Supplementary Materials

A Computational Study of the Mechanism of the Photocyclization Reaction of α-Methylamino Ketone

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Table S1. The vertical excitation energies and oscillator strengths for the fifteen lowest energy triplet excited states of molecule **1** at the TD-DFT/M06-L/6-311G(d,p).

Excited State 1:	3.009-?Sym	0.3744 eV	3311.50 nm	f=0.0000	<S**2>=2.014
78B -> 80B	0.82332				
79B -> 80B	-0.56831				
Excited State 2:	3.009-?Sym	0.3883 eV	3193.08 nm	f=0.0000	<S**2>=2.013
81A -> 85A	0.15334				
78B -> 80B	0.56555				
79B -> 80B	0.81574				
81A <- 85A	0.11608				
Excited State 3:	3.010-?Sym	0.7904 eV	1568.72 nm	f=0.0001	<S**2>=2.015
77B -> 80B	0.99736				
Excited State 4:	3.010-?Sym	1.0367 eV	1195.90 nm	f=0.0005	<S**2>=2.015
81A -> 82A	0.99956				
Excited State 5:	3.011-?Sym	1.1236 eV	1103.50 nm	f=0.0001	<S**2>=2.017
76B -> 80B	0.99600				
Excited State 6:	3.011-?Sym	1.2185 eV	1017.55 nm	f=0.0000	<S**2>=2.017
75B -> 80B	0.99871				
Excited State 7:	3.010-?Sym	1.4497 eV	855.22 nm	f=0.0004	<S**2>=2.015
81A -> 83A	0.99994				
Excited State 8:	3.011-?Sym	1.9779 eV	626.83 nm	f=0.0009	<S**2>=2.017
81A -> 84A	0.99321				
Excited State 9:	3.011-?Sym	2.0381 eV	608.32 nm	f=0.00009	<S**2>=2.017
73B -> 80B	0.99921				
Excited State 10:	3.013-?Sym	2.9240 eV	424.02 nm	f=0.0002	<S**2>=2.020
81A -> 85A	-0.15577				
68B -> 80B	0.75667				
69B -> 80B	-0.41677				
70B -> 80B	-0.44828				
Excited State 11:	3.013-?Sym	3.1597 eV	392.39 nm	f=0.0433	<S**2>=2.020
81A -> 85A	-0.29186				
67B -> 80B	0.88544				
68B -> 80B	-0.25921				
69B -> 80B	-0.20649				
Excited State 12:	3.034-?Sym	3.2088 eV	386.39 nm	f=0.1165	<S**2>=2.052
81A -> 85A	0.65899				
67B -> 80B	0.44444				
68B -> 80B	0.25811				

69B -> 80B	0.39204				
78B -> 82B	-0.26623				
79B -> 82B	-0.15817				
Excited State 13:	3.018-?Sym	3.5132 eV	352.91 nm	f=0.0042	<S**2>=2.028
64B -> 80B	-0.11466				
65B -> 80B	0.45937				
66B -> 80B	0.83400				
68B -> 80B	-0.17382				
70B -> 80B	-0.11264				
Excited State 14:	4.101-?Sym	3.6597 eV	338.78 nm	f=0.0000	<S**2>=3.955
76A -> 82A	0.11707				
76A -> 83A	0.32004				
77A -> 82A	-0.40764				
77A -> 83A	0.10867				
79A -> 82A	-0.31284				
80A -> 82A	-0.30341				
81A -> 86A	0.13069				
75B -> 83B	0.32861				
76B -> 81B	0.43200				
77B -> 81B	0.39492				
79B -> 81B	-0.12192				
Excited State 15:	3.032-?Sym	3.6874 eV	336.24 nm	f=0.0006	<S**2>=2.049
81A -> 86A	0.98754				

Table S2. The vertical excitation energies and oscillator strengths for the fifteen lowest energy singlet excited states of molecule **1** at the TD-DFT/M06-L/6-311G(d,p).

Excited State 1:	Singlet-?Sym	3.6563 eV	339.10 nm	f=0.0004	<S**2>=0.000
80 -> 81	0.70101				
Excited State 2:	Singlet-?Sym	3.9300 eV	315.48 nm	f=0.0000	<S**2>=0.000
79 -> 81	0.69724				
Excited State 3:	Singlet-?Sym	4.3311 eV	286.26 nm	f=0.0000	<S**2>=0.000
79 -> 82	0.12798				
80 -> 82	0.68758				
Excited State 4:	Singlet-?Sym	4.3453 eV	285.33 nm	f=0.0000	<S**2>=0.000
77 -> 81	0.51421				
78 -> 81	-0.47321				
Excited State 5:	Singlet-?Sym	4.4583 eV	278.10 nm	f=0.0000	<S**2>=0.000
75 -> 81	0.69958				
Excited State 6:	Singlet-?Sym	4.6037 eV	269.31 nm	f=0.0146	<S**2>=0.000
77 -> 82	-0.11243				
78 -> 82	0.12171				
79 -> 82	0.67613				
80 -> 82	-0.10434				
Excited State 7:	Singlet-?Sym	4.6496 eV	266.65 nm	f=0.0165	<S**2>=0.000
76 -> 81	0.49917				
76 -> 84	0.14052				
77 -> 81	-0.23846				
77 -> 84	0.13825				
78 -> 81	-0.34048				
78 -> 84	0.12505				
Excited State 8:	Singlet-?Sym	4.7207 eV	262.64 nm	f=0.0101	<S**2>=0.000
80 -> 83	0.69645				
Excited State 9:	Singlet-?Sym	4.8009 eV	258.25 nm	f=0.0031	<S**2>=0.000
80 -> 84	0.70009				
Excited State 10:	Singlet-?Sym	4.9712 eV	249.40 nm	f=0.0016	<S**2>=0.000
75 -> 82	-0.16004				
79 -> 83	0.68511				
Excited State 11:	Singlet-?Sym	5.0048 eV	247.73 nm	f=0.0145	<S**2>=0.000
74 -> 81	0.28896				
77 -> 82	0.40908				
78 -> 82	0.46364				

79 -> 84	-0.10603				
Excited State 12:	Singlet-?Sym	5.0097 eV	247.49 nm	f=0.0425	<S**2>=0.000
74 -> 81	0.58568				
77 -> 82	-0.19382				
78 -> 82	-0.27381				
79 -> 84	-0.13797				
Excited State 13:	Singlet-?Sym	5.0426 eV	245.87 nm	f=0.0167	<S**2>=0.000
74 -> 81	0.24456				
76 -> 81	0.15372				
77 -> 81	0.16789				
78 -> 81	0.15641				
79 -> 84	0.59336				
Excited State 14:	Singlet-?Sym	5.0916 eV	243.51 nm	f=0.0022	<S**2>=0.000
76 -> 82	0.68901				
77 -> 82	0.10925				
Excited State 15:	Singlet-?Sym	5.1462 eV	240.92 nm	f=0.2518	<S**2>=0.000
73 -> 81	0.15576				
76 -> 81	0.35222				
77 -> 81	0.31967				
78 -> 81	0.28214				
78 -> 84	0.13869				
79 -> 84	-0.32453				

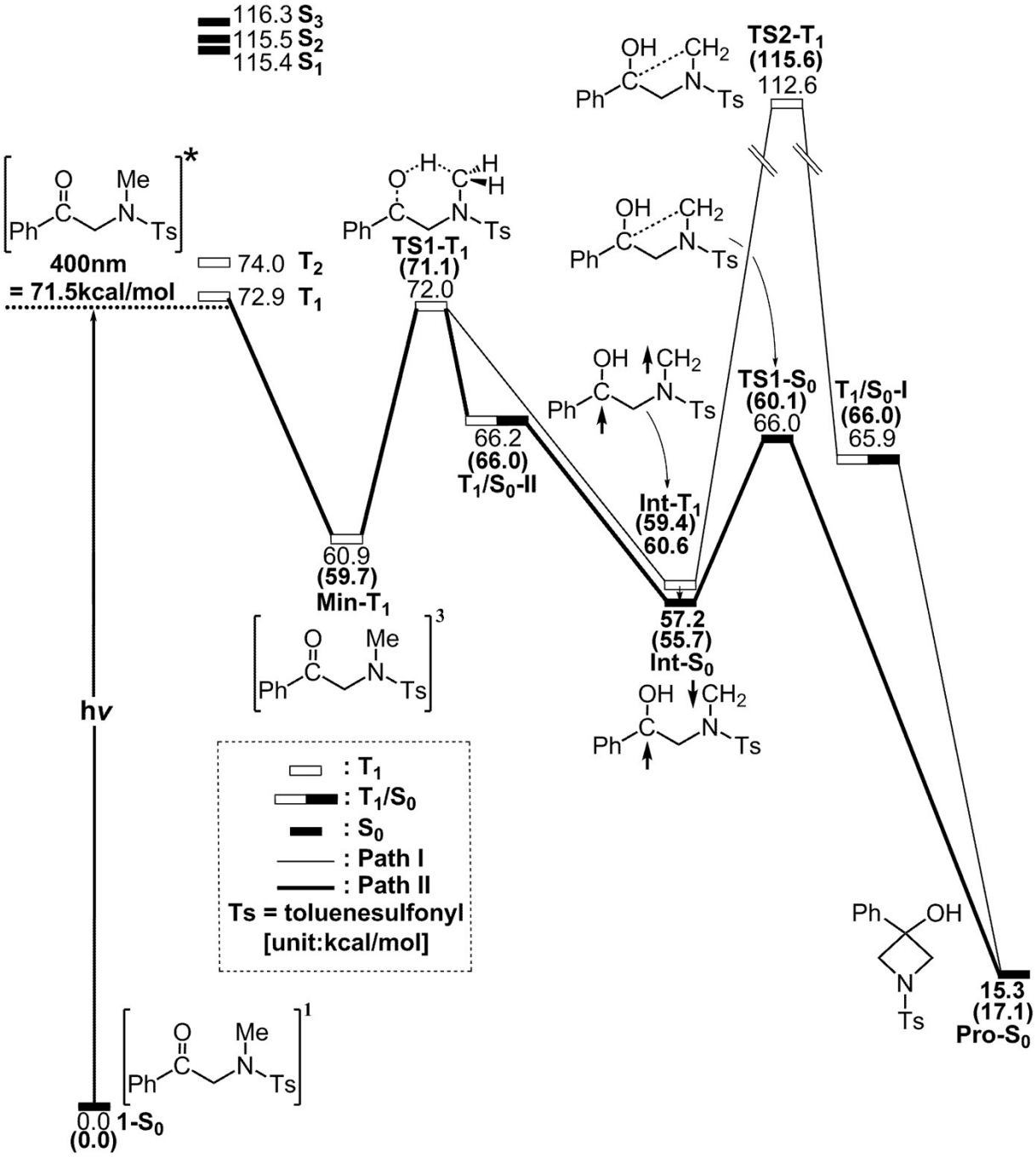
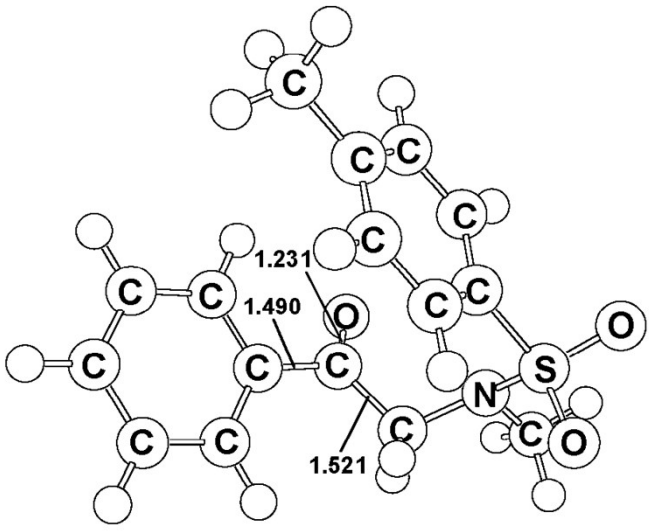


Figure S1 The energy profiles for the photochemical cyclization addition of α-*N*-methylamidoacetophenone (**1**). The relative energies are obtained at the M06-L/6-311G(d,p) level of theory. All energies (in kcal/mol) are given with respect to the reactant (**1**). The solvent effect (SCRF = PCM, solvent = DMA) have been considered using the For the M06-L/6-311G(d,p) + PCM(solvent) = DMA)//M06-L/6-311G(d,p) method, whose computational values are given in the parenthesis. For more information, see IV Conclusion.



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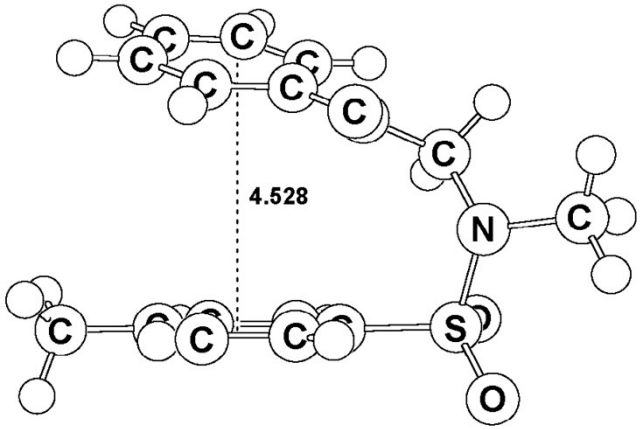

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.146802	-1.601922	0.930757
8	-0.015969	-1.392477	2.137035
6	1.030405	-1.904225	0.016696
1	0.780771	-1.694954	-1.026732
1	1.234581	-2.978638	0.087309
7	2.217418	-1.104178	0.427803
6	3.402479	-1.935999	0.704242
1	3.150036	-2.713097	1.433228
1	4.204476	-1.337115	1.145015
1	3.763669	-2.415729	-0.210296
16	2.538931	0.282832	-0.504811

8	3.636517	1.004899	0.100613
8	2.600844	-0.147195	-1.887482
6	-1.516053	-1.569380	0.341825
6	-4.111186	-1.425439	-0.694958
6	-2.498705	-0.812889	0.994218
6	-1.845953	-2.269133	-0.825095
6	-3.142307	-2.192356	-1.341511
6	-3.791208	-0.737751	0.473929
1	-2.256357	-0.269550	1.906058
1	-1.123460	-2.892286	-1.343610
1	-3.400333	-2.735755	-2.247782
1	-4.546265	-0.143291	0.982275
1	-5.119225	-1.368701	-1.099078
6	1.072183	1.256575	-0.286665
6	-1.262567	2.737955	0.101215
6	0.783149	1.770413	0.979199
6	0.220885	1.496427	-1.367332
6	-0.944354	2.238778	-1.169669
6	-0.382763	2.512661	1.168944
1	1.450893	1.581974	1.817735
1	0.452924	1.114213	-2.358498
1	-1.606087	2.425800	-2.013011
1	-0.604130	2.907669	2.158419
6	-2.504376	3.555528	0.304082
1	-2.289654	4.613302	0.124160
1	-2.885919	3.439299	1.323957
1	-3.298836	3.233504	-0.377389

Figure S2 The geometrical (bond length, Å) conformation with the two aromatic rings stacking for α-*N*-methylamidoacetophenone at the M06-L/6-311G(d,p) level of theory. Its Cartesian coordinate is given as well. The computational result indicates that the energy of this two-rings-stacked structure is above the initial reactant (**1-S$_0$**) by 10.2 kcal/mol.

(All were calculated at the M06-L/6-311G(d,p) level of theory)

1. 1-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-2.927466	2.528514	-0.050430
6	-3.650373	1.722067	-0.113035
6	-5.454401	-0.391871	-0.233225
6	-3.247563	0.446097	0.296165
6	-4.932005	1.934407	-0.596157
6	-5.836874	0.877153	-0.656150
6	-4.162739	-0.610057	0.231937
1	-5.229131	2.923430	-0.930787
1	-6.840841	1.042210	-1.035512
1	-3.879725	-1.606532	0.558502
1	-6.162106	-1.213673	-0.272585
6	-1.855374	0.285174	0.793913
8	-1.181291	1.243190	1.110860
6	-1.314667	-1.139892	0.934806
1	-1.759308	-1.805771	0.182183
1	-1.632634	-1.524693	1.912451
7	0.143180	-1.164942	0.910025
6	0.791453	-2.149557	1.764990
1	0.506180	-1.952009	2.800398
1	1.875490	-2.034107	1.693061
1	0.536707	-3.185360	1.506465
16	0.765702	-1.093158	-0.663417
8	1.119510	-2.420093	-1.148328
8	-0.178136	-0.265819	-1.396730
6	2.277565	-0.204345	-0.380537
6	4.641767	1.206237	0.019086
6	2.224243	1.056195	0.208581
6	3.483486	-0.771642	-0.773630
6	4.658877	-0.059638	-0.570915
6	3.409547	1.749421	0.404045
1	1.266788	1.465157	0.521140
1	3.487692	-1.756491	-1.227982
1	5.607340	-0.496671	-0.870981

1	3.384009	2.730478	0.870332
6	5.913239	1.972401	0.216675
1	5.854736	2.637370	1.080660
1	6.134010	2.596612	-0.655694
1	6.767011	1.305535	0.357560

M06L/6-311G** = -1298.6085446

2. FC-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-2.927466	2.528514	-0.050430
6	-3.650373	1.722067	-0.113035
6	-5.454401	-0.391871	-0.233225
6	-3.247563	0.446097	0.296165
6	-4.932005	1.934407	-0.596157
6	-5.836874	0.877153	-0.656150
6	-4.162739	-0.610057	0.231937
1	-5.229131	2.923430	-0.930787
1	-6.840841	1.042210	-1.035512
1	-3.879725	-1.606532	0.558502
1	-6.162106	-1.213673	-0.272585
6	-1.855374	0.285174	0.793913
8	-1.181291	1.243190	1.110860
6	-1.314667	-1.139892	0.934806
1	-1.759308	-1.805771	0.182183
1	-1.632634	-1.524693	1.912451
7	0.143180	-1.164942	0.910025
6	0.791453	-2.149557	1.764990
1	0.506180	-1.952009	2.800398
1	1.875490	-2.034107	1.693061
1	0.536707	-3.185360	1.506465
16	0.765702	-1.093158	-0.663417
8	1.119510	-2.420093	-1.148328
8	-0.178136	-0.265819	-1.396730
6	2.277565	-0.204345	-0.380537
6	4.641767	1.206237	0.019086
6	2.224243	1.056195	0.208581

6	3.483486	-0.771642	-0.773630
6	4.658877	-0.059638	-0.570915
6	3.409547	1.749421	0.404045
1	1.266788	1.465157	0.521140
1	3.487692	-1.756491	-1.227982
1	5.607340	-0.496671	-0.870981
1	3.384009	2.730478	0.870332
6	5.913239	1.972401	0.216675
1	5.854736	2.637370	1.080660
1	6.134010	2.596612	-0.655694
1	6.767011	1.305535	0.357560

M06L/6-311G** = -1298.4855165

3. Min-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-4.548686	1.709421	0.852084
6	-4.503658	0.676401	0.522750
6	-4.347478	-1.970249	-0.316696
6	-3.358640	0.245597	-0.202666
6	-5.531225	-0.200148	0.804586
6	-5.471018	-1.531956	0.388431
6	-3.307714	-1.109238	-0.615222
1	-6.394327	0.155213	1.359892
1	-6.279851	-2.218151	0.615372
1	-2.437413	-1.498184	-1.131391
1	-4.277741	-3.007147	-0.631684
6	-2.328190	1.198296	-0.456914
8	-2.373770	2.418808	-0.054117
6	-1.132359	0.913024	-1.394833
1	-1.136142	1.669631	-2.186534
1	-1.274567	-0.073403	-1.834375
7	0.170034	0.976329	-0.772023
6	0.551188	2.284800	-0.272684
1	0.504051	2.998441	-1.100669
1	1.573854	2.258817	0.113895
1	-0.140787	2.624363	0.515407

16	0.545636	-0.344528	0.274945
8	0.170757	-0.030077	1.641969
8	0.033866	-1.511051	-0.419955
6	2.318401	-0.320950	0.177480
6	5.099786	-0.318668	0.047634
6	2.946360	-0.688500	-1.009642
6	3.052883	0.047694	1.298707
6	4.439500	0.044356	1.224669
6	4.331366	-0.681361	-1.065534
1	2.352669	-0.979720	-1.870424
1	2.532249	0.324331	2.209694
1	5.021725	0.329509	2.096714
1	4.831255	-0.965276	-1.987682
6	6.595014	-0.349802	-0.011414
1	6.966050	-0.136851	-1.016127
1	6.973578	-1.339135	0.266937
1	7.041561	0.369066	0.678844

M06L/6-311G** = -1298.5114358

4. TS1-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	4.730979	-0.970729	0.037306
6	4.406980	0.063909	0.037915
6	3.557111	2.713151	0.014828
6	3.025607	0.339916	-0.156459
6	5.319283	1.085597	0.205002
6	4.910025	2.422136	0.198114
6	2.628419	1.703258	-0.164945
1	6.370103	0.843690	0.338196
1	5.631977	3.220926	0.331197
1	1.585766	1.972030	-0.307621
1	3.224614	3.747403	0.011305
6	2.115081	-0.735351	-0.345678
8	2.564313	-1.980207	-0.309000
6	0.694884	-0.483735	-0.835076

1	0.706840	-0.193515	-1.900700
1	0.241535	0.355469	-0.295758
7	-0.174551	-1.643474	-0.703765
6	0.390718	-2.876684	-1.083510
16	-1.268322	-1.676711	0.643871
8	-2.038456	-2.886849	0.437658
8	-0.547368	-1.423669	1.876083
6	-2.255257	-0.247751	0.275321
6	-3.850512	1.980767	-0.225640
6	-2.295642	0.786560	1.203919
6	-3.005911	-0.194696	-0.897462
6	-3.790118	0.922541	-1.141061
6	-3.096232	1.890654	0.946771
1	-1.703652	0.713773	2.109990
1	-2.972376	-1.015243	-1.607078
1	-4.371283	0.978808	-2.057307
1	-3.132987	2.701386	1.668676
6	-4.721633	3.170892	-0.479551
1	-4.332321	4.064883	0.011620
1	-5.731447	3.004876	-0.089100
1	-4.821729	3.382503	-1.545842
1	1.601760	-2.698538	-0.622265
1	0.583682	-2.958794	-2.159305
1	-0.121191	-3.738404	-0.651758

M06L/6-311G** = -1298.4938651

5. T_1/S_0-II

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	4.7234453	-1.1727522	0.2626080
6	4.5084340	-0.1198782	0.1205380
6	3.9146657	2.5798690	-0.2337360
6	3.1549598	0.2764755	-0.0220106
6	5.5244570	0.8137348	0.0786545
6	5.2415337	2.1708519	-0.0982719
6	2.8860391	1.6580951	-0.1976681

1	6.5539230	0.4869529	0.1861565
1	6.0443536	2.8994443	-0.1290374
1	1.8626675	2.0050461	-0.2987109
1	3.6831444	3.6319338	-0.3687243
6	2.1096871	-0.6761103	0.0732348
8	2.3950723	-1.9424317	0.3402396
6	0.6742485	-0.3139633	-0.1630591
1	0.6016894	0.3876915	-1.0047755
1	0.2553585	0.2078167	0.7075672
7	-0.1760321	-1.4669684	-0.4482668
6	0.3379353	-2.5312814	-1.2022860
16	-1.4374905	-1.7681129	0.6780289
8	-2.1109721	-2.9517382	0.1899726
8	-0.9041734	-1.6687496	2.0227232
6	-2.4277887	-0.3303082	0.3709665
6	-3.8258313	2.0040921	-0.2203351
6	-2.3928321	0.7326243	1.2675382
6	-3.1634658	-0.2544338	-0.8096955
6	-3.8580371	0.9086245	-1.0933847
6	-3.0943011	1.8924015	0.9631604
1	-1.8244211	0.6396597	2.1869309
1	-3.1821526	-1.0996424	-1.4898509
1	-4.4325597	0.9794752	-2.0124174
1	-3.0677311	2.7311611	1.6531206
6	-4.5777206	3.2555667	-0.5458257
1	-4.1721056	4.1188238	-0.0155930
1	-5.6312489	3.1653514	-0.2617704
1	-4.5550627	3.4700423	-1.6162755
1	1.7115961	-2.5383986	-0.1386295
1	0.8647995	-2.2009987	-2.0983463
1	-0.3376650	-3.3724892	-1.2978892

Difference Gradient:

-1	0.00022141	-0.00000389	-0.00002679
-2	0.00598583	-0.00130143	0.00020146
-3	-0.00074372	-0.00155811	-0.00375763
-4	-0.01917020	-0.00876210	0.02405816
-5	-0.00207285	-0.00315995	-0.00078933
-6	0.00268722	0.00379691	0.00013634
-7	-0.00149737	0.00544191	-0.00097508
-8	0.00036295	-0.00012730	0.00012645

-9	0.00026403	0.00034246	0.00034738
-10	-0.00074083	0.00025570	0.00194815
-11	-0.00010210	0.00062330	-0.00013990
-12	-0.00445134	0.04291085	-0.04034333
-13	0.00144300	-0.10683293	-0.00508932
-14	-0.00431030	0.01891100	-0.01774767
-15	-0.00262259	0.00455469	-0.00302645
-16	-0.00480340	0.00202589	-0.00026318
-17	0.02303910	-0.02796172	0.00070783
-18	-0.05449184	0.03877813	-0.02036963
-19	-0.00914213	0.00082348	0.01382199
-20	0.00182104	-0.00213320	-0.00152732
-21	0.00008598	-0.00186496	-0.00604925
-22	-0.00151587	0.00310462	-0.00112223
-23	-0.00119477	-0.00143146	-0.00292378
-24	-0.00224653	-0.00043336	-0.00022809
-25	0.00208700	-0.00166102	0.00126638
-26	-0.00067868	0.00266615	0.00071445
-27	0.00122718	-0.00224359	0.00241144
-28	0.00073359	0.00056701	-0.00045413
-29	-0.00042726	0.00024331	-0.00012756
-30	0.00003658	0.00002386	0.00001955
-31	0.00007780	-0.00034384	-0.00000265
-32	0.00023873	0.00019584	-0.00017170
-33	0.00003796	-0.00012141	-0.00004686
-34	0.00012856	-0.00016221	0.00013154
-35	0.00002829	-0.00007227	0.00009011
-36	0.06084349	0.04553702	0.05021666
-37	0.00676959	-0.00648102	0.00704833
-38	0.00209245	-0.00414636	0.00193563

M06L/6-311G** = -1298.5030820700

6. Int-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.600422	-2.037144	0.941453

6	3.195029	-1.302396	0.403365
6	4.750419	0.573694	-0.945960
6	2.574855	-0.122578	-0.082032
6	4.544274	-1.525479	0.215446
6	5.334909	-0.599102	-0.476292
6	3.401942	0.821212	-0.743539
1	4.992783	-2.436636	0.599343
1	6.385860	-0.799895	-0.657639
1	2.953737	1.709910	-1.178829
1	5.345836	1.289605	-1.507192
6	1.174125	0.113468	0.073656
8	0.647974	1.329017	-0.251787
6	0.171081	-0.964773	-0.076719
1	0.628204	-1.945383	0.108469
1	-0.253187	-0.984220	-1.089791
7	-0.944503	-0.708806	0.858747
6	-0.598117	-0.823342	2.154268
16	-2.545801	-1.388118	0.339215
8	-3.427686	-1.092860	1.452451
8	-2.754144	-0.865104	-0.996015
6	-2.274044	-3.131225	0.265382
6	-1.625593	-5.846851	0.243939
6	-1.721603	-3.698973	-0.884090
6	-2.473738	-3.895964	1.415241
6	-2.157030	-5.247205	1.388626
6	-1.408884	-5.048067	-0.887211
1	-1.561758	-3.085073	-1.765333
1	-2.907776	-3.434761	2.295816
1	-2.333113	-5.853367	2.273223
1	-0.991901	-5.498081	-1.784229
6	-1.327237	-7.313020	0.212990
1	-0.467966	-7.539330	-0.421958
1	-2.176860	-7.875495	-0.189774
1	-1.127524	-7.707337	1.211292
1	1.292394	2.007071	-0.018100
1	-1.370784	-0.675385	2.897572
1	0.416635	-1.082148	2.426090

M06L/6-311G** = -1298.51739

7. TS1-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.357647	1.179302	1.500883
6	3.267537	1.074197	0.920352
6	5.613684	0.884574	-0.562275
6	3.231230	0.441494	-0.347702
6	4.446084	1.592892	1.423419
6	5.630205	1.498150	0.693168
6	4.439571	0.375926	-1.086808
1	4.440281	2.079577	2.394293
1	6.554009	1.898704	1.098057
1	4.434293	-0.107352	-2.058334
1	6.536697	0.798816	-1.129501
6	2.028111	-0.121785	-0.855858
8	1.966841	-0.372591	-2.183515
6	0.754390	-0.192535	-0.078787
7	0.107062	-1.469526	-0.414751
6	0.967636	-2.536270	-0.107334
16	-1.408090	-1.661454	0.589942
8	-2.021511	-2.879639	0.094979
8	-0.997760	-1.517872	1.982750
6	-2.446706	-0.277298	0.199018
6	-4.222280	1.815734	-0.277186
6	-2.506528	0.788198	1.094291
6	-3.249976	-0.309328	-0.936335
6	-4.127570	0.740108	-1.166264
6	-3.391835	1.825612	0.848039
1	-1.883525	0.775689	1.982228
1	-3.203969	-1.161858	-1.605432
1	-4.767900	0.717569	-2.043444
1	-3.455573	2.652758	1.549712
6	-5.223105	2.906010	-0.497702
1	-4.898628	3.850190	-0.056085
1	-6.182105	2.649326	-0.034534
1	-5.416659	3.071928	-1.559057
1	1.175451	-0.911818	-2.332032

1	1.593306	-2.472873	0.795212
1	0.625305	-3.518543	-0.425015
1	0.061729	0.626239	-0.335679
1	0.966411	-0.130972	0.996974

M06L/6-311G** = -1298.5032994

8. Pro-S_0

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	4.393628	-1.211526	-0.031121
6	3.902313	-0.246204	-0.015292
6	2.622053	2.222794	0.025822
6	2.509010	-0.196134	-0.013556
6	4.647533	0.928638	0.003553
6	4.013002	2.164751	0.024661
6	1.876202	1.051603	0.007430
1	5.731989	0.875047	0.003085
1	4.597629	3.079292	0.040427
1	0.788298	1.111828	0.010356
1	2.115935	3.183697	0.043030
6	1.686951	-1.453812	-0.025165
8	2.549704	-2.568590	-0.052326
6	0.549991	-1.559100	-1.073497
1	0.719503	-2.235806	-1.914065
1	0.219699	-0.581075	-1.444699
7	-0.315728	-2.110970	-0.009375
6	0.576078	-1.587337	1.046948
16	-1.967270	-1.795271	0.021821
8	-2.479832	-2.277897	-1.245026
8	-2.427122	-2.268037	1.311429
6	-2.086453	-0.016805	0.013388
6	-2.118456	2.777612	-0.013080
6	-2.065838	0.685158	1.217128
6	-2.127980	0.662345	-1.203088
6	-2.147559	2.050403	-1.206825
6	-2.084331	2.073340	1.194419

1	-2.071575	0.138023	2.154230
1	-2.179228	0.097032	-2.127893
1	-2.197792	2.581991	-2.152865
1	-2.085434	2.622887	2.131372
6	-2.116863	4.274764	-0.027713
1	-2.585157	4.688106	0.867604
1	-2.640579	4.670443	-0.900166
1	-1.093867	4.665606	-0.063710
1	1.997982	-3.357454	-0.057556
1	0.254870	-0.617904	1.449166
1	0.764598	-2.284969	1.865878

M06L/6-311G** = -1298.5840961

9. Int-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.125310	-0.761547	-0.552703
8	-2.609307	-2.020551	-0.431346
6	-0.745023	-0.595018	-1.106983
1	-0.328760	0.374362	-0.822396
1	-0.748263	-0.618676	-2.208786
7	0.189562	-1.643433	-0.689906
6	0.050269	-2.918668	-1.225710
1	0.692372	-3.684924	-0.812771
1	-0.202310	-2.939349	-2.281398
16	0.977617	-1.421700	0.819666
8	0.034690	-0.821167	1.739981
8	1.651666	-2.674728	1.084240
6	-3.013190	0.306488	-0.296809
6	-4.833399	2.405856	0.227675
6	-4.351281	0.041368	0.103248
6	-2.626627	1.667179	-0.422867
6	-3.522156	2.686596	-0.161713
6	-5.232623	1.073125	0.355962
1	-4.666546	-0.989953	0.207928
1	-1.616966	1.923189	-0.729279

1	-3.198198	3.717855	-0.264605
1	-6.249689	0.841478	0.658780
1	-5.531958	3.211636	0.426293
6	2.177224	-0.188103	0.385523
6	4.101371	1.723801	-0.249236
6	2.044796	1.104882	0.882170
6	3.252637	-0.543412	-0.428093
6	4.201329	0.414460	-0.742127
6	3.011415	2.050691	0.560219
1	1.199463	1.351271	1.516871
1	3.339906	-1.559868	-0.801376
1	5.041951	0.146323	-1.376540
1	2.919974	3.061569	0.949395
6	5.160430	2.734622	-0.560956
1	6.036005	2.590675	0.082534
1	4.806767	3.755656	-0.402901
1	5.509244	2.648574	-1.592824
1	-1.887350	-2.660955	-0.582838

M06L/6-311G** = -1298.511982

10. TS2-T_1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.072498	0.932848	1.514939
6	2.983873	0.991622	0.926991
6	5.433208	0.916817	-0.492676
6	3.080028	0.261565	-0.350359
6	4.020574	1.751505	1.358561
6	5.258969	1.787909	0.640286
6	4.411121	0.160267	-0.956193
1	3.924244	2.324531	2.277387
1	6.080643	2.399650	0.994014
1	4.540477	-0.503504	-1.803001
1	6.407785	0.860124	-0.967036
6	1.952830	-0.337731	-0.952695
8	2.127776	-0.699556	-2.282424

6	0.529566	0.096740	-0.619440
7	0.004431	-1.281205	-0.451235
6	1.297706	-1.900815	-0.165715
16	-1.116256	-1.479665	0.828967
8	-1.592903	-2.844764	0.733957
8	-0.527310	-0.979765	2.066855
6	-2.370654	-0.332414	0.329146
6	-4.354066	1.474861	-0.415803
6	-2.570647	0.815471	1.088713
6	-3.138019	-0.590067	-0.804090
6	-4.119559	0.318030	-1.168915
6	-3.562444	1.708614	0.711615
1	-1.958112	0.985689	1.967397
1	-2.966508	-1.492879	-1.381165
1	-4.724367	0.126449	-2.050694
1	-3.730793	2.602916	1.305161
6	-5.452575	2.420908	-0.785503
1	-5.234133	3.440348	-0.461500
1	-6.392983	2.127169	-0.306341
1	-5.633019	2.434334	-1.862119
1	1.355791	-1.218531	-2.537277
1	1.567821	-1.995907	0.892662
1	1.535250	-2.776308	-0.774534
1	0.040047	0.650359	-1.429093
1	0.484477	0.678771	0.305723

M06L/6-311G** = -1298.4291847

11. T_1/S_0-I

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-4.4308109	-11.6095572	-0.8922872
6	-5.3860679	-12.1147000	-0.7919646
6	-7.8298626	-13.4348641	-0.5328001
6	-6.5425102	-11.5718713	-1.4055113
6	-5.4708272	-13.2837291	-0.0582551
6	-6.6852552	-13.9554533	0.0748280

6	-7.7691934	-12.2638263	-1.2614523
1	-4.5761237	-13.6846384	0.4067546
1	-6.7404165	-14.8780873	0.6421015
1	-8.6605990	-11.8580035	-1.7259501
1	-8.7774043	-13.9545974	-0.4333981
6	-6.4614660	-10.3711801	-2.1524736
8	-7.5378607	-10.0323802	-2.9014502
6	-5.1701509	-9.6546137	-2.4003900
7	-4.7655697	-9.0841723	-1.1206891
6	-5.7812879	-8.3373756	-0.5675153
16	-3.0967615	-8.5237391	-1.0130507
8	-3.0212231	-7.8746641	0.2800511
8	-2.2858012	-9.6720280	-1.3758920
6	-2.9754368	-7.3084476	-2.2910342
6	-3.0577703	-5.4798229	-4.3988509
6	-2.4579672	-7.6667735	-3.5338949
6	-3.5564550	-6.0544198	-2.0930670
6	-3.5907568	-5.1540519	-3.1473424
6	-2.4921589	-6.7473195	-4.5711162
1	-2.0208428	-8.6510215	-3.6663026
1	-3.9472760	-5.7907257	-1.1159083
1	-4.0311969	-4.1724303	-2.9965146
1	-2.0706266	-7.0125442	-5.5362920
6	-3.0627348	-4.4857142	-5.5172823
1	-2.9082470	-4.9675509	-6.4844679
1	-2.2604251	-3.7514770	-5.3894051
1	-3.9996068	-3.9252942	-5.5600361
1	-7.3876056	-9.1602824	-3.2833287
1	-5.6080565	-7.9337597	0.4218540
1	-6.5015836	-7.8486479	-1.2245170
1	-5.3371188	-8.8587672	-3.1516496
1	-4.3707641	-10.2993550	-2.7868438

Difference Gradient:

-1	0.00000325	0.00058684	0.00262671
-2	-0.00245395	-0.00536354	0.00778704
-3	0.00218578	-0.00129680	0.00063548
-4	0.00278099	0.01082167	-0.00491334
-5	0.00342244	0.00241755	-0.00560080
-6	-0.00419579	-0.00432871	0.00136165
-7	-0.00218427	0.00053569	0.00186215

-8	0.00049051	-0.00046088	0.00012498
-9	-0.00024538	0.00038527	0.00110410
-10	0.00005509	0.00005294	-0.00052135
-11	-0.00030165	-0.00032359	0.00006045
-12	0.03769155	-0.05484591	-0.03565190
-13	-0.02388014	0.02191846	-0.00801072
-14	-0.01954286	-0.01178081	-0.00721866
-15	-0.00533894	0.02530214	-0.00101121
-16	0.03960716	0.03995267	0.03162945
-17	-0.00835574	-0.01350840	0.01880458
-18	0.00065124	-0.00119313	-0.00685552
-19	-0.00748951	0.00775586	-0.00305593
-20	-0.00758315	0.00067514	-0.00545925
-21	0.00114107	-0.00175638	-0.00093600
-22	0.00058908	-0.00223308	0.00216755
-23	0.00125763	-0.00027400	-0.00058550
-24	0.00041325	0.00029824	0.00208640
-25	0.00021369	0.00248883	-0.00051528
-26	-0.00030192	0.00014062	-0.00013367
-27	-0.00075868	0.00020195	0.00006669
-28	0.00022107	-0.00039524	0.00015323
-29	-0.00042999	-0.00013209	0.00048988
-30	-0.00034271	-0.00030992	-0.00028966
-31	0.00000879	0.00004973	0.00034006
-32	-0.00019246	-0.00037869	0.00032389
-33	0.00022186	-0.00018972	0.00023489
-34	-0.00269221	-0.00472080	0.00069758
-35	0.00001241	0.00141356	-0.00025128
-36	-0.00693581	-0.00914696	0.00127743
-37	0.00345467	0.00045601	0.00148040
-38	-0.00119635	-0.00281452	0.00569546

M06L/6-311G** = -1298.5035138900