
55	1	0	-7.112923	-1.557733	-1.104226
56	1	0	1.636427	-2.866555	-1.695116
57	1	0	3.168498	-4.646839	-0.880308
58	1	0	3.743342	-4.777268	1.530406
59	1	0	2.783362	-3.133306	3.121232
60	1	0	1.257195	-1.365556	2.312944

Zero-point correction=	0.496940 (Hartree/Particle)
Thermal correction to Energy=	0.529226
Thermal correction to Enthalpy=	0.530170
Thermal correction to Gibbs Free Energy=	0.426606
Sum of electronic and zero-point Energies=	-1463.504412
Sum of electronic and thermal Energies=	-1463.472127
Sum of electronic and thermal Enthalpies=	-1463.471183
Sum of electronic and thermal Free Energies=	-1463.574747

TS: BR+EL

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.713688	5.450291	0.020289
2	1	0	-0.433476	6.382732	-0.478004
3	1	0	-1.802569	5.358976	-0.014097

4	1	0	-0.420149	5.532813	1.071318
5	6	0	-0.039621	4.241666	-0.650496
6	1	0	1.047453	4.399505	-0.643379
7	1	0	-0.336388	4.187803	-1.703107
8	6	0	-0.357933	2.938548	0.026615
9	1	0	-0.076711	2.865274	1.078378
10	6	0	-0.977051	1.897480	-0.549025
11	1	0	-1.272418	1.984410	-1.595100
12	6	0	-1.265365	0.603046	0.097852
13	6	0	-2.521974	-0.073880	-0.267971
14	1	0	-2.843944	0.036900	-1.303309
15	6	0	-3.256149	-0.840595	0.552284
16	1	0	-2.938158	-0.952370	1.589601
17	6	0	-4.513161	-1.565826	0.166909
18	1	0	-4.716814	-1.405063	-0.896762
19	1	0	-4.357960	-2.645912	0.292253
20	6	0	-5.733718	-1.145345	1.002761
21	1	0	-6.620156	-1.720419	0.720179
22	1	0	-5.556286	-1.309701	2.070098
23	1	0	-5.957045	-0.084192	0.862757
24	1	0	-1.081319	0.610736	1.175764
25	6	0	3.731800	-0.081520	0.953474
26	6	0	2.427817	-0.123898	0.466377
27	6	0	1.994022	-1.229496	-0.272400
28	6	0	2.871281	-2.296561	-0.520626
29	6	0	4.168977	-2.252494	-0.027754
30	6	0	4.599210	-1.145161	0.708785
31	1	0	4.071338	0.776794	1.521659
32	1	0	1.746122	0.699813	0.643240
33	1	0	2.518120	-3.144484	-1.095885
34	1	0	4.848934	-3.076075	-0.214807
35	1	0	5.613499	-1.113500	1.091067
36	6	0	0.602154	-1.271551	-0.787033
37	8	0	0.134308	-2.102690	-1.507342
38	1	0	-0.333926	-0.207281	-0.313701

Zero-point correction= 0.318217 (Hartree/Particle)
Thermal correction to Energy= 0.337630
Thermal correction to Enthalpy= 0.338574
Thermal correction to Gibbs Free Energy= 0.265419
Sum of electronic and zero-point Energies= -697.345254
Sum of electronic and thermal Energies= -697.325841
Sum of electronic and thermal Enthalpies= -697.324896
Sum of electronic and thermal Free Energies= -697.398051

TS: EL+ELR (thermneutral reaction)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.854196	0.895850	-3.381828
2	1	0	3.066917	1.118081	-4.431514
3	1	0	2.295248	1.736083	-2.961311
4	1	0	3.810489	0.835079	-2.853346
5	6	0	2.060494	-0.414853	-3.244687

6	1	0	2.631035	-1.219583	-3.728400
7	1	0	1.115277	-0.334115	-3.791794
8	6	0	1.783523	-0.790512	-1.817686
9	1	0	2.657182	-0.948652	-1.184464
10	6	0	0.558886	-0.916572	-1.273252
11	1	0	-0.309427	-0.748403	-1.910525
12	6	0	0.278300	-1.308719	0.105690
13	6	0	-0.985386	-0.894527	0.712339
14	1	0	-1.811834	-0.712216	0.025179
15	6	0	-1.213712	-0.774116	2.032806
16	1	0	-0.389587	-0.950751	2.724324
17	6	0	-2.524839	-0.384633	2.651913
18	1	0	-3.279657	-0.265322	1.867482
19	1	0	-2.876574	-1.199838	3.299080
20	6	0	-2.437992	0.900955	3.492228
21	1	0	-3.400996	1.132563	3.956317
22	1	0	-1.698097	0.799119	4.291981
23	1	0	-2.143546	1.753045	2.873727
24	1	0	1.138800	-1.266931	0.776505
25	6	0	2.650420	-6.371792	3.539193
26	1	0	2.845963	-6.602073	4.590473
27	1	0	2.056470	-7.186217	3.115905
28	1	0	3.611828	-6.355279	3.016863
29	6	0	1.918585	-5.026244	3.395323
30	1	0	2.522013	-4.248092	3.882636
31	1	0	0.966680	-5.062600	3.935517
32	6	0	1.669817	-4.639674	1.966014
33	1	0	2.554430	-4.524272	1.338788
34	6	0	0.456584	-4.455283	1.412714
35	1	0	-0.423276	-4.580533	2.043963
36	6	0	0.205796	-4.050900	0.031565
37	6	0	-1.073665	-4.398905	-0.583594
38	1	0	-1.914175	-4.533795	0.097413
39	6	0	-1.297546	-4.512193	-1.905437
40	1	0	-0.459469	-4.382775	-2.590580
41	6	0	-2.622251	-4.833559	-2.534608
42	1	0	-3.389188	-4.910169	-1.756673
43	1	0	-2.924598	-4.003100	-3.187333
44	6	0	-2.596127	-6.124796	-3.370468
45	1	0	-3.565619	-6.306300	-3.843275
46	1	0	-1.844185	-6.065140	-4.163164
47	1	0	-2.353456	-6.989223	-2.746638
48	1	0	1.067435	-4.138536	-0.633304
49	1	0	0.175737	-2.678104	0.067873

Zero-point correction= 0.434641 (Hartree/Particle)
Thermal correction to Energy= 0.458974
Thermal correction to Enthalpy= 0.459918
Thermal correction to Gibbs Free Energy= 0.375167
Sum of electronic and zero-point Energies= -704.233121
Sum of electronic and thermal Energies= -704.208787
Sum of electronic and thermal Enthalpies= -704.207843
Sum of electronic and thermal Free Energies= -704.292594

Part II : Data from M062X 6-311++g(d,p)

BAPO

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.252244	-1.108778	-0.564276
2	8	0	-0.164856	-0.657668	-1.985373
3	6	0	-1.181857	3.581025	-0.953806
4	6	0	-0.555559	2.414841	-0.522141
5	6	0	-1.314879	1.493564	0.210499
6	6	0	-2.670620	1.714562	0.497201
7	6	0	-3.257135	2.884204	0.024038
8	6	0	-2.529441	3.826672	-0.701018
9	6	0	-0.695819	0.231413	0.703483
10	8	0	-0.567136	-0.063785	1.865726
11	6	0	-3.480518	0.714151	1.285671
12	6	0	0.902754	2.173322	-0.820459
13	6	0	-3.194484	5.073479	-1.222219
14	6	0	-2.362824	-2.642583	-1.364686
15	6	0	-3.424261	-3.527026	-1.203709
16	6	0	-3.676892	-4.087870	0.043678
17	6	0	-2.871917	-3.768345	1.135144
18	6	0	-1.809909	-2.885785	0.985564
19	6	0	-1.556676	-2.326065	-0.270144
20	1	0	-0.600895	4.315599	-1.503254
21	1	0	-4.307171	3.067203	0.231247
22	1	0	-4.530008	1.007375	1.305624
23	1	0	-3.119318	0.643738	2.313391
24	1	0	-3.415337	-0.286892	0.848773
25	1	0	1.382490	3.094455	-1.153461
26	1	0	1.447635	1.810640	0.056496
27	1	0	1.003206	1.426013	-1.612346
28	1	0	-2.481786	5.895269	-1.304633
29	1	0	-4.010514	5.387565	-0.569756
30	1	0	-3.612994	4.894900	-2.216662
31	1	0	-2.150080	-2.187278	-2.325759
32	1	0	-4.053034	-3.775123	-2.050320
33	1	0	-4.504467	-4.776538	0.168315
34	1	0	-3.071565	-4.209156	2.104358
35	1	0	-1.185283	-2.630992	1.832618
36	1	0	6.154278	2.067297	-0.919257
37	6	0	5.577548	2.123231	0.004621
38	6	0	4.536830	1.036799	0.065157
39	1	0	6.266641	2.055985	0.848187
40	1	0	5.101851	3.107228	0.043991
41	6	0	4.090739	0.405593	-1.089917
42	6	0	3.999185	0.639578	1.290792
43	6	0	3.082930	-0.558080	-1.058924
44	1	0	4.538010	0.661439	-2.046192
45	6	0	3.010764	-0.334380	1.380325
46	1	0	4.370463	1.093586	2.204611
47	6	0	2.523247	-0.894239	0.180725

48	6	0	2.691938	-1.238283	-2.348384
49	6	0	2.516541	-0.777455	2.734513
50	6	0	1.331083	-1.791308	0.265267
51	1	0	3.595306	-1.529266	-2.888926
52	1	0	2.101165	-0.572768	-2.979253
53	1	0	2.095631	-2.135840	-2.184617
54	1	0	2.921879	-0.127865	3.510290
55	1	0	1.427991	-0.757393	2.799669
56	1	0	2.836429	-1.801538	2.936706
57	8	0	1.255178	-2.793211	0.921450

Zero-point correction= 0.464935
(Hartree/Particle)
Thermal correction to Energy= 0.495865
Thermal correction to Enthalpy= 0.496810
Thermal correction to Gibbs Free Energy= 0.401126
Sum of electronic and zero-point Energies= -1573.406638
Sum of electronic and thermal Energies= -1573.375708
Sum of electronic and thermal Enthalpies= -1573.374764
Sum of electronic and thermal Free Energies= -1573.470447
SCF Done: E(RM062X) = -1573.87157335

Excited State 1: Triplet-A 2.6606 eV 466.00 nm f=0.0000 <S**2>=2.000
Excited State 3: Singlet-A 3.0719 eV 403.60 nm f=0.0074 <S**2>=0.000

TPO

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.779984	-0.074945	-0.584390
2	8	0	-0.251698	-0.292937	-1.964514
3	6	0	3.792623	-1.363289	-0.445239
4	6	0	2.433920	-1.285260	-0.153545
5	6	0	1.953457	-0.118163	0.455889
6	6	0	2.805857	0.955736	0.761291
7	6	0	4.150473	0.842147	0.422567
8	6	0	4.660736	-0.307379	-0.178594
9	6	0	0.511430	0.009576	0.800367
10	8	0	0.099306	0.272341	1.904828
11	6	0	2.296488	2.211319	1.426148
12	6	0	1.528886	-2.451589	-0.465742
13	6	0	6.116503	-0.395588	-0.553730
14	6	0	-1.571911	2.354304	-1.547211
15	6	0	-2.172116	3.609271	-1.509431
16	6	0	-2.799863	4.045187	-0.348235
17	6	0	-2.831039	3.228382	0.779939
18	6	0	-2.235792	1.973644	0.749729
19	6	0	-1.605310	1.535991	-0.417477
20	1	0	4.181691	-2.272389	-0.893794
21	1	0	4.818999	1.669791	0.639597
22	1	0	3.048570	2.998289	1.369929
23	1	0	2.062200	2.026693	2.476020
24	1	0	1.381689	2.576200	0.952284
25	1	0	2.110560	-3.370357	-0.547871

26	1	0	0.774226	-2.605761	0.310502
27	1	0	1.010310	-2.280253	-1.412433
28	1	0	6.469995	-1.427141	-0.521780
29	1	0	6.734091	0.203029	0.117408
30	1	0	6.270669	-0.022417	-1.570073
31	1	0	-1.077295	1.993501	-2.442296
32	1	0	-2.148368	4.244288	-2.386957
33	1	0	-3.266971	5.022705	-0.319592
34	1	0	-3.320283	3.569782	1.684299
35	1	0	-2.253137	1.346931	1.632473
36	6	0	-3.672046	-3.458685	0.561239
37	6	0	-3.231329	-3.286173	-0.746572
38	6	0	-3.232718	-2.600443	1.565413
39	6	0	-2.354265	-2.251747	-1.054435
40	1	0	-3.566349	-3.958803	-1.527102
41	6	0	-2.358198	-1.561981	1.265950
42	1	0	-3.567224	-2.742777	2.586060
43	6	0	-1.924526	-1.382312	-0.050289
44	1	0	-4.353733	-4.266322	0.800950
45	1	0	-1.989760	-2.108784	-2.065972
46	1	0	-1.999656	-0.913272	2.055805

Zero-point correction= 0.372573
(Hartree/Particle)
Thermal correction to Energy= 0.396408
Thermal correction to Enthalpy= 0.397352
Thermal correction to Gibbs Free Energy= 0.316415
Sum of electronic and zero-point Energies= -1342.270084
Sum of electronic and thermal Energies= -1342.246249
Sum of electronic and thermal Enthalpies= -1342.245305
Sum of electronic and thermal Free Energies= -1342.326242
SCF Done: E(RM062X) = -1342.64265720

Excited State 1: Triplet-A 2.7244 eV 455.09 nm f=0.0000 <S**2>=2.000
Excited State 2: Singlet-A 3.1347 eV 395.52 nm f=0.0065 <S**2>=0.000

TPO-L

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.969499	0.760797	0.646546
2	8	0	-0.424194	0.939290	2.009215
3	6	0	3.805896	0.745924	0.582294
4	6	0	2.491733	1.125007	0.322072
5	6	0	1.696665	0.268079	-0.451186
6	6	0	2.199168	-0.943827	-0.954514
7	6	0	3.509162	-1.292246	-0.642118
8	6	0	4.325924	-0.461342	0.123532
9	6	0	0.283349	0.627115	-0.753752
10	8	0	-0.169613	0.718844	-1.871366
11	6	0	1.354326	-1.864183	-1.801326
12	6	0	1.976841	2.442853	0.845239
13	6	0	5.735071	-0.867880	0.465111
14	6	0	-2.192389	-1.466905	1.653816

15	6	0	-2.903826	-2.661249	1.610688
16	6	0	-3.340398	-3.167185	0.391083
17	6	0	-3.064895	-2.483503	-0.790657
18	6	0	-2.356478	-1.288398	-0.754922
19	6	0	-1.925421	-0.772959	0.471999
20	1	0	4.438752	1.413119	1.160374
21	1	0	3.905453	-2.232833	-1.012873
22	1	0	1.853783	-2.824793	-1.927857
23	1	0	1.176964	-1.431112	-2.787615
24	1	0	0.377713	-2.045747	-1.344628
25	1	0	2.791703	3.165356	0.910134
26	1	0	1.205048	2.870028	0.200413
27	1	0	1.538745	2.308887	1.835856
28	1	0	6.396168	-0.000454	0.501080
29	1	0	6.131324	-1.574556	-0.265392
30	1	0	5.765853	-1.349119	1.446702
31	1	0	-1.827862	-1.064674	2.592782
32	1	0	-3.111251	-3.198743	2.528215
33	1	0	-3.891813	-4.099684	0.358434
34	1	0	-3.399181	-2.883317	-1.740654
35	1	0	-2.126360	-0.767405	-1.677892
36	8	0	-1.890574	1.987414	0.172916
37	6	0	-3.548225	3.331083	-0.871154
38	6	0	-2.957267	1.941679	-0.791294
39	1	0	-2.794677	4.044524	-1.206632
40	1	0	-4.379751	3.340496	-1.578606
41	1	0	-3.914271	3.643675	0.107406
42	1	0	-3.702195	1.213412	-0.458312
43	1	0	-2.552023	1.624220	-1.754711

Zero-point correction= 0.353301
(Hartree/Particle)
Thermal correction to Energy= 0.376167
Thermal correction to Enthalpy= 0.377111
Thermal correction to Gibbs Free Energy= 0.299669
Sum of electronic and zero-point Energies= -1265.120956
Sum of electronic and thermal Energies= -1265.098090
Sum of electronic and thermal Enthalpies= -1265.097146
Sum of electronic and thermal Free Energies= -1265.174589
SCF Done: E(RM062X) = -1265.47425732

Excited State	1:	Triplet-A	2.6742 eV	463.63 nm	f=0.0000	<S**2>=2.000
Excited State	2:	Singlet-A	3.0973 eV	400.29 nm	f=0.0039	<S**2>=0.000