

Origins of Enantioselectivity in Diels-Alder Cycloadditions Catalyzed by Chiral Imidazolidinones.

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Supporting Information:

Reference 18: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A. Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I. R.; Gomperts, R.; Martin, L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M. P.; Gill, M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98*, revision A.6; Gaussian, Inc.: Pittsburgh, PA, 1998.

Reference 21: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision B. 04; Gaussian, Inc.: Pittsburgh, PA, 2003.

Molecular Geometries and Energies:

Cyclopentadiene

B3LYP/6-31G(d) energy= -194.101058

Zero-point correction (ZPC)= 0.092896

Number of Imaginary Frequencies= 0

C	-0.734452	0.991658	0.000154	-0.114736
C	0.735513	0.990865	0.000111	-0.114733
C	1.181003	-0.282318	-0.000356	-0.133728
C	-0.000649	-1.217343	0.000364	-0.345957
C	-1.181309	-0.281064	-0.000382	-0.133832
H	-0.001001	-1.882291	-0.877372	0.167321
H	-0.001009	-1.881545	0.878690	0.167437
H	2.213730	-0.611980	-0.000558	0.128885
H	1.348418	1.886595	0.000215	0.125306
H	-2.214390	-0.609613	-0.000607	0.128868
H	-1.346389	1.888049	0.000288	0.125293

7 s-trans

B3LYP/6-31G(d) energy= -231.2341826

Zero-point correction (ZPC)= 0.090043

Number of Imaginary Frequencies=0

C	-2.431373	-0.166116	0.000246	-0.495963
C	-1.043436	0.391369	-0.000116	-0.077462
C	0.092190	-0.324145	-0.000466	-0.142375
C	1.406135	0.333559	-0.000145	0.229347
O	2.472149	-0.253444	0.000355	-0.415344

H	1.366618	1.447577	-0.000381	0.096340
H	0.088895	-1.412536	-0.000572	0.147077
H	-0.962399	1.480700	0.000297	0.145079
H	-2.989630	0.181637	-0.879341	0.172312
H	-2.432107	-1.260111	0.000534	0.168710
H	-2.989667	0.182286	0.879504	0.172300

7 s-cis

B3LYP/6-31G(d) energy= -231.2320827

Zero-point correction (ZPC)= 0.090103

Number of Imaginary Frequencies=0

C	2.322462	-0.123228	0.000008	-0.498059
C	0.838325	-0.296893	0.000087	-0.047317
C	-0.067902	0.693709	-0.000234	-0.174042
C	-1.519034	0.414999	0.000210	0.221115
O	-2.015057	-0.698095	-0.000197	-0.408830
H	-2.169210	1.317184	0.000989	0.099778
H	0.237476	1.739311	-0.000497	0.129711
H	0.455683	-1.317766	0.000725	0.170046
H	2.615507	0.931248	-0.000281	0.162773
H	2.769030	-0.608127	0.878711	0.172422
H	2.768859	-0.608614	-0.878490	0.172449

TS7 s-trans-endo

B3LYP/6-31G(d) energy= -425.3012094

Zero-point correction (ZPC)= 0.186137
HF/6-31G(d)// B3LYP/6-31G(d) energy=-422.526363
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=2.247$) energy=-422.530462
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-422.543286

Number of Imaginary Frequencies= 1

C	1.329212	-1.183831	-1.057001
C	0.328068	-1.919952	-0.406238
C	0.131538	-1.383263	0.867228
C	1.324280	-0.522064	1.180590
C	1.735313	-0.122863	-0.223633
C	0.187758	1.260861	-0.469465
C	-0.886338	0.712033	0.256998
C	-2.026529	0.075525	-0.395235
O	-3.107808	-0.144830	0.129047
C	0.857461	2.536958	0.008032
H	-1.843930	-0.207719	-1.459007
H	1.154263	0.294059	1.884434
H	2.117526	-1.165535	1.598450
H	0.106973	1.188664	-1.553188
H	-1.053556	1.016947	1.288208
H	2.628228	0.465113	-0.416755
H	-0.555185	-1.770318	1.611292
H	1.036144	2.520769	1.089124
H	1.815184	2.713015	-0.493350
H	0.214183	3.401556	-0.201112
H	-0.273428	-2.701813	-0.857186
H	1.631489	-1.316521	-2.090938

TS7 *s-trans-exo*

B3LYP/6-31G(d) energy= -425.3019534
Zero-point correction (ZPC)= 0.186113
HF/6-31G(d)// B3LYP/6-31G(d) energy= -422.526406
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=2.247$) energy=-422.530353
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-422.542445

Number of Imaginary Frequencies= 1

C	0.570660	-1.218744	1.147556
C	0.139375	-1.613404	-0.239167
C	1.175138	-1.282970	-1.108784
C	2.050121	-0.397007	-0.456881
C	1.531034	-0.094231	0.817100
C	0.030688	1.292294	0.379053
C	0.781099	2.431534	-0.280671
C	-0.932099	0.562498	-0.342213
C	-2.168018	0.091272	0.272470
O	-3.144439	-0.328955	-0.330829
H	-2.180325	0.148687	1.388169
H	-0.939629	0.596795	-1.428105
H	-0.208865	1.466395	1.429942
H	1.154829	-2.049479	1.578527
H	-0.229297	-0.977822	1.849206
H	-0.669109	-2.303024	-0.452578
H	2.113180	0.411491	1.583145
H	1.679676	2.712434	0.279998
H	1.081820	2.167904	-1.299862
H	0.140307	3.320979	-0.345963
H	1.237531	-1.575171	-2.151706
H	2.907419	0.085001	-0.914914

TS7 *s-cis-endo*

B3LYP/6-31G(d) energy= -425.3043932

Zero-point correction (ZPC)= 0.186389
HF/6-31G(d)// B3LYP/6-31G(d) energy= -422.527491
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=2.247$) energy=-422.531043
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-422.541986

Number of Imaginary Frequencies= 1

C	-0.798233	-1.047245	-1.225939	-0.062794
C	-1.694950	-0.980295	-0.145613	-0.082769
C	-0.992858	-1.165160	1.033398	-0.137052
C	0.360620	-1.719501	0.692472	-0.298797
C	0.516704	-1.210432	-0.733518	-0.176642
C	1.150279	0.644829	-0.303179	-0.109475
C	0.343227	1.076113	0.769099	-0.170831
C	-0.879688	1.798167	0.504125	0.227723
O	-1.338899	1.991864	-0.622339	-0.467739
C	2.642918	0.455684	-0.098412	-0.457960
H	-1.423023	2.169726	1.401011	0.079225
H	1.165300	-1.461671	1.383132	0.153335
H	0.294897	-2.820450	0.659791	0.170034
H	0.882779	1.096905	-1.255512	0.175785
H	0.688926	1.004258	1.797510	0.118594
H	1.322166	-1.562318	-1.373392	0.139472
H	-1.417290	-1.169137	2.031043	0.141488
H	2.869302	-0.053851	0.844910	0.147711
H	3.103985	-0.113600	-0.912784	0.146785
H	3.136085	1.435443	-0.065387	0.165483
H	-2.741086	-0.708251	-0.223812	0.148634
H	-1.058971	-0.864923	-2.262396	0.149826

TS7 *s-cis-exo*

B3LYP/6-31G(d) energy= -425.3055613
Zero-point correction (ZPC)= 0.186393
HF/6-31G(d)// B3LYP/6-31G(d) energy= -422.528551
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=2.247$) energy=-422.531691
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-422.541748

Number of Imaginary Frequencies= 1

C	0.324837	-1.255824	1.002877
C	0.461045	-1.639830	-0.440052
C	1.633410	-1.076969	-0.933508
C	2.096034	-0.115516	-0.019713
C	1.158589	0.009577	1.028414
C	-0.270751	1.236444	0.233041
C	0.477973	2.505691	-0.122479
C	-0.899768	0.481055	-0.776124
C	-2.143889	-0.232599	-0.552947
O	-2.676740	-0.426431	0.538718
H	-2.623699	-0.624453	-1.477765
H	-0.591536	0.601526	-1.811516
H	-0.839858	1.289920	1.160852
H	0.835100	-2.018008	1.616599
H	-0.700742	-1.162337	1.366094
H	-0.099116	-2.441281	-0.908623
H	1.391753	0.523036	1.957817
H	1.147760	2.827590	0.682909
H	1.073702	2.377470	-1.032430
H	-0.233010	3.322314	-0.304889
H	2.072557	-1.284564	-1.903847
H	2.956137	0.528046	-0.172000

8 *s-trans*

B3LYP/6-31G(d) energy= -309.8707514000

Zero-point correction (ZPC)= 0.147196

Number of Imaginary Frequencies=0

C 3.244576 -0.316918 0.000015 -0.493412
C 1.750258 -0.426563 0.000056 -0.079484
C 0.904881 0.614805 -0.000179 -0.166693
C -0.578082 0.536579 0.000001 0.446809
C -1.261039 -0.830624 0.000012 -0.361879
C -2.785723 -0.734045 -0.000063 -0.432084
O -1.233562 1.569868 0.000140 -0.468324
H 1.285961 1.635110 -0.000422 0.140296
H 1.349974 -1.440383 0.000331 0.141019
H 3.673094 -0.815456 0.879929 0.167117
H 3.673108 -0.816076 -0.879538 0.167101
H 3.574324 0.726401 -0.000357 0.166848
H -0.907833 -1.394675 0.874856 0.157238
H -0.907723 -1.394743 -0.874745 0.157255
H -3.234164 -1.733202 0.000036 0.136096
H -3.143754 -0.192570 0.880351 0.161051
H -3.143715 -0.192752 -0.880606 0.161026

8 s-cis

B3LYP/6-31G(d) energy=-309.8722712000

Zero-point correction (ZPC)= 0.146965

Number of Imaginary Frequencies=0

C -3.345553 -0.247099 0.000067 -0.497853
C -1.945746 0.279199 0.000092 -0.054181
C -0.829927 -0.463486 -0.000219 -0.182283
C 0.521824 0.162017 -0.000081 0.438247
O 0.679685 1.374766 -0.000088 -0.471398
C 1.705546 -0.799091 0.000104 -0.359230
H -0.884365 -1.551765 -0.000496 0.122006
H -1.817877 1.361815 0.000400 0.165838
H -3.896607 0.114290 0.878920 0.168937
H -3.896696 0.114675 -0.878574 0.168942
H -3.375054 -1.341353 -0.000177 0.159296
H 1.600073 -1.461585 0.873005 0.158199
H 1.600155 -1.461926 -0.872543 0.158174
C 3.062594 -0.100928 0.000051 -0.433146
H 3.876027 -0.834124 0.000259 0.137310
H 3.172284 0.538893 -0.880671 0.160581
H 3.172153 0.539286 0.880501 0.160606

TS8 s-trans-endo

B3LYP/6-31G(d) energy=-503.9365273000

Zero-point correction (ZPC)= 0.2431470000

HF/6-31G(d)// B3LYP/6-31G(d) energy=-500.602436

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-500.616229

Number of Imaginary Frequencies= 1

C 0.820988 -1.268675 1.109594 -0.130428
C 2.178501 -0.667924 0.861844 -0.295954
C 2.110723 -0.483247 -0.641793 -0.157288
C 1.255744 -1.497340 -1.113384 -0.094797
C 0.454298 -1.948909 -0.052616 -0.103033
C 0.827947 1.198773 -0.513427 -0.122961
C 0.001404 0.897077 0.584841 -0.192109
C -1.426306 0.528746 0.520300 0.468185
O -2.109860 0.506269 1.539959 -0.502082
C 1.848033 2.318982 -0.413752 -0.453668
H 2.425656 0.218167 1.447944 0.154648
H 2.942437 -1.434609 1.077485 0.170076
H 0.384355 1.105325 -1.501502 0.143993
H 0.286418 1.268588 1.567298 0.136685
H 2.952061 -0.107849 -1.217498 0.133687

H 0.399340 -1.439260 2.093543 0.158083
H 2.357853 2.319889 0.555987 0.151295
H 2.608566 2.258206 -1.199788 0.145366
H 1.349593 3.292096 -0.516509 0.161769
H -0.389830 -2.624144 -0.144346 0.141296
H 1.137144 -1.782023 -2.154108 0.134014
C -2.052122 0.223474 -0.842362 -0.362044
H -1.390404 -0.449471 -1.403711 0.149262
H -2.067901 1.161496 -1.417562 0.153335
C -3.461742 -0.355257 -0.733602 -0.432441
H -4.114324 0.318493 -0.172120 0.165744
H -3.893388 -0.517094 -1.727380 0.130722
H -3.453515 -1.312169 -0.201260 0.148685

TS8 s-trans-exo

B3LYP/6-31G(d) energy=-503.9349032000

Zero-point correction (ZPC)=0.2431310000

HF/6-31G(d)// B3LYP/6-31G(d) energy=-500.599979

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-500.612769

Number of Imaginary Frequencies= 1

C -2.086852 -1.331686 0.810046 -0.097762
C -2.760681 -0.446106 -0.046778 -0.086175
C -1.906175 -0.100599 -1.111472 -0.167388
C -0.865530 -1.199006 -1.174665 -0.305919
C -0.831429 -1.611191 0.272332 -0.128357
C -0.606731 1.300385 -0.204490 -0.116598
C -1.558553 2.378131 0.276140 -0.450415
C 0.120673 0.535836 0.726014 -0.189632
C 1.534810 0.122389 0.614203 0.458681
O 2.088619 -0.449440 1.549664 -0.496954
H -0.229723 0.502825 1.753902 0.139570
H -0.100640 1.544830 -1.137754 0.139398
H -1.284826 -2.032083 -1.764435 0.170306
H 0.092210 -0.930611 -1.619944 0.156107
H -0.101409 -2.290635 0.696473 0.160580
H -2.252261 0.422812 -1.999028 0.133459
H -2.281815 2.664439 -0.495768 0.140783
H -2.113434 2.047989 1.160327 0.153813
H -1.000295 3.281446 0.557996 0.153952
H -2.437438 -1.652341 1.785438 0.137048
H -3.723794 0.009905 0.157345 0.135088
C 2.343046 0.491232 -0.636712 -0.362125
H 1.753135 0.320683 -1.546027 0.145089
H 2.503972 1.579404 -0.602163 0.159670
C 3.683688 -0.238140 -0.715777 -0.432114
H 4.260617 0.103348 -1.582083 0.132444
H 4.269701 -0.063780 0.189923 0.169538
H 3.539455 -1.320189 -0.804564 0.147708

TS8 s-cis-endo

B3LYP/6-31G(d) energy=-503.9417174000

Zero-point correction (ZPC)= 0.2429760000

HF/6-31G(d)// B3LYP/6-31G(d) energy=-500.606769

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-500.617926

Number of Imaginary Frequencies= 1

C -0.599456 -1.442651 -1.046664 -0.140277
C -1.977513 -0.843818 -1.056635 -0.296075
C -2.133026 -0.498988 0.416363 -0.174693
C -1.307464 -1.410106 1.111085 -0.063920
C -0.359609 -1.945221 0.223802 -0.086463
C -1.073838 1.225648 0.380092 -0.108690
C 0.044114 0.956237 -0.432633 -0.192823

C	1.305310	0.551048	0.177551	0.464626
O	1.382939	0.262310	1.374936	-0.520407
C	-2.111496	2.239495	-0.068954	-0.457857
H	-2.132046	-0.023183	-1.759129	0.151035
H	-2.706248	-1.633965	-1.305749	0.167438
H	-0.842969	1.258832	1.442172	0.172480
H	0.043190	1.243442	-1.481695	0.115091
H	-3.083502	-0.163129	0.823286	0.135848
H	-0.041476	-1.693999	-1.941959	0.137370
H	-2.355329	2.138347	-1.132570	0.146209
H	-3.042700	2.160719	0.502577	0.145678
H	-1.723694	3.255451	0.079834	0.162343
H	0.490078	-2.552034	0.514950	0.144442
H	-1.309639	-1.562211	2.184652	0.145864
C	2.542902	0.509261	-0.722750	-0.351018
H	2.795813	1.549247	-0.980948	0.153259
H	2.277487	0.029742	-1.674831	0.140341
C	3.742216	-0.179698	-0.074098	-0.431020
H	3.989591	0.293293	0.880124	0.164369
H	3.525036	-1.232685	0.134744	0.145331
H	4.620067	-0.133590	-0.727907	0.131255

TS8 s-cis-exo

B3LYP/6-31G(d) energy= -503.9431683000
 Zero-point correction (ZPC)= 0.2431300000
 HF/6-31G(d)// B3LYP/6-31G(d) energy= -500.607996
 CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -500.619013

Number of Imaginary Frequencies= 1

C	1.722627	-1.486200	-1.062951	-0.098487
C	2.654596	-0.674155	-0.396986	-0.084244
C	2.097526	-0.249227	0.827511	-0.172764
C	0.976299	-1.216944	1.142166	-0.320913
C	0.608782	-1.657076	-0.244736	-0.132872
C	0.863979	1.301784	0.257800	-0.106761
C	1.798461	2.286037	-0.417294	-0.454816
C	-0.177125	0.699066	-0.472256	-0.185178
C	-1.483546	0.416389	0.127999	0.449391
O	-1.679612	0.427159	1.345490	-0.509500
H	-0.125990	0.693387	-1.558171	0.116846
H	0.596174	1.555417	1.282991	0.168464
H	1.404237	-2.079690	1.681266	0.167221
H	0.153218	-0.818093	1.738068	0.206607
H	-0.246646	-2.283705	-0.472591	0.141995
H	2.692239	0.215667	1.609713	0.137323
H	2.717586	2.442310	0.158664	0.142579
H	2.078132	1.948764	-1.421036	0.148771
H	1.306596	3.262457	-0.522099	0.155553
H	1.816230	-1.843762	-2.083320	0.131315
H	3.585245	-0.313106	-0.822195	0.134323
C	-2.631803	0.125987	-0.843012	-0.350543
H	-2.277386	-0.576133	-1.610317	0.144467
H	-2.848531	1.059720	-1.384374	0.156813
C	-3.892800	-0.394865	-0.156573	-0.431398
H	-3.701210	-1.348242	0.346903	0.148273
H	-4.237014	0.308555	0.606493	0.164550
H	-4.697953	-0.545593	-0.883928	0.132955

TS9 s-trans-endo

B3LYP/6-31G(d) energy= -484.4644933000
 Zero-point correction (ZPC)= 0.268858
 HF/6-31G(d)// B3LYP/6-31G(d) energy= -481.170826
 CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-481.2417630000

Number of Imaginary Frequencies= 1

C	0.979836	-1.632492	0.979401	-0.090519
C	1.957371	-0.541148	1.270632	-0.325971
C	2.373896	-0.113191	-0.128808	-0.182816
C	2.059169	-1.205210	-0.967796	-0.063314
C	1.149929	-2.070042	-0.317456	-0.103223
C	1.023216	1.240047	-0.612229	-0.143813
C	1.737784	2.524465	-0.216959	-0.466492
C	-0.198590	0.932319	0.062976	-0.152221
C	-1.239097	0.251830	-0.562130	0.115760
N	-2.471929	0.068045	-0.091738	-0.339949
C	-3.481505	-0.671098	-0.852328	-0.338528
C	-2.861201	0.576546	1.224852	-0.342202
H	1.603113	0.242191	1.942926	0.185719
H	2.839439	-0.995435	1.753927	0.227935
H	0.997254	1.088469	-1.689933	0.179733
H	-0.344994	1.327648	1.063544	0.158384
H	3.282958	0.458553	-0.288738	0.192113
H	0.331312	-2.084517	1.722030	0.190356
H	-1.069219	-0.152313	-1.557780	0.178116
H	-3.800669	-1.559095	-0.295671	0.199536
H	-4.354707	-0.036164	-1.033906	0.206924
H	-3.066933	-0.983962	-1.812089	0.190949
H	-2.698788	1.657590	1.282232	0.203209
H	-3.919441	0.371737	1.387626	0.205650
H	-2.281213	0.084920	2.014896	0.187619
H	1.887415	2.591128	0.865711	0.172629
H	2.708395	2.622500	-0.709720	0.181302
H	1.123994	3.380545	-0.521340	0.196758
H	0.660389	-2.924800	-0.770164	0.183038
H	2.400351	-1.317464	-1.992326	0.193304

TS9 s-trans-exo

B3LYP/6-31G(d) energy= -484.4651148000
 Zero-point correction (ZPC)= 0.268754
 HF/6-31G(d)// B3LYP/6-31G(d) energy= -481.171478
 CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-481.2427900000

Number of Imaginary Frequencies= 1

C	-1.801036	-1.511970	1.077530	-0.100224
C	-2.630739	-0.458530	0.616620	-0.046288
C	-2.262582	-0.090639	-0.692303	-0.197362
C	-1.419906	-1.238532	-1.220201	-0.330448
C	-0.997302	-1.923077	0.039842	-0.093722
C	-0.911510	1.359727	-0.427148	-0.144546
C	-1.685214	2.465283	0.265213	-0.463813
C	0.237966	0.818587	0.216806	-0.134940
C	1.367781	0.434345	-0.498616	0.102979
N	2.533592	0.030286	0.004691	-0.339675
C	2.727415	-0.097410	1.450138	-0.342538
C	3.685403	-0.248522	-0.855828	-0.338861
H	0.261489	0.805496	1.301824	0.159217
H	-0.791114	1.524967	-1.499296	0.183231
H	-2.094378	-1.916629	-1.770182	0.228433
H	-0.611869	-0.981109	-1.907697	0.174249
H	-0.246344	-2.704112	0.086498	0.188111
H	-2.949938	0.447422	-1.339282	0.192894
H	-2.668086	2.627780	-0.186861	0.177258
H	-1.818516	2.261753	1.331916	0.171611
H	-1.122752	3.402605	0.173772	0.194785
H	1.343355	0.497578	-1.584685	0.180954
H	2.684268	0.882995	1.937695	0.204601
H	1.954509	-0.744400	1.878660	0.188038
H	3.704276	-0.542488	1.640560	0.204661

H 4.030163 -1.276453 -0.702381 0.200380
H 3.405931 -0.119170 -1.902801 0.192103
H 4.506385 0.437722 -0.622106 0.207614
H -1.796603 -1.910757 2.085449 0.185885
H -3.387583 0.039226 1.213768 0.195333

TS9 s-trans-endo (full optimization in water)

B3LYP/6-31G(d) energy= -484.4651148000

Zero-point correction (ZPC)= 0.268754

CPCM: B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -484.5346300000

Number of Imaginary Frequencies= 1

C 1.961287 -1.287694 -0.947840 -0.074858
C 0.991450 -2.069377 -0.282336 -0.120526
C 0.850202 -1.590138 1.004709 -0.101193
C 1.910034 -0.574494 1.277207 -0.341604
C 2.359457 -0.207737 -0.129120 -0.196743
C 1.083796 1.217867 -0.629223 -0.147395
C 1.856917 2.463112 -0.222941 -0.473260
C -0.150828 0.968116 0.042380 -0.170426
C -1.199446 0.295432 -0.579297 0.100811
N -2.438349 0.145350 -0.113615 -0.339648
C -3.427675 -0.657416 -0.831669 -0.349286
C -2.824029 0.665153 1.197773 -0.353099
H 1.616181 0.247593 1.936473 0.204109
H 2.756858 -1.090769 1.770071 0.229234
H 1.062559 1.061344 -1.710690 0.210755
H -0.285494 1.369360 1.043506 0.173947
H 3.316373 0.297075 -0.305878 0.222553
H 0.158463 -1.967926 1.752669 0.200113
H -1.029387 -0.131980 -1.568086 0.212404
H -3.686224 -1.550813 -0.248414 0.199201
H -4.337250 -0.067972 -0.995678 0.199884
H -3.019280 -0.966327 -1.797274 0.203323
H -2.544820 1.720682 1.285506 0.202332
H -3.906696 0.575077 1.309718 0.203839
H -2.332893 0.097504 2.000009 0.197669
H 1.980552 2.525032 0.864077 0.172460
H 2.845382 2.498160 -0.690218 0.172273
H 1.298960 3.350873 -0.547927 0.178574
H 0.426778 -2.885816 -0.723994 0.189750
H 2.281389 -1.435484 -1.976427 0.194743

TS9 s-trans-exo (full optimization in water)

B3LYP/6-31G(d) energy= -484.4651148000

Zero-point correction (ZPC)= 0.268754

CPCM: B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -484.5356370000

Number of Imaginary Frequencies= 1

C -1.673851 -1.522572 1.106769 -0.117365
C -2.574687 -0.532452 0.644411 -0.065720
C -2.250721 -0.164631 -0.677805 -0.207380
C -1.351661 -1.270040 -1.201500 -0.347586
C -0.858177 -1.896975 0.061602 -0.104111
C -0.970725 1.335976 -0.451188 -0.149146
C -1.787632 2.422113 0.223488 -0.472218
C 0.199319 0.857202 0.204607 -0.154319
C 1.327105 0.463430 -0.509804 0.087868
N 2.501782 0.098066 0.000504 -0.337689
C 2.704108 0.017919 1.446888 -0.353556
C 3.626786 -0.266223 -0.860059 -0.349146
H 0.226506 0.869432 1.291000 0.169551
H -0.858628 1.481830 -1.531560 0.219159
H -2.002837 -2.003643 -1.715303 0.229835
H -0.581166 -0.980256 -1.921511 0.199346
H -0.050215 -2.621700 0.110104 0.197363

H -2.978669 0.336634 -1.329604 0.230295
H -2.783830 2.518235 -0.220367 0.170545
H -1.897979 2.237388 1.297226 0.170540
H -1.272928 3.384363 0.100447 0.175256
H 1.288389 0.479251 -1.599607 0.218653
H 2.565157 1.001447 1.912202 0.202997
H 1.992848 -0.689451 1.891890 0.195678
H 3.720749 -0.327962 1.644177 0.204969
H 3.924616 -1.304820 -0.669917 0.199714
H 3.335315 -0.161679 -1.908203 0.203627
H 4.482285 0.389325 -0.657030 0.200230
H -1.617777 -1.894903 2.125829 0.187791
H -3.343491 -0.062427 1.252245 0.194945

10 s-trans

B3LYP/6-31G(d) energy= -369.0031892000

Zero-point correction (ZPC)= 0.230447

Number of Imaginary Frequencies=0

C 3.540195 -0.564356 0.080611 -0.515343
C 2.215359 0.045454 -0.213738 -0.046656
C 1.027258 -0.554099 0.037898 -0.182396
C -0.270986 0.042293 -0.207760 0.426217
C -0.387225 1.499127 -0.587733 -0.380435
C -0.443311 2.433351 0.642914 -0.457138
N -1.358443 -0.688805 -0.046455 -0.384658
C -1.308475 -2.141371 0.235898 -0.359267
C -2.733094 -0.156813 -0.127665 -0.361861
H 2.246185 1.034823 -0.665523 0.187024
H 1.053467 -1.542801 0.482486 0.179584
H 4.130507 -0.643285 -0.842520 0.214086
H 4.114747 0.091784 0.748515 0.213014
H 3.459656 -1.553869 0.537242 0.191545
H -3.189649 -0.461866 -1.074825 0.224696
H -3.309390 -0.583654 0.696642 0.220793
H -2.752959 0.925159 -0.038080 0.214951
H -0.571582 -2.631195 -0.400828 0.218412
H -1.073023 -2.318468 1.289989 0.222389
H -2.289467 -2.562967 0.018098 0.219616
H -1.258174 1.655067 -1.228169 0.197637
H 0.477128 1.764394 -1.199686 0.198600
H -0.499300 3.471662 0.305271 0.203607
H -1.317478 2.233504 1.270375 0.175372
H 0.450107 2.321836 1.263650 0.180164

10 s-cis1

B3LYP/6-31G(d) energy= -368.9977020000

Zero-point correction (ZPC)= 0.230522

Number of Imaginary Frequencies=0

C 3.579815 -0.439237 -0.022068 -0.509163
C 2.189778 0.069660 -0.199572 -0.049182
C 1.077371 -0.626817 0.119694 -0.189404
C -0.303187 -0.257848 -0.164921 0.396336
C -1.204748 -1.407311 -0.561019 -0.374813
C -2.085814 -1.892604 0.613721 -0.462099
N -0.773602 0.964943 -0.040793 -0.361265
C -0.014255 2.089299 0.543526 -0.359333
C -2.145830 1.362084 -0.415971 -0.355468
H 2.100165 1.047983 -0.668802 0.180115
H 1.192922 -1.645218 0.486300 0.192817
H 4.084408 -0.508690 -0.994899 0.211099
H 4.167842 0.269842 0.575514 0.206362
H 3.607790 -1.419109 0.461016 0.193053
H -2.723086 1.559055 0.492374 0.223035
H -2.085821 2.282092 -1.003059 0.221100

H	-2.641505	0.596687	-1.004833	0.213168
H	0.783856	1.714590	1.181514	0.216966
H	0.401311	2.718717	-0.248815	0.217855
H	-0.707577	2.688075	1.137996	0.216122
H	-0.567035	-2.227303	-0.899753	0.206020
H	-1.828478	-1.134865	-1.417524	0.201919
H	-2.782017	-1.120280	0.953662	0.173448
H	-2.670853	-2.756572	0.287094	0.207371
H	-1.475488	-2.202967	1.467425	0.183962

10 s-cis2

B3LYP/6-31G(d) energy=-368.9987326000

Zero-point correction (ZPC)= 0.230566

Number of Imaginary Frequencies=0

C	-3.485253	0.205378	0.165567	-0.509514
C	-2.038483	-0.138304	0.268920	-0.045946
C	-1.074235	0.373642	-0.526715	-0.185382
C	0.363985	0.183722	-0.378888	0.393979
C	1.210865	1.410575	-0.618902	-0.375313
C	1.299805	2.316514	0.632026	-0.457957
N	0.919859	-0.961575	-0.049261	-0.362203
C	0.205693	-2.252958	-0.004059	-0.361857
C	2.364439	-1.098860	0.240208	-0.362943
H	-1.768721	-0.815033	1.078514	0.179507
H	-1.353927	1.120948	-1.266015	0.191764
H	-4.081756	-0.708309	0.041890	0.206960
H	-3.831958	0.670111	1.098079	0.210437
H	-3.695899	0.881517	-0.666750	0.193882
H	2.480797	-1.858384	1.015686	0.220110
H	2.892913	-1.427134	-0.660674	0.226430
H	2.785431	-0.164900	0.603283	0.218231
H	-0.013185	-2.530974	1.031079	0.217044
H	-0.716070	-2.195541	-0.579428	0.216555
H	0.862221	-3.010424	-0.438898	0.218760
H	0.733089	1.974804	-1.426502	0.207638
H	2.208973	1.141654	-0.972187	0.196138
H	1.879836	3.210028	0.387109	0.206047
H	0.306177	2.633049	0.961339	0.184262
H	1.792163	1.811357	1.469359	0.173438

10 s-cis3

B3LYP/6-31G(d) energy=-368.9969347000

Zero-point correction (ZPC)= 0.230289

Number of Imaginary Frequencies=0

C	-3.418046	-0.252515	0.152974	-0.508861
C	-1.948820	-0.466211	0.287387	-0.048424
C	-1.008138	0.322804	-0.276065	-0.190080
C	0.427707	0.225297	-0.057412	0.390988
C	1.214803	1.505273	0.153451	-0.373514
C	0.493816	2.820285	-0.166353	-0.471126
N	1.072378	-0.922952	-0.026851	-0.362096
C	0.492316	-2.222040	-0.423239	-0.361256
C	2.506282	-1.012108	0.324405	-0.358474
H	-1.330629	1.199654	-0.829089	0.196825
H	-3.898186	-1.161949	-0.232023	0.206046
H	-3.865650	-0.066806	1.138346	0.210617
H	-3.659780	0.583275	-0.508408	0.192943
H	2.694564	-2.005970	0.732240	0.220632
H	3.120883	-0.872082	-0.571301	0.225890
H	2.773411	-0.269853	1.074334	0.216271
H	0.261968	-2.821714	0.462091	0.217104
H	-0.407523	-2.069305	-1.015262	0.216272
H	1.238851	-2.750222	-1.021162	0.218227
H	2.145692	1.445318	-0.423272	0.204074

H	1.520034	1.519114	1.211166	0.215686
H	1.177010	3.649809	0.034192	0.198629
H	0.203081	2.883605	-1.219671	0.181709
H	-0.394130	2.965310	0.455020	0.183074
H	-1.645769	-1.292241	0.929860	0.179152

TS10a s-trans-endo

B3LYP/6-31G(d) energy= -563.0916423000

Zero-point correction (ZPC)= 0.326393

HF/6-31G(d)// B3LYP/6-31G(d) energy=-559.234649

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy=-559.2995020000

Number of Imaginary Frequencies= 1

C	1.100718	1.129322	0.710316	-0.148275
C	0.022314	0.208538	0.873842	-0.195218
C	1.532532	-1.839749	-0.609147	-0.098850
C	2.485109	-1.204614	0.351093	-0.325628
C	2.582274	0.211842	-0.199023	-0.177713
C	1.477766	-1.088752	-1.764668	-0.097111
C	2.183528	0.117137	-1.552528	-0.073586
C	-1.129260	0.134672	0.065713	0.414166
C	-1.276499	1.039207	-1.139702	-0.373421
C	-1.958914	2.385195	-0.817339	-0.453821
C	1.786521	1.612981	1.982336	-0.463694
N	-2.137965	-0.698467	0.382699	-0.405389
C	-3.416879	-0.764933	-0.335240	-0.348095
C	-2.002982	-1.660005	1.481557	-0.343647
H	2.231310	-1.309156	1.407105	0.182966
H	3.472004	-1.679310	0.215434	0.224901
H	0.943719	1.935955	-0.000624	0.178258
H	0.053313	-0.398804	1.771050	0.153180
H	3.404918	0.862277	0.083405	0.188350
H	1.077496	-2.813414	-0.463395	0.186395
H	-3.457035	-1.658063	-0.970497	0.197037
H	-4.228299	-0.821030	0.395463	0.203203
H	-3.580360	0.117001	-0.948433	0.199413
H	-1.973597	-1.153173	2.452515	0.202289
H	-2.858893	-2.334652	1.467529	0.201654
H	-1.090258	-2.252964	1.360012	0.180312
H	2.068987	0.783071	2.638210	0.170425
H	2.679786	2.205226	1.767059	0.178314
H	1.092223	2.252667	2.539829	0.193015
H	0.965533	-1.365556	-2.679104	0.180143
H	2.334025	0.890902	-2.298975	0.188971
H	-0.278566	1.233143	-1.542614	0.170585
H	-1.817286	0.521857	-1.937061	0.179804
H	-1.398533	2.941302	-0.059721	0.171616
H	-2.015562	2.999466	-1.720749	0.187113
H	-2.976540	2.247484	-0.438598	0.172443

TS10a s-trans-exo

B3LYP/6-31G(d) energy= -563.0906441000

Zero-point correction (ZPC)= 0.32641

HF/6-31G(d)// B3LYP/6-31G(d) energy=-559.233596

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy=-559.2981890000

Number of Imaginary Frequencies= 1

C	-0.952534	1.281126	0.464577	-0.146366
C	0.001489	0.243766	0.676265	-0.186083
C	-1.657187	-1.600777	-1.003704	-0.095779
C	-1.757092	-0.267796	-1.671522	-0.334201
C	-2.450967	0.568271	-0.607430	-0.196166
C	-2.539145	-1.650210	0.053324	-0.100803
C	-3.089553	-0.360520	0.243380	-0.050169

C	1.224401	0.082586	-0.004571	0.400069
C	1.669693	1.074409	-1.062873	-0.373782
C	2.507293	2.237481	-0.490042	-0.452868
C	-1.626111	1.889792	1.684068	-0.460666
N	2.061800	-0.917448	0.333724	-0.401610
C	1.660134	-1.944888	1.298941	-0.345399
C	3.423972	-1.084712	-0.187098	-0.348236
H	-0.189951	-0.401118	1.525724	0.153998
H	-0.679672	2.032315	-0.274434	0.179365
H	-2.453647	-0.361919	-2.521945	0.224251
H	-0.822411	0.122933	-2.075709	0.181043
H	-1.073072	-2.431109	-1.385259	0.185934
H	-2.934214	1.507829	-0.863062	0.189705
H	-2.513429	2.471969	1.416982	0.173554
H	-1.914361	1.125928	2.412506	0.169142
H	-0.922400	2.570075	2.178850	0.188744
H	1.622592	-1.542854	2.317962	0.201344
H	0.676773	-2.347534	1.036588	0.182076
H	2.389150	-2.755257	1.272533	0.200634
H	3.480311	-1.981249	-0.815248	0.198044
H	3.745315	-0.224816	-0.766947	0.199471
H	4.114665	-1.205499	0.653354	0.203448
H	-2.767344	-2.523948	0.653168	0.183494
H	-3.834598	-0.109826	0.990992	0.192693
H	2.221253	0.560916	-1.855747	0.181648
H	0.785391	1.493556	-1.548248	0.172444
H	3.425437	1.887138	-0.008647	0.171480
H	2.788480	2.923372	-1.294519	0.188274
H	1.936758	2.800064	0.255137	0.171185

TS10b s-trans-endo

B3LYP/6-31G(d) energy=-563.0874099000
Zero-point correction (ZPC)= 0.326276
HF/6-31G(d)// B3LYP/6-31G(d) energy=-559.229718
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-559.2949180000
Number of Imaginary Frequencies= 1

C	-2.449880	-0.344864	1.244164	-0.330003
C	-2.610257	0.164146	-0.181758	-0.179968
C	-2.209966	1.518022	-0.146303	-0.063837
C	-1.465748	1.773481	1.028941	-0.098518
C	-1.495132	0.647397	1.822431	-0.097006
C	-0.047773	-0.936591	-0.314111	-0.197103
C	1.185351	-0.262830	-0.405380	0.406891
N	2.202548	-0.612504	0.410189	-0.399720
C	1.995746	-1.529828	1.533209	-0.343695
C	-1.187086	-0.776509	-1.160252	-0.153529
C	-1.922657	-2.053304	-1.554873	-0.461053
C	3.601885	-0.214729	0.218142	-0.347389
H	-2.172011	-1.392893	1.368444	0.184308
H	-3.421324	-0.217023	1.751893	0.226460
H	-1.078771	-0.096014	-2.000276	0.179337
H	-0.094237	-1.784260	0.360155	0.151409
H	-3.463108	-0.134682	-0.783754	0.189019
H	-1.009135	0.537535	2.785834	0.188816
H	3.921587	0.465878	1.015355	0.198481
H	4.230292	-1.110239	0.253795	0.202161
H	3.754498	0.267184	-0.743613	0.197582
H	1.875985	-2.565626	1.193075	0.199794
H	2.864463	-1.479255	2.190899	0.201066
H	1.109869	-1.235078	2.103404	0.178964
H	-2.161842	-2.675668	-0.686472	0.170027
H	-2.847533	-1.844232	-2.098926	0.178141
H	-1.275692	-2.642543	-2.215301	0.193778

H	-0.958176	2.701724	1.263923	0.184105
H	-2.385974	2.237471	-0.939915	0.189825
C	1.434520	0.819804	-1.439061	-0.368443
H	2.246746	0.501388	-2.104512	0.193021
H	0.558659	0.895868	-2.083360	0.170710
C	1.743760	2.216098	-0.864499	-0.458105
H	2.656564	2.237610	-0.264047	0.170886
H	1.870996	2.926921	-1.686444	0.186671
H	0.923723	2.571710	-0.235374	0.156931

TS10b s-trans-exo

B3LYP/6-31G(d) energy=-563.0881443000
Zero-point correction (ZPC)= 0.326414
HF/6-31G(d)// B3LYP/6-31G(d) energy=-559.230566
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy=-559.2955610000
Number of Imaginary Frequencies= 1

C	-3.014681	-0.556304	-0.341656	-0.049790
C	-2.490246	0.726145	-0.079164	-0.194997
C	-1.650636	1.080991	-1.293650	-0.338095
C	-1.391101	-0.260809	-1.899118	-0.095492
C	-2.285725	-1.173673	-1.387905	-0.101925
C	-1.122900	0.441793	1.334244	-0.148994
C	-1.926096	-0.123393	2.494610	-0.459535
C	-0.060831	-0.352413	0.814386	-0.189174
C	1.233079	0.069990	0.451239	0.400783
N	2.149468	-0.844741	0.068420	-0.398325
C	3.594759	-0.599470	0.000102	-0.347583
C	1.663564	1.523642	0.532463	-0.371452
C	2.107827	2.156622	-0.801369	-0.463652
C	1.773190	-2.235314	-0.199495	-0.345267
H	-0.231941	-1.422170	0.853328	0.153522
H	-0.919236	1.504763	1.450011	0.181543
H	-2.293764	1.650506	-1.986159	0.224706
H	-0.766826	1.693451	-1.113364	0.181977
H	-0.686800	-0.440925	-2.703940	0.186689
H	-3.087736	1.479146	0.427855	0.190281
H	-2.863152	0.419764	2.650318	0.174003
H	-2.155017	-1.183735	2.351887	0.169127
H	-1.335919	-0.032261	3.414580	0.190478
H	1.604615	-2.795218	0.728613	0.199221
H	0.866232	-2.269609	-0.809365	0.182255
H	2.583344	-2.714585	-0.751095	0.200057
H	3.944042	-0.642736	-1.037608	0.198613
H	3.859671	0.364458	0.425945	0.197436
H	4.110296	-1.377464	0.572262	0.202531
H	-2.409128	-2.199222	-1.717015	0.183431
H	-3.809143	-1.032278	0.223351	0.192943
H	0.839431	2.109776	0.940464	0.173066
H	2.467486	1.617710	1.273453	0.195018
H	1.316504	2.103961	-1.555655	0.164157
H	2.344156	3.212593	-0.640151	0.189934
H	2.995400	1.680410	-1.224794	0.172457

I1 s-trans

B3LYP/6-31G(d) energy=-310.2186323000
Zero-point correction (ZPC)= 0.159901
Number of Imaginary Frequencies=0

C	-3.269026	-0.291343	0.000022	-0.520819
C	-1.796231	-0.433679	-0.000029	-0.024776
C	-0.918407	0.608100	-0.000188	-0.160321
C	0.492895	0.437110	-0.000025	0.443936
O	1.164487	1.550019	0.000112	-0.488751
C	1.228380	-0.874590	-0.000064	-0.372802

C	2.758214	-0.766758	0.000022	-0.536813
H	-1.274368	1.635078	-0.000405	0.219214
H	-1.413546	-1.454291	0.000155	0.202502
H	-3.690375	-0.810541	-0.873177	0.229394
H	-3.689619	-0.807262	0.875603	0.229439
H	-3.597989	0.749721	-0.001591	0.211609
H	0.885480	-1.443086	-0.874778	0.236106
H	0.885357	-1.443122	0.874575	0.236105
H	3.187905	-1.771439	-0.000086	0.229911
H	3.141546	-0.265556	-0.897168	0.195372
H	3.141543	-0.265868	0.897402	0.195379
H	2.133216	1.403165	0.000144	0.475459

11 s-cis

B3LYP/6-31G(d) energy=-310.2205131000

Zero-point correction (ZPC)=0.159591

Number of Imaginary Frequencies=0

C	-3.348365	-0.240076	0.000253	-0.523609
C	-1.963596	0.276504	-0.000024	-0.006111
C	-0.841009	-0.499979	-0.000173	-0.173525
C	0.471367	0.043162	-0.000189	0.442358
O	0.600909	1.338655	-0.000236	-0.508592
C	1.683378	-0.834970	-0.000309	-0.370424
C	3.034416	-0.114924	0.000503	-0.535108
H	-0.917085	-1.583490	-0.000155	0.205055
H	-1.843175	1.359589	0.000103	0.224366
H	-3.887336	0.155051	0.874029	0.231241
H	-3.887900	0.155583	-0.872921	0.231252
H	-3.403404	-1.330607	-0.000035	0.206654
H	1.589048	-1.502500	0.869442	0.242207
H	1.589531	-1.501353	-0.871015	0.242243
H	3.838552	-0.854709	0.000372	0.230448
H	3.178735	0.500864	-0.895921	0.192671
H	3.178037	0.499988	0.897621	0.192703
H	1.540578	1.614034	0.000009	0.476235

Complex 11 s-trans-endo

B3LYP/6-31G(d) energy=-504.3310393

Zero-point correction (ZPC)=0.25433

Number of Imaginary Frequencies=0

C	-0.791243	-2.073773	-0.780216
C	-0.977972	-1.818622	0.646220
C	0.231234	-1.808717	1.262730
C	1.300378	-2.127068	0.254088
C	0.534539	-2.225399	-1.036496
C	0.676138	0.813204	-1.664629
C	0.965181	1.183918	-0.381083
C	-0.015280	1.489488	0.591536
O	0.464735	1.823960	1.763641
C	1.698183	0.638393	-2.730000
C	-1.495340	1.592171	0.346445
C	-2.364622	1.639761	1.609352
H	2.125003	-1.401950	0.233704
H	1.770163	-3.095009	0.492292
H	-0.361958	0.726458	-1.975393
H	1.998506	1.274687	-0.055886
H	0.982477	-2.484319	-1.988796
H	0.418892	-1.683964	2.323104
H	2.716531	0.596126	-2.336212
H	1.496036	-0.252555	-3.332934
H	1.631604	1.493119	-3.421233
H	-1.943835	-1.700046	1.126743
H	-1.597380	-2.166261	-1.500857
H	-1.797209	0.760126	-0.295664

H	-1.650027	2.505659	-0.247716
H	-2.196535	2.546158	2.205893
H	-3.418745	1.663133	1.322043
H	-2.215344	0.756970	2.240168
H	-0.244143	2.045770	2.398533

Complex 11 s-trans-exo

B3LYP/6-31G(d) energy=-504.3285712

Zero-point correction (ZPC)=0.253773

Number of Imaginary Frequencies=0

C	-0.448742	2.426737	-0.876103
C	-0.766966	2.350924	0.594242
C	0.512195	1.829595	1.193958
C	1.437114	1.688111	0.213114
C	0.840915	2.059940	-1.070846
C	-0.640818	-0.883724	-1.744074
C	0.367956	-1.357052	-0.957604
C	0.246611	-1.592568	0.433621
C	-1.023479	-1.535423	1.235179
C	-0.837098	-1.458320	2.756209
C	-0.544224	-0.713435	-3.215266
O	1.345405	-2.008496	1.008070
H	1.344093	-1.567055	-1.387141
H	-1.606193	-0.652778	-1.297831
H	-1.004829	3.349472	0.993481
H	-1.651090	1.735462	0.821159
H	0.671678	1.693945	2.257986
H	-1.142621	2.789127	-1.626134
H	-0.869323	0.292003	-3.507272
H	0.462020	-0.899097	-3.597464
H	-1.242254	-1.409553	-3.704427
H	2.470623	1.385172	0.344861
H	1.373867	2.063692	-2.015744
H	-1.590426	-2.442697	0.973975
H	-1.626261	-0.695885	0.880432
H	-1.815968	-1.379013	3.235525
H	-0.371926	-2.360788	3.174657
H	-0.252806	-0.579732	3.047587
H	1.222080	-2.171964	1.963804

Complex 11 s-cis-endo

B3LYP/6-31G(d) energy=-504.3326942

Zero-point correction (ZPC)=0.254204

Number of Imaginary Frequencies=0

C	-0.725284	-2.069776	-0.798139
C	-0.841832	-1.836981	0.636364
C	0.398818	-1.765846	1.183773
C	1.424470	-2.020084	0.113248
C	0.590404	-2.147037	-1.132593
C	0.546470	0.790347	-1.795300
C	0.689581	1.211631	-0.498454
C	-0.403010	1.402376	0.372715
O	-1.611448	1.221226	-0.107623
C	1.658747	0.722494	-2.778303
C	-0.228851	1.923252	1.769846
C	-1.411542	1.694006	2.718249
H	2.207451	-1.252322	0.052349
H	1.955883	-2.964175	0.314154
H	-0.456498	0.599518	-2.167725
H	1.675107	1.423744	-0.094559
H	0.994205	-2.378413	-2.111266
H	0.638179	-1.646789	2.234588
H	2.644753	0.785295	-2.311065
H	1.596367	-0.180813	-3.393323

H	1.555122	1.568810	-3.475734
H	-1.783971	-1.769793	1.170682
H	-1.566190	-2.190766	-1.472628
H	-0.031870	3.003452	1.670872
H	0.691754	1.494973	2.178300
H	-2.316868	2.232942	2.407852
H	-1.644145	0.629264	2.825274
H	-1.160670	2.078421	3.709920
H	-2.293461	1.368238	0.575288

Complex 11 s-cis-exo

B3LYP/6-31G(d) energy= -504.3314165

Zero-point correction (ZPC)= 0.253872

Number of Imaginary Frequencies=0

C	-0.742645	2.082961	-1.439917
C	-0.867671	2.475928	-0.144814
C	0.467314	2.351515	0.539258
C	1.338503	1.746273	-0.526151
C	0.621352	1.629982	-1.675243
C	-1.778338	-0.434162	0.469451
C	-3.125021	-0.368942	-0.151917
C	-0.685572	-1.022362	-0.112717
C	0.552265	-1.193436	0.537922
O	0.641708	-0.833097	1.804704
C	1.708394	-1.902160	-0.092144
C	1.732213	-3.400837	0.308466
H	1.640205	-1.805454	-1.178338
H	-0.741205	-1.375490	-1.137611
H	-1.689021	-0.074633	1.492863
H	0.846446	3.345797	0.825000
H	0.433219	1.773829	1.473030
H	2.397129	1.544500	-0.404821
H	-1.747812	2.905732	0.319781
H	-3.574185	0.621230	-0.022056
H	-3.116514	-0.634075	-1.211760
H	-3.787856	-1.071686	0.377296
H	0.997217	1.283582	-2.632269
H	-1.519984	2.110972	-2.195890
H	2.643499	-1.419918	0.220942
H	2.598079	-3.877807	-0.157922
H	1.814903	-3.531557	1.392153
H	0.830031	-3.915485	-0.033357
H	1.528652	-1.008975	2.170183

TS11 s-trans-endo

B3LYP/6-31G(d) energy= -504.3239278000

Zero-point correction (ZPC)= 0.25588600

HF/6-31G(d)// B3LYP/6-31G(d) energy= -500.997797

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -501.074224

Number of Imaginary Frequencies=1

C	1.262131	-1.349424	-1.148509	-0.070593
C	0.516142	-2.097974	-0.195981	-0.109806
C	0.917039	-1.726496	1.063967	-0.086312
C	2.081821	-0.795754	0.969097	-0.335923
C	2.066897	-0.403932	-0.497096	-0.184072
C	0.861252	1.296802	-0.522368	-0.135705
C	-0.071967	1.152337	0.538251	-0.163512
C	-1.367952	0.688092	0.407485	0.409725
O	-2.103396	0.701268	1.516759	-0.554755
C	1.923988	2.368742	-0.399908	-0.471528
C	-2.017214	0.265230	-0.887276	-0.361169
C	-3.264156	-0.617825	-0.739287	-0.510400
H	2.089935	0.014342	1.701244	0.196890

H	3.001457	-1.379343	1.147870	0.235294
H	0.476989	1.178356	-1.531583	0.188330
H	0.212196	1.485624	1.533240	0.181479
H	2.930423	0.038222	-0.981710	0.197952
H	0.519008	-2.106484	1.998581	0.202394
H	2.419193	2.350959	0.575740	0.183314
H	2.679607	2.297309	-1.185729	0.186296
H	1.435097	3.346492	-0.502732	0.207542
H	-0.241060	-2.836641	-0.432831	0.186499
H	1.189527	-1.467020	-2.225582	0.196138
H	-1.267249	-0.248853	-1.498192	0.180923
H	-2.275552	1.178793	-1.442237	0.218940
H	-4.105993	-0.086557	-0.276330	0.176072
H	-3.613255	-0.925933	-1.728178	0.206817
H	-3.059068	-1.525586	-0.161469	0.180090
H	-3.011972	0.397392	1.345568	0.449012

TS11 s-trans-exo

B3LYP/6-31G(d) energy= -504.3225669000

Zero-point correction (ZPC)= 0.25563000

HF/6-31G(d)// B3LYP/6-31G(d) energy= -500.997563

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -501.074623

Number of Imaginary Frequencies=1

C	-1.876178	-0.282064	-0.941895	-0.199619
C	-0.901958	-1.437740	-1.012365	-0.348259
C	-0.925592	-1.972023	0.384699	-0.092448
C	-1.968057	-1.414531	1.075730	-0.097194
C	-2.592956	-0.436154	0.245747	-0.048018
C	-0.626723	1.383843	-0.436347	-0.130562
C	0.216915	0.977970	0.626176	-0.151601
C	1.520025	0.531599	0.514545	0.410209
C	2.342087	0.413293	-0.741785	-0.380788
C	3.176279	-0.878029	-0.843622	-0.477215
C	-1.624955	2.492764	-0.211980	-0.470886
O	2.132331	0.272574	1.671314	-0.551552
H	-0.150048	1.085631	1.643888	0.182588
H	-0.202393	1.365132	-1.438109	0.192391
H	-1.328206	-2.196993	-1.689732	0.234636
H	0.094469	-1.215315	-1.402387	0.181606
H	-0.253028	-2.737574	0.755568	0.195135
H	-2.298032	0.178130	-1.829415	0.196832
H	-2.411901	2.506427	-0.970868	0.184749
H	-2.081376	2.442745	0.780204	0.184353
H	-1.090578	3.450128	-0.282262	0.205661
H	-2.271881	-1.661890	2.086040	0.193320
H	-3.472790	0.135383	0.522705	0.198518
H	3.015324	1.283759	-0.767412	0.217147
H	1.698455	0.512296	-1.618623	0.179811
H	3.711148	-0.890897	-1.796740	0.205596
H	3.938929	-0.957665	-0.059593	0.164937
H	2.548011	-1.773004	-0.793299	0.176033
H	3.061927	0.019551	1.536105	0.444675

TS11 s-cis-endo

B3LYP/6-31G(d) energy= -504.3293613000

Zero-point correction (ZPC)= 0.25556300

HF/6-31G(d)// B3LYP/6-31G(d) energy= -501.006776

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -501.081351

Number of Imaginary Frequencies=1

C	-1.303204	-1.265520	1.193272	-0.052992
C	-0.336523	-2.043874	0.483160	-0.105568
C	-0.564847	-1.912741	-0.859095	-0.105729

C	-1.803223	-1.103582	-1.086482	-0.337429
C	-2.103167	-0.563899	0.295964	-0.187177
C	-1.098323	1.393046	0.286877	-0.106787
C	0.089539	1.197420	-0.452744	-0.175866
C	1.284706	0.809647	0.120770	0.427012
O	1.288477	0.556365	1.432238	-0.574405
C	-2.207252	2.235524	-0.284865	-0.482498
C	2.585573	0.732206	-0.627118	-0.373497
C	3.411846	-0.538080	-0.353387	-0.473290
H	-1.724542	-0.366868	-1.891096	0.189918
H	-2.621566	-1.782897	-1.378987	0.232105
H	-0.996030	1.423552	1.366961	0.213843
H	0.092834	1.392294	-1.520353	0.172894
H	-3.064475	-0.143339	0.566855	0.195911
H	0.005859	-2.379258	-1.654662	0.192254
H	-2.396541	2.019944	-1.340789	0.183351
H	-3.139858	2.140022	0.275644	0.191291
H	-1.896537	3.287923	-0.215441	0.212350
H	0.444200	-2.636593	0.945421	0.178570
H	-1.383232	-1.215832	2.274205	0.194105
H	3.176854	1.618107	-0.348138	0.212599
H	2.378672	0.826594	-1.696453	0.195584
H	3.731024	-0.624557	0.693246	0.155667
H	2.852062	-1.440498	-0.616868	0.174037
H	4.325077	-0.514715	-0.953416	0.207193
H	2.177636	0.304318	1.737859	0.446572

TS11 *s-cis-exo*

B3LYP/6-31G(d) energy= -504.3282576000

Zero-point correction (ZPC)= 0.25533500

HF/6-31G(d)// B3LYP/6-31G(d) energy= -501.005641

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -501.079322

Number of Imaginary Frequencies=1

C	1.021945	-1.305980	1.211858	-0.356913
C	0.666065	-2.066334	-0.025253	-0.107240
C	1.533353	-1.746603	-1.033914	-0.100507
C	2.425828	-0.730500	-0.566733	-0.056179
C	2.066509	-0.333261	0.715544	-0.194225
C	0.871822	1.473470	0.200746	-0.106017
C	1.891161	2.370738	-0.442957	-0.479558
C	-0.256614	1.030798	-0.524893	-0.160378
C	-1.471195	0.703069	0.043683	0.413805
O	-1.581287	0.728857	1.377335	-0.574729
C	-2.702686	0.389462	-0.757463	-0.375808
C	-3.414153	-0.913932	-0.343164	-0.467730
H	-0.204814	1.000683	-1.608473	0.173468
H	0.727947	1.618735	1.268901	0.215939
H	1.501041	-1.991465	1.931292	0.231405
H	0.169547	-0.868444	1.740161	0.205797
H	-0.123553	-2.808123	-0.074579	0.188390
H	2.717445	0.223607	1.380437	0.196605
H	2.848309	2.364160	0.085173	0.189136
H	2.056267	2.126714	-1.495825	0.183741
H	1.508270	3.400484	-0.396393	0.209608
H	1.553846	-2.184537	-2.025055	0.186956
H	3.242625	-0.313562	-1.146595	0.193109
H	-2.433525	0.352085	-1.816078	0.197307
H	-3.396645	1.236391	-0.642529	0.209347
H	-2.755757	-1.779528	-0.464566	0.173754
H	-3.768156	-0.896496	0.694987	0.155831
H	-4.294260	-1.063694	-0.973592	0.206687
H	-2.490501	0.526582	1.659338	0.448327

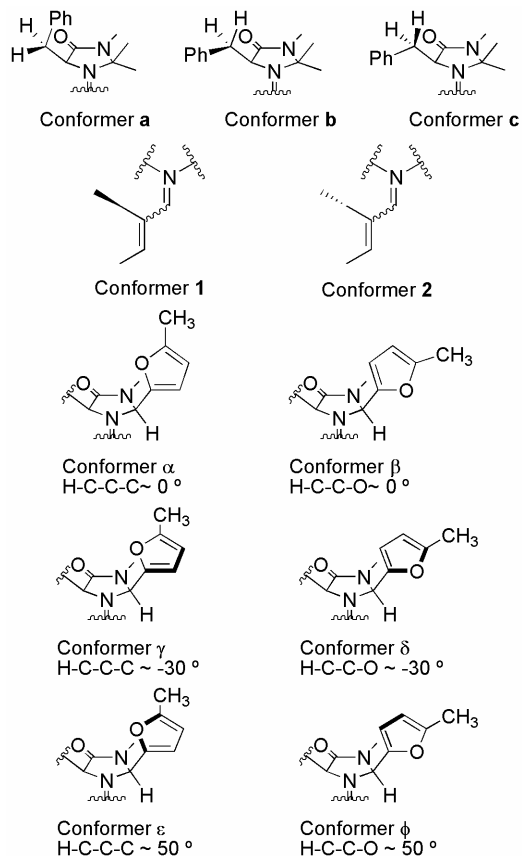


Figure 1. Nomenclature for iminium complexes.

13(E)-a1

B3LYP/6-31G(d) energy= -924.7976362000

Zero-point correction (ZPC)= 0.4307520000

Number of Imaginary Frequencies=0

N	-0.577680	-0.891213	-0.027277	-0.485650
C	-0.011190	-0.721944	-1.398061	-0.078095
C	1.296457	-1.494813	-1.347794	0.632526
N	1.470829	-1.972180	-0.087234	-0.462627
C	0.402921	-1.666953	0.870974	0.337782
C	0.246513	0.744323	-1.847480	-0.383735
C	1.064307	1.586460	-0.890687	0.150280
C	2.461510	1.465740	-0.831264	-0.194528
C	3.202033	2.241938	0.062050	-0.133646
C	2.560485	3.154736	0.902680	-0.127065
C	1.173171	3.296599	0.838540	-0.132749
C	0.433064	2.517197	-0.053369	-0.198427
O	2.049791	-1.618840	-2.295291	-0.499625
C	2.670232	-2.723716	0.268834	-0.348713
C	0.955545	-0.804012	2.014338	-0.471545
C	-0.230781	-2.990087	1.340741	-0.465194
C	-1.793941	-0.489796	0.298124	0.433239
C	-2.697822	-0.052947	-0.754033	-0.175113
C	-3.965444	0.379174	-0.555925	-0.055630
C	-4.900856	0.755113	-1.651448	-0.513716
C	-2.281160	-0.442239	1.729607	-0.371849
C	-2.216289	0.990496	2.314613	-0.468709
H	-0.662405	-1.218480	-2.124320	0.213882
H	3.246426	-2.209660	1.043637	0.185878
H	3.272693	-2.789613	-0.638120	0.230052
H	2.424821	-3.735023	0.605738	0.184956
H	1.742568	-1.364314	2.527053	0.187811
H	1.387241	0.119940	1.623328	0.208906

H	0.200184	-0.561791	2.762320	0.173720
H	0.537981	-3.590008	1.835114	0.195074
H	-0.607135	-3.556929	0.484357	0.184083
H	-1.038784	-2.857729	2.060495	0.181620
H	-5.233287	1.794224	-1.522893	0.209847
H	-5.809452	0.140186	-1.597894	0.211058
H	-4.456314	0.645237	-2.643753	0.190742
H	-4.363904	0.471444	0.451962	0.184030
H	-2.356640	-0.124048	-1.778710	0.179561
H	-3.310179	-0.809555	1.759181	0.195673
H	-1.705796	-1.103729	2.368083	0.185465
H	0.763771	0.636776	-2.807601	0.218665
H	-0.706480	1.239709	-2.052293	0.167114
H	-0.644387	2.654484	-0.119254	0.124346
H	0.669832	4.024789	1.468522	0.151412
H	3.140106	3.765462	1.588679	0.159355
H	4.283665	2.145122	0.088743	0.159615
H	2.970659	0.773879	-1.496695	0.171051
H	-2.856036	1.686664	1.766562	0.172933
H	-2.555515	0.961621	3.354163	0.196277
H	-1.196580	1.384148	2.294831	0.189665
XX	1.824160	2.358173	-0.003511	0.000000

13(E)-a2

B3LYP/6-31G(d) energy=-924.7978469000

Zero-point correction (ZPC)=0.4308070000

Number of Imaginary Frequencies=0

N	-0.657506	0.683946	0.166586	-0.481100
C	0.005349	0.332429	1.457798	-0.083096
C	1.157744	1.319050	1.551409	0.635324
N	1.166646	2.084401	0.427329	-0.464672
C	0.166313	1.742493	-0.590674	0.337450
C	0.511843	-1.129569	1.598385	-0.379277
C	1.417690	-1.621276	0.490170	0.149372
C	2.786144	-1.309353	0.486314	-0.194015
C	3.612181	-1.761978	-0.543797	-0.132948
C	3.085264	-2.536775	-1.580032	-0.127304
C	1.728196	-2.864151	-1.578339	-0.128500
C	0.902479	-2.408979	-0.548756	-0.194961
O	1.927940	1.377392	2.491360	-0.498070
C	2.198491	3.096058	0.221301	-0.349034
C	0.855872	1.146434	-1.829469	-0.469993
C	-0.673619	2.989775	-0.906683	-0.468744
C	-1.809469	0.158939	-0.202269	0.432765
C	-2.531960	-0.689303	0.737366	-0.178816
C	-3.530092	-1.538511	0.404639	-0.057100
C	-4.281188	-2.374028	1.382975	-0.513156
C	-2.451035	0.427340	-1.544569	-0.376044
C	-3.738455	1.277908	-1.461653	-0.458097
H	-0.681228	0.555134	2.281252	0.214847
H	2.804352	2.874284	-0.662241	0.184975
H	2.836434	3.069592	1.105746	0.230254
H	1.765371	4.095937	0.126214	0.186012
H	1.496140	1.913532	-2.274691	0.186559
H	1.476475	0.292136	-1.554044	0.212574
H	0.147627	0.836289	-2.599480	0.176630
H	-0.000676	3.784575	-1.238949	0.196161
H	-1.198226	3.341692	-0.013648	0.182003
H	-1.390651	2.830554	-1.711073	0.180121
H	-4.165585	-3.438725	1.139522	0.209305
H	-5.356529	-2.162885	1.309925	0.209214
H	-3.957888	-2.209081	2.413910	0.190158
H	-3.818712	-1.662244	-0.637556	0.181570
H	-2.258214	-0.626279	1.784511	0.181389

H	-2.695205	-0.548761	-1.979207	0.200400
H	-1.747593	0.885285	-2.232545	0.186419
H	1.042008	-1.129829	2.557442	0.216638
H	-0.343216	-1.802116	1.705789	0.167812
H	-0.149217	-2.688923	-0.540441	0.115940
H	1.316114	-3.484226	-2.369559	0.150467
H	3.731916	-2.896935	-2.374817	0.159031
H	4.671471	-1.521901	-0.528276	0.159674
H	3.204944	-0.720373	1.297891	0.169932
H	-4.506678	0.793019	-0.855371	0.176138
H	-3.544112	2.264860	-1.033016	0.179783
H	-4.137033	1.418784	-2.470289	0.196129
XX	2.237349	-2.080291	-0.547840	0.000000

13(E)-b1

B3LYP/6-31G(d) energy=-924.7941150000

Zero-point correction (ZPC)=0.4304910000

Number of Imaginary Frequencies=0

C	2.419970	-2.091193	-0.403445	-0.197812
C	1.554807	-1.561000	0.567138	0.161332
C	2.100372	-0.816452	1.620633	-0.189139
C	3.475837	-0.584965	1.693840	-0.130563
C	4.324281	-1.099975	0.712978	-0.130215
C	3.793425	-1.859238	-0.334478	-0.130170
C	0.069707	-1.823139	0.483697	-0.376394
C	-0.747559	-1.020774	-0.575269	-0.087277
N	-1.035493	0.395882	-0.209117	-0.488576
C	-2.511196	0.544913	0.206313	0.336501
N	-3.030414	-0.783215	-0.138594	-0.462890
C	-2.126319	-1.656862	-0.661885	0.618855
C	-0.156351	1.379627	-0.335660	0.423496
C	-0.372892	2.737870	0.295439	-0.370446
C	0.473208	2.898726	1.582405	-0.461476
O	-2.338213	-2.783004	-1.065938	-0.485204
C	-4.439818	-1.146437	-0.024213	-0.347930
C	-2.654856	0.797143	1.715117	-0.460439
C	-3.237018	1.586630	-0.666459	-0.469674
C	1.079359	1.151468	-1.060074	-0.151793
C	1.975627	2.117217	-1.373110	-0.062623
C	3.204216	1.879576	-2.180664	-0.510479
H	-0.273875	-1.071653	-1.556802	0.212070
H	-4.815419	-0.949445	0.983483	0.181868
H	-4.500788	-2.216618	-0.226616	0.231099
H	-5.058297	-0.616031	-0.754990	0.187727
H	-3.714721	0.772599	1.983781	0.192968
H	-2.141563	0.019138	2.286667	0.183397
H	-2.268802	1.771952	2.016703	0.179157
H	-4.310879	1.505543	-0.478469	0.196631
H	-3.061642	1.381594	-1.726423	0.186159
H	-2.960174	2.618284	-0.452879	0.184025
H	4.089736	2.209889	-1.621652	0.204386
H	3.179371	2.487589	-3.095444	0.204821
H	3.330141	0.828998	-2.452182	0.190900
H	1.824705	3.142384	-1.042402	0.177627
H	1.295842	0.149561	-1.402200	0.181683
H	-0.101064	3.512242	-0.426240	0.196975
H	-1.413276	2.908764	0.545766	0.180685
H	-0.401776	-1.672359	1.461413	0.168685
H	-0.107803	-2.869332	0.208422	0.223013
H	2.018105	-2.707447	-1.205629	0.150492
H	4.451979	-2.288954	-1.084036	0.160674
H	5.395415	-0.931100	0.774710	0.159873
H	3.884991	-0.017743	2.525180	0.154605
H	1.448727	-0.433703	2.403364	0.130477

H 0.304474 3.898011 1.994183 0.195996
H 0.183496 2.165725 2.341347 0.175612
H 1.541354 2.778678 1.388608 0.181084

13(E)-b2

B3LYP/6-31G(d) energy=-924.7944169000

Zero-point correction (ZPC)= 0.4305770000

Number of Imaginary Frequencies=0

C 2.550281 -1.930208 -0.589387 -0.194140
C 1.565078 -1.658862 0.372559 0.171254
C 1.952337 -1.086235 1.591512 -0.193137
C 3.289010 -0.768108 1.837760 -0.131487
C 4.258225 -1.026301 0.866583 -0.133665
C 3.886600 -1.614875 -0.346147 -0.130519
C 0.119916 -2.002956 0.105973 -0.377301
C -0.707372 -0.991617 -0.745012 -0.097699
N -0.963105 0.324088 -0.095372 -0.481754
C -2.390645 0.341643 0.479731 0.334774
N -2.972615 -0.814467 -0.213474 -0.461159
C -2.099676 -1.571349 -0.936035 0.625124
C -0.079735 1.310990 -0.074901 0.429402
C -0.284791 2.566557 0.745844 -0.379957
C -0.565484 3.841373 -0.080069 -0.457392
O -2.346501 -2.572083 -1.579121 -0.483834
C -4.384052 -1.175907 -0.126470 -0.348870
C -2.372671 0.109205 2.000888 -0.458744
C -3.179952 1.597893 0.082689 -0.474281
C 1.122346 1.221567 -0.884281 -0.153342
C 2.178596 2.062191 -0.794531 -0.053400
C 3.373249 2.002148 -1.682313 -0.509056
H -0.249404 -0.849340 -1.723812 0.212624
H -4.718140 -1.212855 0.914531 0.180609
H -4.478468 -2.169199 -0.567732 0.230997
H -5.015986 -0.480995 -0.688023 0.188916
H -3.401237 0.019845 2.362303 0.192900
H -1.844728 -0.814592 2.248908 0.184407
H -1.908618 0.935652 2.543809 0.180934
H -4.235744 1.418349 0.301660 0.198094
H -3.086858 1.793372 -0.989289 0.185052
H -2.893931 2.485660 0.643957 0.182288
H 4.282909 1.876357 -1.082034 0.205251
H 3.489296 2.953334 -2.219825 0.202158
H 3.314893 1.189110 -2.409772 0.187193
H 2.200023 2.838618 -0.033051 0.176261
H 1.183735 0.430820 -1.620327 0.172971
H 0.638153 2.710437 1.318870 0.203110
H -1.064300 2.422234 1.488558 0.181922
H -0.408945 -2.168542 1.050791 0.173497
H 0.045441 -2.939647 -0.458174 0.218786
H 2.271954 -2.411251 -1.525087 0.148516
H 4.640911 -1.846832 -1.092742 0.159919
H 5.301377 -0.795053 1.062482 0.159536
H 3.576193 -0.338630 2.793482 0.154886
H 1.206786 -0.907977 2.363858 0.129296
H -0.687116 4.688024 0.601648 0.194032
H 0.255095 4.069615 -0.763465 0.176155
H -1.478802 3.749915 -0.672992 0.178956

13(E)-c1

B3LYP/6-31G(d) energy=-924.7958224000

Zero-point correction (ZPC)= 0.4308450000

Number of Imaginary Frequencies=0

C 2.746074 -1.870605 -0.170346 -0.194789
C 2.266564 -0.811129 0.614946 0.142252

C 3.162601 0.177771 1.043081 -0.200043
C 4.513296 0.115303 0.691671 -0.129650
C 4.980037 -0.936221 -0.097473 -0.124317
C 4.093900 -1.927983 -0.525282 -0.129159
C 0.803275 -0.741968 1.013473 -0.373834
C -0.176009 -0.782131 -0.208133 -0.074962
N -1.274067 0.228051 -0.150371 -0.492114
C -2.642762 -0.460854 -0.064321 0.336347
N -2.244841 -1.871513 -0.117635 -0.463497
C -0.912128 -2.108722 -0.265762 0.608731
C -1.037289 1.524955 -0.251430 0.417470
C -2.107017 2.569803 -0.028137 -0.371754
C -1.976073 3.234401 1.363776 -0.461212
O -0.369604 -3.192069 -0.378157 -0.483781
C -3.203631 -2.972417 -0.105494 -0.349016
C -3.347727 -0.166169 1.268421 -0.461022
C -3.498178 -0.138268 -1.303805 -0.464544
C 0.317782 1.967249 -0.532688 -0.177680
C 0.670659 3.249846 -0.789173 -0.059594
C 2.057919 3.675591 -1.121861 -0.517899
H 0.375827 -0.653519 -1.143085 0.224019
H -3.810473 -2.959945 0.804241 0.184651
H -2.617383 -3.892000 -0.129890 0.232361
H -3.858270 -2.947837 -0.981980 0.186328
H -4.228129 -0.808921 1.353630 0.194402
H -2.683891 -0.384225 2.109847 0.184334
H -3.697275 0.864046 1.344900 0.179701
H -4.394190 -0.764550 -1.285466 0.195822
H -2.941492 -0.365931 -2.217365 0.186298
H -3.837180 0.896979 -1.344988 0.182788
H 2.383421 4.467691 -0.434083 0.205410
H 2.083267 4.121473 -2.125877 0.209787
H 2.771714 2.849263 -1.080630 0.199873
H -0.073535 4.043351 -0.771042 0.181029
H 1.106491 1.226223 -0.569360 0.198832
H -2.018936 3.329762 -0.809394 0.198372
H -3.102894 2.151684 -0.126794 0.183148
H 0.617781 0.168691 1.591871 0.162841
H 0.555985 -1.583988 1.669643 0.209713
H 2.063952 -2.655308 -0.488183 0.178084
H 4.454424 -2.755237 -1.129869 0.158250
H 6.029747 -0.987987 -0.371309 0.156836
H 5.198389 0.882829 1.040748 0.150059
H 2.807451 0.991989 1.672030 0.127090
H -2.780394 3.965457 1.486192 0.198519
H -2.061731 2.497787 2.168100 0.178426
H -1.021250 3.752289 1.480641 0.177278

13(E)-c2

B3LYP/6-31G(d) energy=-924.7962335000

Zero-point correction (ZPC)= 0.4309060000

Number of Imaginary Frequencies=0

C 2.820341 -1.738556 -0.420115 -0.195147
C 2.349940 -0.792957 0.503696 0.141620
C 3.236046 0.173995 0.997420 -0.199787
C 4.567900 0.200639 0.576753 -0.129741
C 5.025473 -0.737777 -0.348706 -0.124121
C 4.148939 -1.706224 -0.844154 -0.129266
C 0.909402 -0.822773 0.981152 -0.370091
C -0.132382 -0.760966 -0.185825 -0.084505
N -1.263583 0.186848 0.040359 -0.487612
C -2.572273 -0.586109 0.250034 0.333597
N -2.151683 -1.939773 -0.127578 -0.461778
C -0.823338 -2.099191 -0.380017 0.612596

C	-1.085485	1.495995	0.058315	0.420873
C	-2.209782	2.475065	0.311299	-0.376014
C	-2.677601	3.214425	-0.963398	-0.458960
O	-0.253944	-3.131897	-0.679752	-0.483196
C	-3.067044	-3.075539	-0.186778	-0.349573
C	-2.974309	-0.547834	1.735286	-0.455034
C	-3.694910	-0.133433	-0.695652	-0.470920
C	0.245440	2.022563	-0.196039	-0.178225
C	0.599525	3.322783	-0.061009	-0.059769
C	1.967969	3.842672	-0.332829	-0.517699
H	0.363216	-0.498122	-1.123621	0.225283
H	-3.637218	-3.173350	0.741548	0.182144
H	-2.449477	-3.964596	-0.321962	0.231905
H	-3.756757	-2.994346	-1.032358	0.189089
H	-3.832612	-1.206775	1.893849	0.193866
H	-2.151702	-0.900470	2.363686	0.185333
H	-3.267445	0.451102	2.065435	0.180376
H	-4.500558	-0.870845	-0.648693	0.197812
H	-3.337589	-0.089761	-1.728414	0.185635
H	-4.133560	0.824510	-0.420414	0.181754
H	2.348358	4.382510	0.544492	0.204901
H	1.932515	4.580450	-1.146688	0.209026
H	2.672150	3.051285	-0.600521	0.199971
H	-0.126410	4.061797	0.272250	0.180923
H	1.024093	1.332112	-0.497004	0.196461
H	-1.845878	3.207457	1.038560	0.199231
H	-3.055382	1.987327	0.787184	0.184122
H	0.729434	0.012797	1.664783	0.164134
H	0.723738	-1.740268	1.551325	0.207092
H	2.147016	-2.505791	-0.794250	0.178916
H	4.502335	-2.446208	-1.556469	0.158315
H	6.060655	-0.720098	-0.676762	0.156862
H	5.246288	0.948558	0.977707	0.149604
H	2.889115	0.899050	1.731185	0.126246
H	-3.484786	3.903688	-0.699785	0.196758
H	-1.868096	3.792618	-1.414873	0.177000
H	-3.056118	2.520361	-1.718250	0.179828

13(Z)-a1

B3LYP/6-31G(d) energy=-924.7963599000

Zero-point correction (ZPC)=0.4307420000

Number of Imaginary Frequencies=0

C	1.303247	-2.340233	-0.247041	-0.204670
C	1.847376	-1.311128	0.534359	0.148151
C	3.103613	-0.792605	0.181603	-0.190977
C	3.783532	-1.278956	-0.935716	-0.132638
C	3.224585	-2.295325	-1.713954	-0.127475
C	1.983696	-2.829867	-1.363682	-0.128967
C	1.106155	-0.782650	1.746031	-0.383634
C	0.330309	0.548557	1.546211	-0.088880
N	-0.701806	0.558866	0.467802	-0.474951
C	-0.288816	1.528085	-0.660254	0.339924
N	0.885326	2.165102	-0.053461	-0.462418
C	1.276323	1.670112	1.151100	0.634057
C	-1.852398	-0.080821	0.555640	0.421576
C	-2.247356	-0.781286	1.841390	-0.376226
C	-2.349940	-2.318552	1.744786	-0.466760
O	2.225965	2.025898	1.823357	-0.498596
C	1.639139	3.231709	-0.704495	-0.348539
C	0.117801	0.783032	-1.942006	-0.474579
C	-1.373825	2.593162	-0.890334	-0.463147
C	-2.780036	-0.141106	-0.563399	-0.173792
C	-4.088808	-0.465651	-0.459680	-0.055151
C	-5.026648	-0.548078	-1.614280	-0.513155

H	-5.487471	-1.544205	-1.654045	0.209509
H	-1.577329	-0.513027	2.655992	0.195866
H	-3.229029	-0.378622	2.119240	0.201695
H	-0.137887	0.834416	2.492035	0.216014
H	2.456770	3.487276	-0.029115	0.230168
H	1.020459	4.119266	-0.864577	0.184940
H	2.057135	2.899221	-1.659303	0.185618
H	-0.730729	0.334555	-2.462011	0.176164
H	0.565188	1.502563	-2.633458	0.187523
H	0.852578	0.005814	-1.724981	0.214471
H	-0.985041	3.341506	-1.585948	0.194187
H	-1.622255	3.095757	0.048944	0.182291
H	-2.285220	2.189956	-1.330583	0.175117
H	-2.393584	0.070667	-1.550262	0.171969
H	-4.537409	-0.346984	-2.570814	0.186885
H	-5.854211	0.161702	-1.481355	0.209534
H	-4.527949	-0.665879	0.515542	0.182976
H	1.813210	-0.552196	2.551001	0.216234
H	0.423769	-1.543232	2.134956	0.168964
H	0.347509	-2.781716	0.027101	0.125249
H	1.551361	-3.636020	-1.949729	0.151934
H	3.760166	-2.679558	-2.577137	0.158733
H	4.758670	-0.873002	-1.189228	0.159191
H	3.553157	-0.013271	0.790416	0.172308
H	-2.681629	-2.712457	2.709499	0.198246
H	-3.065824	-2.633507	0.982117	0.173695
H	-1.384557	-2.774557	1.511001	0.191232
XX	2.546429	-1.787351	-0.581229	0.000000

13(Z)-a2

B3LYP/6-31G(d) energy=-924.7975495000

Zero-point correction (ZPC)=0.4308820000

Number of Imaginary Frequencies=0

C	-1.467164	2.296105	0.632629	-0.195068
C	-1.920735	1.020513	0.996905	0.149494
C	-3.141670	0.563866	0.476341	-0.191759
C	-3.877793	1.359412	-0.402810	-0.133461
C	-3.409468	2.623504	-0.769316	-0.127448
C	-2.203815	3.093537	-0.245372	-0.129212
C	-1.112756	0.164975	1.948802	-0.387198
C	-0.233071	-0.943074	1.296295	-0.082153
N	0.706940	-0.500258	0.225587	-0.476717
C	0.282076	-1.074895	-1.139076	0.341592
N	-0.799715	-1.976105	-0.726733	-0.462108
C	-1.118546	-1.961155	0.595427	0.630832
C	1.808999	0.182963	0.475167	0.420314
C	2.269102	0.347236	1.909311	-0.377243
C	3.197365	-0.818021	2.331210	-0.464684
O	-1.982588	-2.610910	1.153623	-0.498561
C	-1.529593	-2.823652	-1.664100	-0.348454
C	-0.260586	0.006911	-2.086552	-0.473495
C	1.420405	-1.910567	-1.750618	-0.464316
C	2.626439	0.736776	-0.587751	-0.167948
C	3.829208	1.330475	-0.403024	-0.053984
C	4.646792	1.921750	-1.497968	-0.513752
H	4.849030	2.980422	-1.286479	0.211066
H	1.423284	0.398735	2.590843	0.200861
H	2.793978	1.298361	2.011282	0.193040
H	0.328843	-1.461077	2.078017	0.211764
H	-2.275694	-3.361488	-1.077575	0.229810
H	-0.868416	-3.548714	-2.147526	0.184452
H	-2.037844	-2.226309	-2.426606	0.185712
H	0.513914	0.689746	-2.439482	0.175078
H	-0.677689	-0.482908	-2.971014	0.186183

H	-1.049372	0.585784	-1.603650	0.215117
H	1.040266	-2.422039	-2.638828	0.194469
H	1.760991	-2.668958	-1.039669	0.181295
H	2.274380	-1.312318	-2.068095	0.174639
H	2.241518	0.702146	-1.596137	0.167348
H	4.165780	1.841151	-2.476077	0.187602
H	5.628706	1.431284	-1.542847	0.210293
H	4.265259	1.392058	0.591524	0.185115
H	-1.774542	-0.395258	2.619061	0.218527
H	-0.494245	0.806656	2.582489	0.174642
H	-0.540719	2.680575	1.055533	0.120331
H	-1.844083	4.084403	-0.507987	0.151712
H	-3.989336	3.245186	-1.445241	0.158704
H	-4.826125	0.997266	-0.789506	0.159071
H	-3.520595	-0.411402	0.769798	0.169796
H	3.519076	-0.662085	3.364689	0.203587
H	2.684889	-1.783972	2.280466	0.178926
H	4.087754	-0.875239	1.698994	0.176153
XX	-2.673162	1.805615	0.115164	0.000000

13(Z)-b1

B3LYP/6-31G(d) energy=-924.7919857000

Zero-point correction (ZPC)= 0.4302260000

Number of Imaginary Frequencies=0

C	3.020587	-1.412618	-0.723852	-0.193311
C	2.117348	-1.281059	0.342691	0.170438
C	2.540935	-0.623373	1.505222	-0.200747
C	3.836378	-0.107906	1.603509	-0.130093
C	4.722286	-0.237913	0.533401	-0.126056
C	4.310451	-0.890516	-0.632302	-0.128033
C	0.747860	-1.916935	0.274858	-0.379470
C	-0.317398	-1.288950	-0.671106	-0.098774
N	-0.893785	0.010924	-0.222683	-0.467457
C	-2.259576	-0.240446	0.450920	0.333575
N	-2.533537	-1.608291	-0.003873	-0.459453
C	-1.520976	-2.220975	-0.679161	0.621727
C	-0.378845	1.198559	-0.487058	0.418735
C	0.768704	1.361165	-1.463827	-0.370125
C	2.003204	2.118142	-0.937468	-0.459328
O	-1.522040	-3.338676	-1.154869	-0.482761
C	-3.796933	-2.297515	0.241032	-0.348500
C	-2.140273	-0.189077	1.983378	-0.461103
C	-3.359414	0.684533	-0.094233	-0.465285
C	-0.918863	2.401725	0.132295	-0.182134
C	-0.833213	3.640274	-0.400127	-0.051893
C	-1.370836	4.872609	0.242708	-0.512771
H	-0.571570	5.617137	0.355859	0.208943
H	1.093884	0.398870	-1.850244	0.192646
H	0.342777	1.908812	-2.318264	0.197474
H	0.069201	-1.203149	-1.685556	0.212243
H	-3.644368	-3.337915	-0.049552	0.231136
H	-4.610829	-1.880552	-0.360107	0.188549
H	-4.068278	-2.257130	1.300076	0.180577
H	-1.896020	0.809576	2.352756	0.180696
H	-3.099634	-0.471532	2.426572	0.193137
H	-1.381759	-0.889383	2.340483	0.185815
H	-4.323884	0.300904	2.483886	0.195644
H	-3.361871	0.679248	-1.188033	0.183067
H	-3.281938	1.710504	0.260092	0.176817
H	-1.410761	2.293396	1.090808	0.174328
H	-1.811816	4.677738	1.223922	0.184644
H	-2.128717	5.338289	-0.401417	0.207059
H	-0.373452	3.779293	-1.376676	0.183805
H	0.318640	-1.985910	1.280061	0.170059

H	0.835515	-2.946873	-0.091878	0.222996
H	2.724300	-1.954524	-1.620294	0.145529
H	5.001739	-1.012076	-1.461279	0.160464
H	5.732301	0.153647	0.610515	0.161499
H	4.154278	0.382628	2.519115	0.157240
H	1.864703	-0.539333	2.353372	0.131843
H	2.752590	2.154629	-1.732643	0.187112
H	1.770172	3.143637	-0.643991	0.161101
H	2.443822	1.602700	-0.082515	0.198476

13(Z)-b2

B3LYP/6-31G(d) energy=-924.7965413000

Zero-point correction (ZPC)= 0.4303920000

Number of Imaginary Frequencies=0

C	2.746074	-1.870605	-0.170346	-0.194789
C	2.266564	-0.811129	0.614946	0.142252
C	3.162601	0.177771	1.043081	-0.200043
C	4.513296	0.115303	0.691671	-0.129650
C	4.980037	-0.936221	-0.097473	-0.124317
C	4.093900	-1.927983	-0.525282	-0.129159
C	0.803275	-0.741968	1.013473	-0.373834
C	-0.176009	-0.782131	-0.208133	-0.074962
N	-1.274067	0.228051	-0.150371	-0.492114
C	-2.642762	-0.460854	-0.064321	0.336347
N	-2.244841	-1.871513	-0.117635	-0.463497
C	-0.912128	-2.108722	-0.265762	0.608731
C	-1.037289	1.524955	-0.251430	0.417470
C	-2.107017	2.569803	-0.028137	-0.371754
C	-1.976073	3.234401	1.363776	-0.461212
O	-0.369604	-3.192069	-0.378157	-0.483781
C	-3.203631	-2.972417	-0.105494	-0.349016
C	-3.347727	-0.166169	1.268421	-0.461022
C	-3.498178	-0.138268	-1.303805	-0.464544
C	0.317782	1.967249	-0.532688	-0.177680
C	0.670659	3.249846	-0.789173	-0.059594
C	2.057919	3.675591	-1.121861	-0.517899
H	0.375827	-0.653519	-1.143085	0.224019
H	-3.810473	-2.959945	0.804241	0.184651
H	-2.617383	-3.892000	-0.129890	0.232361
H	-3.858270	-2.947837	-0.981980	0.186328
H	-4.228129	-0.808921	1.353630	0.194402
H	-2.683891	-0.384225	2.109847	0.184334
H	-3.697275	0.864046	1.344900	0.179701
H	-4.394190	-0.764550	-1.285466	0.195822
H	-2.941492	-0.365931	-2.217365	0.186298
H	-3.837180	0.896979	-1.344988	0.182788
H	2.383421	4.467691	-0.434083	0.205410
H	2.083267	4.121473	-2.125877	0.209787
H	2.771714	2.849263	-1.080630	0.199873
H	-0.073535	4.043351	-0.771042	0.181029
H	1.106491	1.226223	-0.569360	0.198832
H	-2.018936	3.329762	-0.809394	0.198372
H	-3.102894	2.151684	-0.126794	0.183148
H	0.617781	0.168691	1.591871	0.162841
H	0.555985	-1.583988	1.669643	0.209713
H	2.063952	-2.655308	-0.488183	0.178084
H	4.454424	-2.755237	-1.129869	0.158250
H	6.029747	-0.987987	-0.371309	0.156836
H	5.198389	0.882829	1.040748	0.150059
H	2.807451	0.991989	1.672030	0.127090
H	-2.780394	3.965457	1.486192	0.198519
H	-2.061731	2.497787	2.168100	0.178426
H	-1.021250	3.752289	1.480641	0.177278

13(Z)-c1

B3LYP/6-31G(d) energy=-924.7939203000

Zero-point correction (ZPC)= 0.4305700000

Number of Imaginary Frequencies=0

C	-3.227614	-1.372624	0.861172	-0.200040
C	-2.696691	-0.145069	0.444022	0.147201
C	-3.453445	0.665889	-0.415893	-0.197501
C	-4.707947	0.244405	-0.856659	-0.129699
C	-5.227104	-0.983803	-0.440572	-0.123774
C	-4.486347	-1.790008	0.423544	-0.126504
C	-1.334182	0.305642	0.941360	-0.371930
C	-0.361416	0.725551	-0.209599	-0.087251
N	1.038156	0.221494	-0.067333	-0.480565
C	2.004645	1.386609	0.194532	0.335309
N	1.115187	2.532794	-0.011865	-0.461902
C	-0.189704	2.234904	-0.261246	0.612001
C	1.365865	-1.046251	-0.229807	0.417709
C	0.303909	-2.064948	-0.592348	-0.384314
C	0.079818	-3.141949	0.492726	-0.458523
O	-1.093215	3.025028	-0.460364	-0.481494
C	1.571431	3.918578	0.042200	-0.349186
C	2.499867	1.360211	1.651054	-0.459893
C	3.135164	1.440658	-0.845963	-0.463259
C	2.728779	-1.519137	-0.040256	-0.174678
C	3.205228	-2.682557	-0.538088	-0.052896
C	4.598565	-3.172235	-0.343311	-0.513537
H	4.585157	-4.167794	0.120366	0.210028
H	-0.648764	-1.587465	-0.814676	0.211376
H	0.627011	-2.551925	-1.520892	0.201373
H	-0.756475	0.397501	-1.173583	0.226621
H	0.679925	4.541078	-0.045004	0.232495
H	2.248163	4.152340	-0.785170	0.187881
H	2.067587	4.135868	0.992547	0.182890
H	3.158065	0.515730	1.864197	0.181333
H	3.070340	2.271209	1.851925	0.194538
H	1.652470	1.328124	2.341576	0.186448
H	3.687316	2.374045	-0.707859	0.195451
H	2.720695	1.436327	-1.858217	0.185782
H	3.854064	0.627813	-0.753217	0.175893
H	3.407483	-0.906390	0.535953	0.169974
H	5.198850	-2.501989	0.277383	0.186080
H	5.095627	-3.298689	-1.314435	0.209804
H	2.564083	-3.318169	-1.145528	0.183989
H	-0.870168	-0.492614	1.528094	0.158939
H	-1.445622	1.160630	1.618654	0.206493
H	-2.665158	-2.000844	1.548378	0.125810
H	-4.886382	-2.741986	0.760846	0.150527
H	-6.206151	-1.306381	-0.782564	0.155826
H	-5.285087	0.882726	-1.519534	0.156426
H	-3.064802	1.632942	-0.724509	0.178307
H	-0.734861	-3.797356	0.173646	0.199830
H	0.970117	-3.752401	0.657689	0.171399
H	-0.204076	-2.695761	1.450029	0.179248

13(Z)-c2

B3LYP/6-31G(d) energy=-924.7962599000

Zero-point correction (ZPC)= 0.4305050000

Number of Imaginary Frequencies=0

C	3.134474	-1.383897	-1.129277	-0.196007
C	2.668805	-0.158836	-0.633844	0.144716
C	3.488741	0.583784	0.229657	-0.195786
C	4.745233	0.099638	0.592913	-0.129922
C	5.201348	-1.124305	0.096827	-0.124271
C	4.395141	-1.864414	-0.767810	-0.127156

C	1.301461	0.358157	-1.042194	-0.372480
C	0.366591	0.674523	0.176117	-0.085535
N	-1.033460	0.192139	0.002194	-0.476668
C	-1.985054	1.373427	-0.214182	0.336902
N	-1.098962	2.496225	0.110732	-0.461573
C	0.201147	2.173730	0.361148	0.611254
C	-1.351543	-1.087250	0.076467	0.413513
C	-0.300844	-2.071779	0.547522	-0.385606
C	-0.318807	-2.223325	2.088439	-0.463436
O	1.102695	2.940568	0.642591	-0.482508
C	-1.551493	3.883216	0.156304	-0.348828
C	-2.429412	1.456383	-1.684664	-0.457553
C	-3.152680	1.355170	0.785955	-0.465926
C	-2.678752	-1.571313	-0.251185	-0.170930
C	-3.102651	-2.841063	-0.047521	-0.051813
C	-4.459630	-3.338126	-0.405159	-0.514181
H	-4.378016	-4.193424	-1.089450	0.211738
H	0.696168	-1.770655	0.225301	0.217722
H	-0.486088	-3.039462	0.078624	0.189994
H	0.785146	0.254390	1.092211	0.222743
H	-0.659390	4.496075	0.292817	0.231778
H	-2.231488	4.058172	0.995578	0.187821
H	-2.043191	4.170288	-0.777832	0.182242
H	-3.071438	0.624804	-1.981707	0.179389
H	-3.000407	2.376625	-1.836415	0.193448
H	-1.559001	1.481079	-2.346206	0.186761
H	-3.694984	2.300766	0.703802	0.196247
H	-2.775539	1.265689	1.808757	0.185236
H	-3.872690	0.558851	0.601683	0.175871
H	-3.375664	-0.884862	-0.709654	0.166101
H	-5.083161	-2.570190	-0.870034	0.187007
H	-4.970646	-3.717228	0.490279	0.210915
H	-2.442837	-3.572244	0.414229	0.187109
H	0.806028	-0.373543	-1.688971	0.161591
H	1.407042	1.274273	-1.635096	0.205147
H	2.517162	-1.959570	-1.816632	0.126198
H	4.745534	-2.812587	-1.165526	0.151240
H	6.182496	-1.495227	0.378474	0.156004
H	5.373135	0.684482	1.258973	0.156837
H	3.144139	1.543496	0.606644	0.178048
H	0.448810	-2.944141	2.382809	0.205021
H	-0.101594	-1.277376	2.594366	0.178616
H	-1.286580	-2.583893	2.448688	0.173097

14(E)-a1u

B3LYP/6-31G(d) energy=-1114.3211932000

Zero-point correction (ZPC)= 0.452872

Number of Imaginary Frequencies=0

C	1.256310	3.135738	0.190607	-0.188389
C	0.886709	1.837494	0.405995	0.164411
O	1.657401	0.998011	-0.349277	-0.184920
C	2.526144	1.779623	-1.068276	-0.131868
C	2.312904	3.096674	-0.768340	-0.129659
C	-0.057041	1.253900	1.396006	-0.131616
N	0.580249	0.405419	2.385161	-0.387185
C	0.081157	-0.855948	2.494217	-0.075040
C	-1.076586	-1.004441	1.510164	0.637409
N	-1.157005	0.337634	0.866112	-0.455615
C	-0.887587	-2.239916	0.591987	0.082705
C	0.309680	-2.261283	-0.334870	-0.467640
C	0.148181	-1.985839	-1.698997	0.350151
C	1.223324	-2.094228	-2.582330	-0.470640
C	2.478528	-2.478904	-2.107443	0.357128
C	2.652704	-2.746699	-0.747624	-0.210637

C	1.575931	-2.642402	0.132901	-0.194342
O	0.466781	-1.738959	3.234865	-0.530580
C	1.686382	0.892993	3.197356	-0.339546
C	-2.160182	0.754805	0.118461	-0.493911
C	-3.300241	-0.115128	-0.100497	0.429676
C	-4.357977	0.191482	-0.887845	-0.364397
C	-5.544149	-0.687452	-1.077027	-0.461948
C	3.472585	1.081712	-1.977227	-0.176944
C	-2.133663	2.127689	-0.507986	-0.052845
C	-1.600061	2.088097	-1.960314	-0.513926
H	-1.985929	-1.151574	2.103999	0.212659
H	2.548718	1.140493	2.571580	0.194724
H	1.951457	0.090841	3.887151	0.225043
H	1.385445	1.779534	3.766424	0.179087
H	-5.666298	-0.931542	-2.141063	0.209777
H	-6.458174	-0.153216	-0.784190	0.210878
H	-5.477555	-1.616522	-0.505388	0.190879
H	-4.376240	1.130352	-1.437175	0.184952
H	-3.323679	-1.063511	0.420991	0.180038
H	-3.146435	2.536828	-0.492984	0.191081
H	-1.515766	2.806476	0.078264	0.188954
H	-0.823659	-3.070976	1.304189	0.214517
H	-1.798285	-2.399306	0.008309	0.164767
H	-0.835211	-1.718905	-2.081695	0.116537
H	1.074798	-1.903410	-3.641781	0.145379
H	3.312026	-2.587752	-2.795775	0.151688
H	3.622765	-3.063217	-0.374658	0.154122
H	1.710692	-2.883357	1.183706	0.168546
H	-2.235663	1.474672	-2.605230	0.168498
H	-1.584067	3.105310	-2.361239	0.193964
H	-0.584399	1.687828	-1.997563	0.196025
H	-0.560144	2.098154	1.888593	0.193828
H	0.838484	4.014478	0.664929	0.167648
H	2.853822	3.938063	-1.177718	0.172519
H	4.123215	1.812639	-2.463344	0.185845
H	4.096311	0.369205	-1.426181	0.191640
H	2.939283	0.516812	-2.749328	0.186701
XX	1.399765	-2.375435	-1.205895	0.000000

14(E)-a2 α

B3LYP/6-31G(d) energy=-1114.3212477000

Zero-point correction (ZPC)= 0.452851

Number of Imaginary Frequencies=0

C	0.628775	-2.396444	-1.123162	-0.462735
C	0.743383	-2.228733	0.262807	0.348955
C	2.018115	-2.269475	0.846662	-0.195273
C	3.149500	-2.481583	0.059137	-0.208669
C	3.022746	-2.661481	-1.320308	0.359414
C	1.759262	-2.612693	-1.912458	0.078923
C	-0.497999	-2.116881	1.121961	-0.453180
C	-0.943536	-0.711414	1.599323	0.639027
C	0.091319	-0.064276	2.517486	-0.075792
N	0.345987	1.193760	2.061468	-0.463495
C	-0.293839	1.549576	0.809322	-0.386320
N	-1.199726	0.342050	0.576610	0.166201
C	0.666138	1.906321	-0.271350	-0.184351
O	1.664919	1.028127	-0.586194	-0.130892
C	2.493188	1.656919	-1.479849	-0.132169
C	2.031620	2.921073	-1.723299	-0.130005
C	0.853991	3.087592	-0.935950	-0.186064
C	3.663868	0.889900	-1.979000	-0.493020
C	1.291625	2.092582	2.709267	-0.339325
O	0.569768	-0.602497	3.496124	0.426596
C	-2.206898	0.338575	-0.273328	-0.174738

C	-2.440450	1.518546	-1.183428	-0.053858
C	-3.477637	2.506562	-0.599700	-0.513944
C	-3.153107	-0.761537	-0.262229	-0.531468
C	-4.125818	-0.951166	-1.183933	-0.378453
C	-5.119870	-2.058664	-1.137389	-0.461691
H	-1.859964	-0.830275	2.189687	0.212478
H	2.163399	2.269366	2.072314	0.194554
H	1.607423	1.608298	3.634103	0.224975
H	0.812471	3.049425	2.942420	0.178877
H	-5.047029	-2.669121	-2.047623	0.210210
H	-6.138848	-1.648567	-1.130921	0.209699
H	-4.992429	-2.704680	-0.265235	0.190566
H	-4.212765	-0.278909	-2.035351	0.183693
H	-3.093341	-1.470292	0.554965	0.179959
H	-0.346160	-2.658602	2.062863	0.213619
H	-1.333471	-2.605768	0.613424	0.164187
H	-0.356150	-2.395677	-1.586557	0.115135
H	1.650888	-2.767168	-2.982571	0.146252
H	3.902271	-2.855919	-1.927880	0.151801
H	4.128401	-2.533180	0.527528	0.153584
H	2.119723	-2.160531	1.923016	0.167089
H	-3.152750	2.924748	0.358813	0.172731
H	-3.614546	3.336259	-1.298704	0.198266
H	-4.446843	2.024825	-0.444096	0.177738
H	-0.950834	2.417676	0.948133	0.191961
H	0.238514	3.975032	-0.861644	0.167033
H	2.486120	3.648996	-2.380197	0.172462
H	4.252614	1.515577	-2.654138	0.185164
H	4.306477	0.566498	-1.152484	0.189833
H	3.347299	-0.009800	-2.516734	0.190267
H	-2.798531	1.147853	-2.147102	0.193264
H	-1.499524	2.028420	-1.385506	0.201064
XX	1.888427	-2.444735	-0.513219	0.000000

14(E)-a1 β

B3LYP/6-31G(d) energy=-1114.3247280000

Zero-point correction (ZPC)= 0.45319

Number of Imaginary Frequencies=0

C	0.576059	1.608600	-2.103616	-0.487895
C	0.546275	2.279806	-0.873477	0.343957
C	-0.497838	3.183620	-0.622059	-0.185588
C	-1.490416	3.402519	-1.579424	-0.218428
C	-1.451502	2.725460	-2.801390	0.358825
C	-0.414833	1.827486	-3.062323	0.077736
C	1.652840	2.074930	0.139372	-0.461125
C	1.365937	1.090761	1.304394	0.633043
C	0.220472	1.589801	2.182599	-0.077427
N	-0.728652	0.615123	2.248218	-0.465101
C	-0.451804	-0.586383	1.487664	-0.383133
N	0.946535	-0.292581	0.948442	0.153160
C	-1.501360	-0.916229	0.480422	-0.193610
O	-1.966969	-2.210529	0.531834	-0.139045
C	-2.965776	-2.324658	-0.398115	-0.131318
C	-3.134102	-1.124142	-1.030692	-0.126295
C	-2.193869	-0.210918	-0.461270	-0.188465
C	-3.635386	-3.648670	-0.508817	-0.493939
C	-1.940444	0.740731	3.047428	-0.339265
O	0.192477	2.681853	2.714959	0.428400
C	1.728612	-1.206616	0.409729	-0.177831
C	1.188881	-2.573392	0.066411	-0.052650
C	0.768511	-2.673019	-1.420312	-0.513732
C	3.119768	-0.890312	0.144998	-0.533423
C	3.996581	-1.732975	-0.449433	-0.379125
C	5.432540	-1.418885	-0.684832	-0.464953

H	2.257216	1.027179	1.938250	0.214614
H	-2.829380	0.694706	2.412253	0.193033
H	-1.893685	1.708994	3.547311	0.224792
H	-1.988798	-0.056293	3.797778	0.181770
H	5.662284	-1.483332	-1.757063	0.209061
H	6.066449	-2.170843	-0.195675	0.210786
H	5.713286	-0.427473	-0.320616	0.190126
H	3.665415	-2.710199	-0.794433	0.185037
H	3.491436	0.075569	0.464141	0.178359
H	1.961764	-3.314231	0.285044	0.190859
H	0.332129	-2.825232	0.690782	0.208613
H	1.873162	3.018628	0.651280	0.215471
H	2.569919	1.774123	-0.375172	0.167356
H	1.397085	0.930207	-2.327001	0.122022
H	-0.368326	1.310361	-4.016549	0.150708
H	-2.215687	2.909264	-3.551123	0.157476
H	-2.283799	4.116533	-1.377335	0.160044
H	-0.522080	3.728509	0.317688	0.171904
H	1.611818	-2.487297	-2.091505	0.166926
H	0.392972	-3.681492	-1.614504	0.190984
H	-0.023087	-1.957594	-1.656724	0.195853
H	-0.356471	-1.449775	2.159974	0.206851
H	-2.060714	0.830780	-0.716336	0.188631
H	-3.855672	-0.911064	-1.806918	0.169557
H	-4.111131	-3.933942	0.436758	0.193854
H	-4.406433	-3.609658	-1.281887	0.191475
H	-2.923786	-4.439899	-0.772896	0.180618
XX	-0.456458	2.512548	-1.822349	0.000000

14(E)-a2β

B3LYP/6-31G(d) energy=-1114.3243655000

Zero-point correction (ZPC)=0.453035

Number of Imaginary Frequencies=0

C	0.859839	-1.858896	-1.926754	-0.486407
C	0.900087	-2.325222	-0.606004	0.341919
C	2.145045	-2.634726	-0.035769	-0.177328
C	3.320490	-2.471350	-0.771372	-0.217194
C	3.267846	-2.002436	-2.086827	0.360530
C	2.034003	-1.696994	-2.663923	0.070990
C	-0.382226	-2.557257	0.164350	-0.456799
C	-0.826715	-1.465015	1.172480	0.633011
C	0.218260	-1.227985	2.261409	-0.082747
N	0.543071	0.096243	2.267141	-0.459041
C	-0.089613	0.902923	1.244135	-0.378287
N	-1.087989	-0.095606	0.651808	0.153221
C	0.877872	1.518546	0.289165	-0.194763
O	0.645135	2.843896	-0.011882	-0.139196
C	1.660522	3.262836	-0.831050	-0.130808
C	2.526561	2.227383	-1.043329	-0.124550
C	2.027261	1.102750	-0.318053	-0.182668
C	1.619945	4.679363	-1.283592	-0.492557
C	1.483915	0.677007	3.216456	-0.338765
O	0.657566	-2.096250	2.988970	0.423051
C	-2.141701	0.257843	-0.055161	-0.174190
C	-2.384363	1.709878	-0.386288	-0.053362
C	-3.351897	2.374734	0.622144	-0.513848
C	-3.119244	-0.745373	-0.435867	-0.533300
C	-4.175768	-0.520019	-1.250965	-0.393554
C	-5.193916	-1.546841	-1.605767	-0.458822
H	-1.736271	-1.812984	1.673834	0.213254
H	2.347311	1.100738	2.696210	0.192853
H	1.809296	-0.128358	3.876082	0.224760
H	0.996193	1.459876	3.807826	0.180817
H	-5.223998	-1.687931	-2.694633	0.209495

H	-6.195263	-1.197629	-1.319611	0.209697
H	-5.005463	-2.511329	-1.127619	0.189929
H	-4.320244	0.459607	-1.702047	0.183595
H	-3.007896	-1.742644	-0.027354	0.178452
H	-1.447805	2.263558	-0.420630	0.222635
H	-2.810351	1.770216	-1.390860	0.190647
H	-0.284525	-3.453876	0.787251	0.211565
H	-1.199535	-2.749231	-0.537195	0.166901
H	-0.099263	-1.643044	-2.393345	0.121203
H	1.983618	-1.346424	-3.690838	0.150644
H	4.182000	-1.891029	-2.662837	0.156571
H	4.275603	-2.728490	-0.322221	0.159293
H	2.190781	-3.017611	0.980057	0.171705
H	-2.950718	2.361877	1.640827	0.174311
H	-3.503676	3.419009	0.335809	0.198319
H	-4.324726	1.875851	0.637217	0.174868
H	-0.677083	1.710842	1.697228	0.202512
H	2.472786	0.120316	-0.256176	0.187060
H	3.426289	2.264415	-1.641248	0.169411
H	1.636548	5.370410	-0.432762	0.192123
H	2.487285	4.890697	-1.913505	0.191774
H	0.714717	4.890664	-1.865319	0.181141
XX	2.088282	-2.169171	-1.329772	0.000000

14(E)-b1α

B3LYP/6-31G(d) energy=-1114.32632820

Zero-point correction (ZPC)=0.452661

Number of Imaginary Frequencies=0

O	-2.223655	-0.771909	-0.885074	-0.485270
C	-2.449080	-0.497206	0.438712	0.381931
C	-3.353283	-1.382413	0.950074	-0.198814
C	-3.704979	-2.262599	-0.121019	-0.214112
C	-2.998176	-1.857467	-1.217327	0.363797
C	-1.787859	0.702332	1.025452	0.030025
N	-2.143584	1.963331	0.401863	-0.439393
C	-1.118755	2.607290	-0.229226	0.622210
C	0.130355	1.730549	-0.109328	-0.092340
N	-0.276573	0.716916	0.901594	-0.446322
C	0.470891	1.177820	-1.523888	-0.380845
C	1.755216	0.392719	-1.647375	0.153149
C	1.743816	-1.008450	-1.625090	-0.191003
C	2.933223	-1.733075	-1.725013	-0.129740
C	4.151716	-1.063563	-1.849760	-0.130475
C	4.174603	0.333621	-1.886712	-0.130467
C	2.984248	1.055534	-1.789461	-0.197191
O	-1.168543	3.660751	-0.828823	-0.479310
C	-3.508779	2.466924	0.430505	-0.339729
C	0.531198	0.041258	1.698942	0.419434
C	1.962934	0.244147	1.616774	-0.159169
C	2.859942	-0.276247	2.486781	-0.061658
C	4.328565	-0.042971	2.404493	-0.511456
C	-2.916846	-2.335319	-2.623358	-0.536412
C	-0.025564	-0.967463	2.676351	-0.363667
C	0.110077	-2.414852	2.147292	-0.457053
H	0.951661	2.330529	0.285929	0.210690
H	-4.191579	1.770352	-0.065898	0.190605
H	-3.508385	3.419433	-0.101063	0.227066
H	-3.841379	2.625761	1.462592	0.178800
H	4.859136	-1.003464	2.361862	0.203158
H	4.683607	0.458480	3.315316	0.204911
H	4.608293	0.554497	1.533641	0.191895
H	2.529941	-0.902511	3.312985	0.177402
H	2.344745	0.846295	0.802937	0.188748
H	0.514516	-0.868190	3.621242	0.195092

H	-1.072529	-0.769196	2.901471	0.182517
H	-0.379568	0.581314	-1.865831	0.191328
H	0.510401	2.074084	-2.153675	0.213011
H	3.007516	2.142257	-1.843973	0.149502
H	5.116621	0.860054	-2.012306	0.159239
H	5.076761	-1.625889	-1.938177	0.157739
H	2.907170	-2.819245	-1.718835	0.151051
H	0.794650	-1.534068	-1.546169	0.133459
H	1.155292	-2.679586	1.968182	0.174987
H	-0.299840	-3.105208	2.889945	0.191695
H	-0.446783	-2.548041	1.216264	0.185731
H	-2.047759	0.735594	2.089370	0.195363
H	-3.736715	-1.403332	1.961875	0.170030
H	-4.401743	-3.087968	-0.082810	0.175515
H	-1.898527	-2.646139	-2.885642	0.184866
H	-3.581567	-3.191321	-2.761539	0.193825
H	-3.216040	-1.550375	-3.327630	0.195825

14(E)-b2a

B3LYP/6-31G(d) energy=-1114.32764380

Zero-point correction (ZPC)= 0.452854

Number of Imaginary Frequencies=0

O	2.173814	-1.230009	-0.565420	-0.482490
C	2.405582	0.114173	-0.696201	0.380866
C	3.292336	0.335493	-1.711059	-0.197513
C	3.623774	-0.948868	-2.244481	-0.212657
C	2.923910	-1.872090	-1.521336	0.365017
C	1.776345	1.037955	0.291967	0.030115
N	2.148296	0.800947	1.674882	-0.436378
C	1.136521	0.348386	2.473557	0.623430
C	-0.126562	0.235154	1.614404	-0.092814
N	0.265329	0.947801	0.370272	-0.443069
C	-0.482759	-1.270639	1.458856	-0.381279
C	-1.769570	-1.580412	0.731057	0.153580
C	-1.759976	-1.898657	-0.633985	-0.190627
C	-2.949792	-2.175320	-1.309773	-0.129615
C	-4.166770	-2.138798	-0.626667	-0.130900
C	-4.187911	-1.834070	0.737323	-0.131038
C	-2.996925	-1.558931	1.411066	-0.196862
O	1.204615	0.042342	3.645354	-0.478808
C	3.523323	0.944862	2.129506	-0.339553
C	-0.542882	1.572512	-0.466438	0.420732
C	-1.972696	1.545622	-0.251676	-0.157703
C	-2.871363	2.198740	-0.1025459	-0.060351
C	-4.340632	2.189478	-0.784268	-0.511136
C	2.826966	-3.355364	-1.565553	-0.536833
C	0.044530	2.367029	-1.610539	-0.379021
C	0.263599	3.854885	-1.250975	-0.461794
H	-0.938724	0.778079	2.101250	0.209850
H	4.185876	0.253394	1.599155	0.190635
H	3.533511	0.713376	3.195465	0.226921
H	3.874454	1.971289	1.975989	0.177758
H	-4.865814	1.835554	-1.681266	0.204197
H	-4.701171	3.211987	-0.606013	0.204091
H	-4.620801	1.558303	0.062202	0.192262
H	-2.539886	2.776839	-1.885675	0.177360
H	-2.352251	0.957688	0.574260	0.185882
H	0.361769	-1.769363	0.976183	0.193185
H	-0.528498	-1.638414	2.490283	0.211229
H	-3.018098	-1.346985	2.478282	0.148699
H	-5.128865	-1.830451	1.280367	0.158550
H	-5.092156	-2.365344	-1.148384	0.157049
H	-2.925490	-2.432152	-2.365206	0.151156
H	-0.811647	-1.944101	-1.165037	0.133792

H	0.955750	3.980668	-0.411807	0.174028
H	0.683582	4.377130	-2.115142	0.197499
H	-0.677201	4.341842	-0.979964	0.179118
H	2.048416	2.058416	0.004358	0.192192
H	3.678993	1.293712	-2.033129	0.170425
H	4.302215	-1.160034	-3.058842	0.175836
H	3.480006	-3.745034	-2.349990	0.193839
H	3.130209	-3.802137	-0.611594	0.195297
H	1.802906	-3.685891	-1.776481	0.186522
H	-0.633748	2.295724	-2.463499	0.195562
H	0.979579	1.909156	-1.937276	0.193674

14(E)-b1b

B3LYP/6-31G(d) energy=-1114.32468830

Zero-point correction (ZPC)= 0.452709

Number of Imaginary Frequencies=0

O	-2.853529	-1.330871	0.053054	-0.486602
C	-2.448377	-0.044956	-0.201352	0.377394
C	-2.844524	0.328307	-1.453587	-0.203299
C	-3.528732	-0.797513	-2.009420	-0.208275
C	-3.514290	-1.782675	-1.063749	0.360274
C	-1.743602	0.658605	0.913340	0.035692
N	-1.876375	2.096948	0.846821	-0.449374
C	-0.728794	2.760384	0.511216	0.620508
C	0.380647	1.718639	0.334106	-0.098513
N	-0.229885	0.493370	0.913777	-0.439159
C	0.767070	1.625687	-1.169009	-0.372867
C	1.984036	0.787653	-1.486121	0.153949
C	1.850028	-0.529059	-1.946489	-0.189184
C	2.977652	-1.306465	-2.218610	-0.128473
C	4.254911	-0.775225	-2.033232	-0.129789
C	4.400699	0.541020	-1.585774	-0.130142
C	3.272663	1.317623	-1.317941	-0.197271
O	-0.590332	3.954066	0.347777	-0.476782
C	-3.142310	2.767495	1.114612	-0.339750
C	0.416227	-0.497440	1.500038	0.413020
C	1.863574	-0.460048	1.586821	-0.162670
C	2.600460	-1.295811	2.354582	-0.061248
C	4.084681	-1.232753	2.463714	-0.511543
C	-4.059895	-3.165294	-1.009662	-0.535634
C	-0.331600	-1.687620	2.054627	-0.369891
C	-0.152165	-2.944531	1.171829	-0.454277
H	1.238229	2.021994	0.936440	0.213337
H	-3.915003	2.438540	0.413864	0.189455
H	-2.968230	3.837465	0.992360	0.227065
H	-3.473744	2.566614	2.139575	0.182762
H	4.521470	-2.207197	2.207498	0.202924
H	4.380666	-1.032192	3.502491	0.204947
H	4.518604	-0.468894	1.814058	0.191216
H	2.116920	-2.066587	2.951476	0.177476
H	2.390062	0.284883	1.004315	0.189812
H	0.040914	-1.887773	3.063825	0.195366
H	-1.396638	-1.485270	2.148930	0.196864
H	-0.102198	1.262901	-1.726100	0.173421
H	0.931642	2.666717	-1.470643	0.213941
H	3.393583	2.349425	-0.993438	0.149633
H	5.391876	0.969244	-1.465715	0.159649
H	5.132671	-1.375649	-2.253940	0.158445
H	2.858341	-2.321449	-2.587158	0.152687
H	0.857033	-0.941783	-2.111489	0.135415
H	0.896991	-3.237869	1.089158	0.172884
H	-0.710245	-3.772418	1.618137	0.190053
H	-0.544648	-2.773216	0.166505	0.180121
H	-2.118480	0.288990	1.872875	0.205185

H	-2.691296	1.291801	-1.920207	0.177471
H	-3.987724	-0.860173	-2.985984	0.175586
H	-4.776249	-3.278731	-0.187656	0.193042
H	-4.573978	-3.395769	-1.945771	0.194227
H	-3.266009	-3.907520	-0.863827	0.181345

14(E)-b2δ

B3LYP/6-31G(d) energy=-1114.32644170

Zero-point correction (ZPC)= 0.452947

Number of Imaginary Frequencies=0

O	-2.703519	-1.396653	-0.551159	-0.485724
C	-2.401603	-0.063628	-0.432080	0.380419
C	-2.789035	0.602079	-1.559367	-0.202295
C	-3.358435	-0.380136	-2.429293	-0.214299
C	-3.287739	-1.579848	-1.781209	0.365656
C	-1.779077	0.360720	0.859952	0.032090
N	-1.940681	1.772412	1.127417	-0.445647
C	-0.800644	2.510809	0.958502	0.620209
C	0.336258	1.547048	0.591877	-0.098273
N	-0.266027	0.221775	0.889007	-0.435178
C	0.771443	1.786815	-0.880797	-0.373101
C	2.024127	1.066558	-1.322862	0.153820
C	1.947653	-0.110385	-2.079257	-0.186912
C	3.107609	-0.778913	-2.475719	-0.128608
C	4.360699	-0.277611	-2.119435	-0.130541
C	4.449510	0.901000	-1.373184	-0.130856
C	3.288948	1.569573	-0.980954	-0.197464
O	-0.683663	3.713826	1.054964	-0.476186
C	-3.228345	2.353506	1.485257	-0.339809
C	0.367603	-0.861245	1.298261	0.412415
C	1.812600	-0.863348	1.377620	-0.161687
C	2.546706	-1.888540	1.870268	-0.060457
C	4.032471	-1.875732	1.970092	-0.511948
C	-3.709559	-2.963684	-2.125499	-0.534075
C	-0.424607	-2.072770	1.738127	-0.392008
C	-0.732363	-2.058709	3.253829	-0.460713
H	1.171392	1.725812	1.271472	0.212680
H	-3.969214	2.178514	0.699729	0.188933
H	-3.071258	3.426091	1.607900	0.226959
H	-3.592790	1.928586	2.427125	0.181924
H	4.451561	-2.745184	1.446429	0.203664
H	4.341940	-1.976528	3.019521	0.204355
H	4.470795	-0.965827	1.553523	0.192454
H	2.058264	-2.792719	2.228118	0.178086
H	2.342910	0.005682	1.008983	0.187714
H	-1.346154	-2.152350	1.160648	0.217490
H	0.153977	-2.966166	1.494234	0.192016
H	-0.066519	1.533266	-1.536644	0.175029
H	0.914652	2.871958	-0.945801	0.212950
H	3.366792	2.500592	-0.422674	0.148907
H	5.422002	1.311089	-1.115574	0.159063
H	5.263964	-0.790635	-2.436689	0.157917
H	3.032424	-1.683160	-3.073162	0.152975
H	0.974524	-0.496983	-2.374516	0.136382
H	-1.344203	-1.197803	3.542813	0.172830
H	-1.283284	-2.965815	3.517561	0.197988
H	0.184656	-2.028804	3.848978	0.176963
H	-2.188001	-0.234525	1.681136	0.201521
H	-2.701989	1.663617	-1.746431	0.177786
H	-3.781270	-0.211295	-3.409559	0.176021
H	-4.442783	-3.347491	-1.406511	0.192204
H	-4.165873	-2.974213	-3.118116	0.194026
H	-2.857409	-3.653750	-2.132686	0.182677

14(E)-c1α

B3LYP/6-31G(d) energy=-1114.3256856000

Zero-point correction (ZPC)= 0.452729

Number of Imaginary Frequencies=0

O	-2.331836	-0.704797	1.075773	-0.485611
C	-2.781978	-0.120490	-0.079240	0.381480
C	-4.063263	0.318570	0.085791	-0.197509
C	-4.428158	-0.010504	1.429375	-0.214961
C	-3.349549	-0.630181	1.994964	0.363353
C	-1.860095	-0.146089	-1.248497	0.023123
N	-1.491588	-1.478514	-1.693408	-0.437058
C	-0.194973	-1.827913	-1.449525	0.613605
C	0.521676	-0.616186	-0.857467	-0.079064
N	-0.504632	0.455400	-0.953755	-0.450349
C	1.039277	-0.892863	0.592453	-0.366788
C	2.551286	-0.978875	0.673738	0.141468
C	3.265687	-0.131402	1.530910	-0.201247
C	4.658050	-0.213377	1.615804	-0.129849
C	5.350310	-1.142292	0.838773	-0.125038
C	4.645210	-1.992456	-0.017161	-0.128878
C	3.255117	-1.915198	-0.099134	-0.193729
O	0.322555	-2.908996	-1.648401	-0.479862
C	-2.488238	-2.411876	-2.198920	-0.340433
C	-0.250622	1.744753	-0.861984	0.420622
C	1.112266	2.171532	-0.611880	-0.181927
C	1.527414	3.460009	-0.640453	-0.057646
C	2.934077	3.884003	-0.399312	-0.516782
C	-3.084871	-1.211968	3.337818	-0.533929
C	-1.360073	2.761294	-0.977416	-0.364262
C	-1.795036	3.316508	0.399176	-0.459593
H	1.354972	-0.358795	-1.515692	0.223545
H	-3.255530	-2.613183	-1.444468	0.191241
H	-1.964949	-3.337498	-2.442056	0.226835
H	-2.963675	-2.013213	-3.101617	0.180125
H	2.972126	4.618339	0.416550	0.204903
H	3.328228	4.399252	-1.286097	0.209247
H	3.588707	3.043406	-0.156266	0.198059
H	0.822715	4.260502	-0.858127	0.180957
H	1.853558	1.411199	-0.391924	0.198132
H	-1.007141	3.580857	-1.610090	0.196602
H	-2.227196	2.336554	-1.483129	0.184059
H	0.668534	-0.106843	1.257409	0.166139
H	0.587475	-1.827737	0.940531	0.209392
H	2.708924	-2.589065	-0.755279	0.175324
H	5.178262	-2.724645	-0.616887	0.157309
H	6.432351	-1.209411	0.904127	0.155435
H	5.197382	0.442585	2.293484	0.148693
H	2.729920	0.584183	2.152010	0.126219
H	-0.964550	3.804259	0.916095	0.171633
H	-2.588122	4.054770	0.250595	0.193436
H	-2.186493	2.523349	1.041042	0.189359
H	-2.325903	0.406599	-2.071766	0.196649
H	-4.681018	0.807530	-0.656091	0.170135
H	-5.376226	0.182009	1.911305	0.175134
H	-2.237252	-0.719428	3.828753	0.184084
H	-3.965645	-1.092350	3.973066	0.193023
H	-2.852756	-2.281097	3.268810	0.195256

14(E)-c2α

B3LYP/6-31G(d) energy=-1114.3267550000

Zero-point correction (ZPC)= 0.45269

Number of Imaginary Frequencies=0

O	-2.258049	-1.061053	1.060616	-0.482186
C	-2.769934	-0.138909	0.186379	0.380859

C	-4.029974	0.220910	0.570022	-0.195876
C	-4.313107	-0.521548	1.758934	-0.213442
C	-3.212161	-1.286519	2.022442	0.364420
C	-1.930060	0.210591	-0.994876	0.021045
N	-1.602780	-0.915674	-1.851573	-0.433044
C	-0.307790	-1.341675	-1.760203	0.614161
C	0.456743	-0.358775	-0.873693	-0.079449
N	-0.551468	0.701913	-0.619213	-0.445348
C	1.030427	-1.039026	0.412240	-0.365365
C	2.541495	-1.164507	0.387565	0.141292
C	3.318378	-0.585031	1.399484	-0.201728
C	4.710552	-0.704329	1.385024	-0.129711
C	5.339687	-1.401539	0.353559	-0.124841
C	4.572121	-1.983626	-0.658689	-0.128879
C	3.182275	-1.869351	-0.643055	-0.193803
O	0.176331	-2.326685	-2.280657	-0.479401
C	-2.637766	-1.660995	-2.553934	-0.340685
C	-0.278515	1.918584	-0.195395	0.418782
C	1.092133	2.260134	0.122757	-0.181947
C	1.500557	3.490264	0.514994	-0.057423
C	2.915033	3.838310	0.821366	-0.516518
C	-2.870847	-2.264023	3.089743	-0.534229
C	-1.384934	2.940826	-0.096750	-0.375299
C	-1.557894	3.745848	-1.405831	-0.461524
H	1.267775	0.070596	-1.466978	0.222675
H	-3.367909	-2.076601	-1.851834	0.190893
H	-2.141900	-2.473808	-3.086071	0.226650
H	-3.153332	-1.014821	-3.272335	0.179589
H	2.990229	4.251842	1.836046	0.205905
H	3.261021	4.633352	0.146390	0.208895
H	3.586020	2.980361	0.732484	0.197987
H	0.780391	4.299565	0.620739	0.181251
H	1.843769	1.481843	0.042854	0.196551
H	0.713521	-0.462991	1.286936	0.166871
H	0.567221	-2.026341	0.509830	0.208119
H	2.587491	-2.334755	-1.425616	0.175440
H	5.056368	-2.535867	-1.458989	0.156947
H	6.421469	-1.497559	0.341021	0.155084
H	5.299228	-0.259666	2.182622	0.148275
H	2.831900	-0.055208	2.216474	0.126183
H	-1.811744	3.102625	-2.254731	0.174034
H	-2.365738	4.471902	-1.279100	0.198656
H	-0.644987	4.290774	-1.662407	0.179307
H	-2.444293	0.987955	-1.568738	0.193503
H	-4.686381	0.916644	0.063698	0.170504
H	-5.223465	-0.495023	2.340816	0.175334
H	-3.711131	-2.365828	3.780490	0.193069
H	-2.649465	-3.251422	2.668291	0.194650
H	-1.992596	-1.942416	3.661959	0.185323
H	-1.159041	3.623960	0.724707	0.193668
H	-2.319450	2.445433	0.174785	0.194929

14(E)-c1β

B3LYP/6-31G(d) energy=-1114.3240994000

Zero-point correction (ZPC)= 0.452691

Number of Imaginary Frequencies=0

O	-3.758813	0.097229	-0.031525	-0.484914
C	-2.593551	-0.588738	0.204062	0.368382
C	-2.583983	-1.063207	1.484493	-0.202376
C	-3.814187	-0.641203	2.076366	-0.205768
C	-4.500356	0.056339	1.121081	0.356959
C	-1.651886	-0.688405	-0.950969	0.053855
N	-1.127834	-2.022146	-1.161346	-0.451865
C	0.216747	-2.158907	-0.968997	0.609944

C	0.787714	-0.790816	-0.603099	-0.081888
N	-0.374246	0.115513	-0.792563	-0.457607
C	1.395648	-0.775498	0.838248	-0.374399
C	2.909214	-0.669816	0.844984	0.143459
C	3.543327	0.378129	1.525263	-0.200356
C	4.937049	0.475231	1.541382	-0.129695
C	5.709605	-0.474053	0.872148	-0.124394
C	5.084505	-1.523141	0.192906	-0.129114
C	3.693555	-1.624359	0.179700	-0.193546
O	0.866428	-3.182732	-1.045805	-0.478842
C	-2.000215	-3.132082	-1.521643	-0.340083
C	-0.290067	1.426410	-0.894815	0.416309
C	1.012902	2.053898	-0.789227	-0.182233
C	1.246578	3.369186	-1.009873	-0.056764
C	2.591813	4.000528	-0.919507	-0.516790
C	-5.830552	0.721595	1.090521	-0.533882
C	-1.531770	2.265153	-1.071065	-0.373725
C	-1.971529	2.930972	0.254489	-0.459917
H	1.553078	-0.535075	-1.339884	0.225781
H	-2.755686	-3.297645	-0.747897	0.191712
H	-1.369718	-4.017321	-1.614407	0.226836
H	-2.496561	-2.935176	-2.478314	0.183281
H	2.568909	4.835756	-0.206604	0.205141
H	2.866875	4.439660	-1.888350	0.209343
H	3.367386	3.292464	-0.617029	0.197421
H	0.428609	4.034211	-1.280085	0.181394
H	1.861204	1.432066	-0.524891	0.196455
H	-1.323920	3.035276	-1.819394	0.194878
H	-2.358377	1.670278	-1.458849	0.200426
H	0.959538	0.058104	1.398262	0.167627
H	1.083507	-1.693733	1.349301	0.204032
H	3.211105	-2.450140	-0.338008	0.176000
H	5.681831	-2.270408	-0.321520	0.158120
H	6.793216	-0.402057	0.884809	0.156343
H	5.415738	1.286754	2.082313	0.149814
H	2.946187	1.112150	2.063157	0.127833
H	-1.200656	3.601213	0.643653	0.170890
H	-2.876924	3.516836	0.073442	0.191913
H	-2.195767	2.183669	1.020210	0.187652
H	-2.166899	-0.333001	-1.851385	0.208670
H	-1.806983	-1.654145	1.950564	0.172304
H	-4.154277	-0.844608	3.082034	0.174912
H	-6.484845	0.267305	0.337327	0.195292
H	-6.313842	0.626490	2.065754	0.193092
H	-5.742455	1.788246	0.853105	0.181830

14(E)-c2δ

B3LYP/6-31G(d) energy=-1114.3252398000

Zero-point correction (ZPC)= 0.45267

Number of Imaginary Frequencies=0

O	-3.507487	0.269511	0.605030	-0.484599
C	-2.546838	-0.664203	0.305936	0.377229
C	-2.535577	-1.641055	1.259961	-0.200142
C	-3.547451	-1.288561	2.205681	-0.209816
C	-4.114444	-0.123671	1.772444	0.363545
C	-1.757760	-0.432555	-0.941877	0.033392
N	-1.277867	-1.660159	-1.538815	-0.443067
C	0.057000	-1.894758	-1.352271	0.607489
C	0.667856	-0.665727	-0.676514	-0.084178
N	-0.453935	0.304926	-0.698489	-0.442880
C	1.244219	-0.981163	0.742679	-0.370020
C	2.756954	-0.886233	0.798627	0.141494
C	3.384491	-0.006397	1.690019	-0.200100
C	4.778505	0.075424	1.744670	-0.130207

C	5.557445	-0.719901	0.903929	-0.124771
C	4.938846	-1.601373	0.013368	-0.128655
C	3.548015	-1.687504	-0.039126	-0.193194
O	0.673697	-2.895135	-1.658314	-0.477674
C	-2.181615	-2.623560	-2.154946	-0.339827
C	-0.327307	1.612506	-0.606103	0.411185
C	0.984640	2.170501	-0.349154	-0.181602
C	1.255561	3.496228	-0.299746	-0.057154
C	2.610839	4.058646	-0.048155	-0.516511
C	-5.211347	0.740458	2.283783	-0.533932
C	-1.528088	2.503662	-0.819615	-0.389310
C	-1.694860	2.904372	-2.304394	-0.460209
H	1.460757	-0.290883	-1.327836	0.224710
H	-2.925616	-2.978288	-1.435630	0.190358
H	-1.572108	-3.462182	-2.494342	0.226455
H	-2.692216	-2.172570	-3.012563	0.182891
H	2.582291	4.740268	0.812531	0.205283
H	2.929817	4.668777	-0.904514	0.208433
H	3.358948	3.282848	0.133010	0.197317
H	0.461210	4.224573	-0.451985	0.181423
H	1.807107	1.483196	-0.180068	0.195148
H	0.793496	-0.296523	1.467939	0.171266
H	0.924796	-1.990571	1.025672	0.202680
H	3.070089	-2.384684	-0.723875	0.172964
H	5.540984	-2.230188	-0.636163	0.157864
H	6.641018	-0.659656	0.946595	0.156147
H	5.252432	0.753572	2.448831	0.149862
H	2.782221	0.604070	2.360230	0.129306
H	-1.854119	2.033224	-2.948322	0.173116
H	-2.564172	3.560170	-2.404245	0.198664
H	-0.816645	3.439144	-2.677061	0.177107
H	-2.352044	0.145179	-1.656643	0.202583
H	-1.901202	-2.516604	1.283607	0.176006
H	-3.829052	-1.841316	3.090776	0.175841
H	-5.613561	0.318777	3.207928	0.193940
H	-4.857053	1.756182	2.496100	0.182645
H	-6.028815	0.818101	1.557455	0.193373
H	-1.407923	3.401931	-0.210308	0.190381
H	-2.432216	2.014251	-0.454876	0.217452

14(Z)-a1 α

B3LYP/6-31G(d) energy=-1114.3194936000

Zero-point correction (ZPC)= 0.452811

Number of Imaginary Frequencies=0

C	1.640688	-1.249591	-1.966328	-0.461748
C	1.818887	-1.621937	-0.628033	0.347348
C	3.015024	-1.267828	0.015032	-0.198075
C	4.002129	-0.556191	-0.666670	-0.209453
C	3.815943	-0.197858	-2.003600	0.358567
C	2.630348	-0.545287	-2.653114	0.084619
C	0.790181	-2.488985	0.071141	-0.458144
C	-0.146837	-1.840160	1.122390	-0.085007
N	-1.078442	-0.762910	0.679726	0.637104
C	-0.789237	0.535467	1.429140	-0.452244
N	0.213102	0.104532	2.384984	0.416990
C	0.630877	-1.185422	2.261533	-0.374624
C	-0.385708	1.715593	0.616920	-0.467710
O	0.752211	1.647697	-0.135406	-0.385676
C	0.969798	2.896257	-0.658912	0.164050
C	-0.012806	3.748660	-0.236817	-0.188241
C	-0.888414	2.987845	0.594197	-0.131899
C	2.159494	3.069052	-1.532191	-0.130335
C	-2.176521	-0.949128	-0.026435	-0.132045
C	-3.052725	0.172442	-0.310740	-0.193714
C	-4.325486	0.051421	-0.753963	-0.493171

C	-5.223351	1.202604	-1.047380	-0.339911
O	1.468373	-1.754705	2.933454	-0.529790
C	0.749593	1.019648	3.382683	-0.172940
C	-2.537259	-2.324002	-0.540382	-0.057041
C	-2.411843	-2.470516	-2.072732	-0.512161
H	-5.576396	1.147724	-2.086081	0.208681
H	-1.940631	-3.091512	-0.049114	0.195730
H	-3.575381	-2.515006	-0.246405	0.199608
H	-0.749341	-2.637722	1.569650	0.214463
H	1.451920	0.449250	3.991770	0.225435
H	-0.052763	1.409455	4.018653	0.178787
H	1.271303	1.854421	2.905342	0.194626
H	-2.650780	1.167889	-0.166149	0.182839
H	-4.735277	2.167604	-0.890014	0.187923
H	-6.123743	1.150574	-0.420418	0.208307
H	-4.762866	-0.934139	-0.902630	0.181663
H	1.303609	-3.268051	0.647318	0.212690
H	0.180118	-3.009550	-0.672816	0.166279
H	0.735213	-1.542556	-2.493454	0.126737
H	2.484476	-0.289559	-3.699173	0.146591
H	4.597498	0.332104	-2.540896	0.151749
H	4.929748	-0.305754	-0.159642	0.153852
H	3.183361	-1.572757	1.043719	0.171095
H	-2.699646	-3.485832	-2.359093	0.197651
H	-3.060264	-1.767221	-2.600951	0.174468
H	-1.385445	-2.301600	-2.408701	0.191569
H	-1.717531	0.811328	1.947733	0.192285
H	-1.764221	3.345310	1.120813	0.165762
H	-0.094998	4.797424	-0.484536	0.171918
H	2.083537	2.451975	-2.434049	0.187522
H	2.248018	4.116482	-1.830476	0.184999
H	3.076554	2.771927	-1.012188	0.192044
XX	2.824962	-0.915579	-1.298012	0.000000

14(Z)-a2 α

B3LYP/6-31G(d) energy=-1114.3197200000

Zero-point correction (ZPC)= 0.452859

Number of Imaginary Frequencies=0

C	1.516265	-0.913434	-2.275364	-0.461678
C	1.634661	-1.618926	-1.071014	0.346859
C	2.845719	-1.556484	-0.366055	-0.198207
C	3.913275	-0.807243	-0.860482	-0.209652
C	3.788177	-0.116893	-2.068256	0.358611
C	2.584869	-0.167641	-2.774435	0.088195
C	0.512042	-2.520046	-0.603072	-0.464441
C	-0.429648	-2.012577	0.522750	-0.075739
N	-1.143832	-0.716477	0.336541	0.635435
C	-0.737180	0.282209	1.417421	-0.454000
N	0.116661	-0.532474	2.261041	0.418329
C	0.342818	-1.801636	1.823744	-0.377246
C	-0.115563	1.561737	0.980207	-0.464417
O	1.061156	1.532910	0.287843	-0.395361
C	1.479521	2.830818	0.141639	0.167769
C	0.584613	3.672227	0.742701	-0.185789
C	-0.445415	2.852147	1.292438	-0.131836
C	2.748138	3.058513	-0.597782	-0.129908
C	-2.180597	-0.532831	-0.459105	-0.131193
C	-2.833853	0.758132	-0.520587	-0.184477
C	-3.948792	1.012933	-1.245748	-0.493538
C	-4.615153	2.342093	-1.316052	-0.339807
O	1.037874	-2.647782	2.351049	-0.530177
C	0.710529	0.003068	3.478169	-0.165765
C	-2.737894	-1.698594	-1.242828	-0.055726
C	-3.872690	-2.409746	-0.464998	-0.512471

H	-4.673187	2.678152	-2.360210	0.209837
H	-3.115001	-1.337908	-2.201977	0.194850
H	-1.954873	-2.416474	-1.475963	0.197928
H	-1.179700	-2.788189	0.708694	0.210881
H	1.263544	-0.812059	3.946455	0.225095
H	-0.067789	0.357612	4.162704	0.178512
H	1.393495	0.826291	3.248947	0.194836
H	-2.382991	1.577391	0.024199	0.178378
H	-4.099627	3.103740	-0.726002	0.188646
H	-5.653972	2.262574	-0.967639	0.208588
H	-4.419604	0.221464	-1.825333	0.183047
H	0.929047	-3.437188	-0.170464	0.216058
H	-0.081849	-2.832781	-1.466429	0.175763
H	0.593797	-0.977112	-2.849728	0.116380
H	2.485799	0.351420	-3.723935	0.146607
H	4.630214	0.442751	-2.466014	0.151476
H	4.852713	-0.785389	-0.315237	0.153497
H	2.960064	-2.118995	0.556494	0.166828
H	-4.241429	-3.249035	-1.061084	0.202565
H	-3.523622	-2.806885	0.493549	0.178947
H	-4.709746	-1.735402	-0.265122	0.175813
H	-1.657840	0.550227	1.954275	0.190826
H	-1.307016	3.178595	1.861038	0.165268
H	0.658931	4.749239	0.793260	0.171497
H	2.674720	2.702816	-1.630976	0.188363
H	2.980067	4.126243	-0.609334	0.184756
H	3.580763	2.523573	-0.128071	0.190884
XX	2.717426	-0.875948	-1.556403	0.000000

14(Z)-a1β

B3LYP/6-31G(d) energy=-1114.3231390000

Zero-point correction (ZPC)=0.45312

Number of Imaginary Frequencies=0

C	1.855048	-0.481552	-2.138650	-0.489969
C	2.340296	-0.950232	-0.910624	0.345933
C	3.458496	-0.317909	-0.343361	-0.177054
C	4.065143	0.761874	-0.987584	-0.218511
C	3.569821	1.220781	-2.211088	0.362812
C	2.463104	0.594859	-2.786785	0.070250
C	1.717098	-2.157546	-0.239828	-0.453482
C	0.734561	-1.904200	0.933165	-0.090308
N	-0.514449	-1.145624	0.649601	0.632394
C	-0.514039	0.182998	1.411975	-0.457502
N	0.626503	0.010774	2.286995	0.412570
C	1.379495	-1.102989	2.062586	-0.373223
C	-0.445598	1.422113	0.583829	-0.467331
O	-1.622844	2.132777	0.486349	-0.380127
C	-1.358795	3.265445	-0.239651	0.150837
C	-0.039154	3.278452	-0.592629	-0.194499
C	0.553406	2.092653	-0.059558	-0.138154
C	-2.493803	4.199741	-0.467494	-0.131760
C	-1.583475	-1.628597	0.048123	-0.125538
C	-2.783949	-0.819687	-0.056162	-0.189912
C	-3.992178	-1.302642	-0.429674	-0.492363
C	-5.229080	-0.478287	-0.520076	-0.338890
O	2.390826	-1.437358	2.647197	-0.534239
C	0.926880	0.973641	3.338843	-0.187328
C	-1.569441	-3.025733	-0.530690	-0.058583
C	-1.547898	-3.059352	-2.075232	-0.512560
H	-5.649838	-0.540021	-1.532852	0.206356
H	-0.726568	-3.597899	-0.144100	0.194064
H	-2.469320	-3.536755	-0.172661	0.199719
H	0.452551	-2.873884	1.355077	0.216119
H	1.815834	0.612815	3.857708	0.224946

H	0.092631	1.040350	4.046137	0.181199
H	1.121912	1.962344	2.914598	0.192477
H	-2.713912	0.234644	0.181415	0.208044
H	-5.053134	0.571029	-0.270837	0.189041
H	-6.000316	-0.879535	0.151330	0.208394
H	-4.112652	-2.356399	-0.673218	0.180605
H	2.503301	-2.771825	0.214243	0.211912
H	1.222997	-2.786864	-0.985927	0.168960
H	1.006827	-0.973913	-2.609255	0.128717
H	2.080058	0.934832	-3.744736	0.151344
H	4.053376	2.050304	-2.718970	0.156793
H	4.937434	1.231704	-0.542088	0.159346
H	3.862205	-0.681602	0.597334	0.173370
H	-1.564897	-4.100474	-2.409270	0.197794
H	-2.412159	-2.546401	-2.504180	0.174670
H	-0.644277	-2.591205	-2.474893	0.189131
H	-1.445016	0.210713	1.992453	0.203366
H	1.587368	1.789281	-0.140705	0.187827
H	0.458675	4.052084	-1.160135	0.170038
H	-2.917565	4.551241	0.480486	0.191776
H	-2.148272	5.069593	-1.031131	0.193210
H	-3.301095	3.723458	-1.036977	0.177626
XX	2.965226	0.130861	-1.543634	0.000000

14(Z)-a2β

B3LYP/6-31G(d) energy=-1114.3235341000

Zero-point correction (ZPC)=0.453083

Number of Imaginary Frequencies=0

C	3.442779	-0.574849	-0.412024	-0.175956
C	2.293675	-0.966048	-1.117281	0.346105
C	1.913997	-0.231960	-2.248915	-0.490616
C	2.658513	0.871883	-2.668117	0.363318
C	3.796859	1.256408	-1.957355	-0.219435
C	4.186408	0.531106	-0.828085	0.072494
C	1.523524	-2.204386	-0.709984	-0.457179
C	0.498404	-2.078773	0.451503	-0.084141
N	-0.632539	-1.123471	0.297320	0.631151
C	-0.504070	0.024539	1.301567	-0.458928
N	0.572041	-0.453202	2.144721	-0.384213
C	1.174117	-1.606805	1.738244	0.153118
C	-0.265803	1.384837	0.737761	-0.181609
C	0.822121	2.049069	0.251781	-0.125366
C	0.383417	3.377513	-0.038375	-0.131423
C	-0.939885	3.448161	0.293133	-0.138911
O	-1.351967	2.233017	0.775445	-0.194047
C	-1.955413	4.534338	0.247226	0.412814
C	-1.720928	-1.343281	-0.413801	-0.377577
C	-2.796055	-0.372119	-0.421341	-0.463353
C	-3.967943	-0.546038	-1.077590	-0.338836
C	-5.079252	0.444542	-1.078167	-0.492652
O	2.097982	-2.183071	2.277576	-0.534153
C	0.942675	0.245600	3.368475	-0.183727
C	-1.872812	-2.650264	-1.158218	-0.057365
C	-2.633045	-3.702975	-0.315709	-0.513195
H	-5.320901	0.739498	-2.108280	0.207426
H	-2.407918	-2.467033	-2.092423	0.195129
H	-0.899486	-3.046398	-1.441537	0.197410
H	0.083289	-3.072355	0.644175	0.211846
H	1.760570	-0.316094	3.821430	0.224729
H	0.095055	0.280529	4.062229	0.180841
H	1.271364	1.264407	3.146617	0.192683
H	-2.654209	0.557541	0.115513	0.205609
H	-4.845016	1.339011	-0.495809	0.189562
H	-5.992447	-0.013759	-0.674525	0.208386

H	-4.149602	-1.453916	-1.649135	0.181733
H	2.218710	-2.969774	-0.345798	0.213458
H	1.028037	-2.629464	-1.587802	0.175807
H	1.042670	-0.538882	-2.824048	0.121850
H	2.357375	1.421213	-3.555534	0.151269
H	4.386141	2.106240	-2.289677	0.156721
H	5.081582	0.813477	-0.281229	0.159172
H	3.763761	-1.147805	0.453612	0.171535
H	-2.734648	-4.622127	-0.899278	0.201469
H	-2.099384	-3.949093	0.607844	0.179560
H	-3.633254	-3.355536	-0.043500	0.176328
H	-1.446973	0.052844	1.863072	0.202522
H	1.817186	1.649124	0.120828	0.187716
H	0.982560	4.184827	-0.435444	0.169643
H	-2.366043	4.738976	1.242885	0.191627
H	-1.497468	5.452136	-0.129124	0.193118
H	-2.793282	4.276581	-0.411872	0.176837
XX	3.052927	0.138181	-1.522517	0.000000

14(Z)-b1a

B3LYP/6-31G(d) energy=-1114.3239753000

Zero-point correction (ZPC)= 0.452708

Number of Imaginary Frequencies=0

O	1.730862	-1.275235	-1.068001	-0.481294
C	2.248513	-0.118931	-0.546874	0.377577
C	3.224375	0.364980	-1.370846	-0.197942
C	3.310101	-0.543035	-2.471788	-0.212332
C	2.386963	-1.524620	-2.249437	0.365570
C	1.777836	0.325822	0.796501	0.033265
N	0.279721	0.542333	0.918677	-0.431885
C	-0.318981	-0.577700	1.692958	-0.097524
C	0.893810	-1.154855	2.430695	0.621275
N	2.018768	-0.617289	1.873103	-0.436140
C	-0.294788	1.680423	0.584080	0.418398
C	-1.730242	1.975843	0.951469	-0.371537
C	-2.641767	2.338917	-0.238748	-0.458490
C	-0.966094	-1.714775	0.857520	-0.382530
C	-2.236990	-1.386037	0.107364	0.165551
C	-2.216675	-1.226328	-1.284827	-0.203060
C	-3.396822	-0.987651	-1.994084	-0.132306
C	-4.613081	-0.895215	-1.315654	-0.125942
C	-4.645030	-1.048279	0.073188	-0.128212
C	-3.466712	-1.297333	0.777575	-0.195147
O	0.833798	-1.977996	3.319565	-0.477353
C	3.368074	-0.993133	2.268455	-0.339886
C	1.983059	-2.744394	-2.998103	-0.537999
C	0.488259	2.681024	-0.126908	-0.183288
C	0.220940	4.005229	-0.102773	-0.054262
C	1.022017	5.040687	-0.814092	-0.511228
H	0.374521	5.619333	-1.486465	0.207684
H	-2.173955	1.134831	1.480371	0.196308
H	-1.699360	2.815908	1.660275	0.196540
H	-1.022881	-0.182701	2.425517	0.210559
H	3.273823	-1.707364	3.087561	0.227248
H	3.928106	-0.116315	2.612492	0.178473
H	3.903709	-1.459764	1.435693	0.190370
H	1.336475	2.330034	-0.705291	0.180251
H	1.841297	4.611192	-1.396423	0.184216
H	1.434972	5.762391	-0.096718	0.206253
H	-0.615090	4.377080	0.487074	0.182768
H	-0.210135	-2.099608	0.168121	0.191752
H	-1.155298	-2.503566	1.595304	0.213386
H	-3.507858	-1.454092	1.854014	0.144916
H	-5.590685	-0.995731	0.605132	0.158565

H	-5.532870	-0.718598	-1.865488	0.158856
H	-3.366608	-0.885708	-3.075360	0.152651
H	-1.272878	-1.313944	-1.818396	0.135544
H	-3.652829	2.515909	0.137517	0.188140
H	-2.307132	3.239837	-0.757448	0.161649
H	-2.688438	1.518050	-0.957059	0.195463
H	2.269579	1.280098	1.017205	0.194320
H	3.826659	1.249373	-1.207684	0.168414
H	3.978632	-0.478534	-3.318535	0.175620
H	0.930560	-2.700837	-3.302942	0.186992
H	2.594670	-2.844184	-3.897888	0.194102
H	2.115712	-3.646376	-2.389580	0.195708

14(Z)-b2a

B3LYP/6-31G(d) energy=-1114.3270697000

Zero-point correction (ZPC)= 0.452668

Number of Imaginary Frequencies=0

C	-3.315890	-1.860376	0.348265	-0.194518
C	-2.019952	-1.646659	-0.145440	0.150022
C	-1.864848	-1.228283	-1.474892	-0.197836
C	-2.979578	-1.014423	-2.288669	-0.130981
C	-4.264686	-1.217830	-1.783042	-0.128563
C	-4.430729	-1.645666	-0.463196	-0.125394
C	-0.815546	-1.852952	0.742783	-0.375442
C	-0.399263	-0.632592	1.615171	-0.099453
N	0.113365	0.536712	0.857950	-0.438142
C	1.629739	0.526581	0.869945	0.039743
N	1.896279	-0.359585	1.989658	-0.439264
C	0.806810	-1.032537	2.468112	0.620930
C	2.280533	0.132181	-0.412729	0.377339
O	1.959297	-1.082393	-0.958658	-0.481859
C	2.747825	-1.255711	-2.071149	0.365102
C	3.560047	-0.168808	-2.224795	-0.213211
C	3.261717	0.728256	-1.151849	-0.198159
C	2.564770	-2.520630	-2.831296	-0.536697
C	-0.603968	1.544410	0.399194	0.421709
C	0.046369	2.598093	-0.355304	-0.173389
C	-0.560059	3.747198	-0.733727	-0.052672
C	0.100623	4.826353	-1.518218	-0.512354
O	0.780763	-1.841576	3.371556	-0.477900
C	3.244167	-0.552620	2.503312	-0.339797
C	-2.074780	1.632746	0.729806	-0.380417
C	-2.308411	2.402755	2.052051	-0.466293
H	-0.462413	5.018797	-2.441440	0.208740
H	-2.592684	2.130967	-0.091680	0.192122
H	-2.512318	0.637704	0.793778	0.218170
H	-1.218635	-0.324526	2.265055	0.209236
H	3.171014	-1.254790	3.334889	0.226920
H	3.660407	0.395333	2.862403	0.178068
H	3.901358	-0.966345	1.731868	0.190302
H	1.073377	2.438461	-0.662249	0.173435
H	1.135077	4.586705	-1.776930	0.185750
H	0.083914	5.768396	-0.953448	0.208266
H	-1.596372	3.932364	-0.458529	0.184762
H	0.051648	-2.154950	0.149589	0.192687
H	-1.003261	-2.650303	1.470661	0.209349
H	-3.452050	-2.212110	1.368983	0.148041
H	-5.427206	-1.825926	-0.070206	0.159654
H	-5.131939	-1.059132	-2.417294	0.158015
H	-2.843883	-0.701553	-3.320313	0.149938
H	-0.864548	-1.087814	-1.878285	0.134848
H	-3.383213	2.456959	2.246496	0.199732
H	-1.838108	1.901299	2.904226	0.176744
H	-1.917091	3.423120	2.005285	0.171330

H	1.968032	1.541696	1.109778	0.192124
H	3.731767	1.682259	-0.950511	0.168121
H	4.291166	-0.026848	-3.007981	0.175147
H	1.542112	-2.614359	-3.215605	0.187417
H	3.252588	-2.545256	-3.679820	0.193348
H	2.763931	-3.395201	-2.201157	0.195364

14(Z)-b1δ

B3LYP/6-31G(d) energy=-1114.3233024000
 Zero-point correction (ZPC)= 0.452741
 Number of Imaginary Frequencies=0

O	-2.628824	0.569383	1.045732	-0.487519
C	-2.094817	-0.611522	0.594364	0.379559
C	-2.176722	-1.560639	1.572240	-0.200668
C	-2.789219	-0.925439	2.697801	-0.215430
C	-3.048160	0.366022	2.338551	0.367667
C	-1.612784	-0.621862	-0.820668	0.032934
N	-0.174179	-0.155236	-1.005678	-0.425055
C	0.697459	-1.355556	-1.094588	-0.102818
C	-0.288007	-2.439896	-1.550833	0.618489
N	-1.555402	-1.950979	-1.387045	-0.446795
C	0.143194	1.094955	-1.276837	0.406905
C	1.546563	1.476517	-1.686432	-0.368558
C	2.233426	2.486966	-0.744017	-0.458975
C	1.374898	-1.797814	0.229557	-0.374652
C	2.523601	-0.948039	0.725079	0.168295
C	2.392226	-0.183624	1.891783	-0.201877
C	3.471029	0.555017	2.385628	-0.129990
C	4.692907	0.543799	1.711660	-0.125952
C	4.835303	-0.215473	0.546894	-0.128425
C	3.760116	-0.959775	0.061318	-0.195708
O	0.029452	-3.537542	-1.956356	-0.474667
C	-2.757439	-2.697551	-1.735890	-0.339635
C	-3.670081	1.524127	3.033870	-0.534997
C	-0.883388	2.124927	-1.194993	-0.193598
C	-0.812270	3.309350	-1.842731	-0.055392
C	-1.861847	4.365097	-1.780565	-0.511502
H	-1.425111	5.309041	-1.427663	0.205464
H	2.180882	0.596319	-1.771127	0.192625
H	1.470168	1.907637	-2.693805	0.195843
H	1.441446	-1.217855	-1.879060	0.212915
H	-2.431696	-3.662699	-2.126465	0.227210
H	-3.328901	-2.166989	-2.505721	0.182578
H	-3.390694	-2.851523	-0.857515	0.188721
H	-1.750451	1.927748	-0.574313	0.204205
H	-2.692945	4.092067	-1.125337	0.186295
H	-2.254174	4.570877	-2.785473	0.205947
H	0.043123	3.531510	-2.478257	0.181191
H	0.605371	-1.876477	1.002837	0.172462
H	1.724100	-2.816916	0.022196	0.215426
H	3.892808	-1.578048	-0.824939	0.144244
H	5.789559	-0.244309	0.028719	0.158568
H	5.534528	1.111039	2.098196	0.159188
H	3.358410	1.128882	3.301170	0.154596
H	1.448049	-0.185805	2.432176	0.138158
H	3.234682	2.698984	-1.128328	0.188463
H	1.683521	3.428567	-0.679745	0.162620
H	2.338823	2.073080	0.260922	0.195208
H	-2.243458	0.030875	-1.433587	0.203135
H	-1.859627	-2.592094	1.501083	0.178382
H	-3.019733	-1.378121	3.651835	0.176368
H	-4.562647	1.875851	2.503233	0.190463
H	-3.966420	1.232205	4.044125	0.194891
H	-2.973494	2.367403	3.111759	0.183061

14(Z)-b2δ

B3LYP/6-31G(d) energy= -1114.3252398000
 Zero-point correction (ZPC)= 0.45267
 Number of Imaginary Frequencies=0

O	-2.740750	0.722596	0.687576	-0.488042
C	-2.147655	-0.499892	0.494848	0.379570
C	-2.349707	-1.290263	1.589554	-0.201458
C	-3.102851	-0.505422	2.518018	-0.213331
C	-3.320258	0.708988	1.933342	0.366031
C	-1.489781	-0.712163	-0.830888	0.038149
N	-0.029385	-0.291876	-0.898119	-0.430073
C	0.820097	-1.496786	-0.736493	-0.105549
C	-0.129670	-2.625428	-1.152561	0.619374
N	-1.396915	-2.108378	-1.199022	-0.449544
C	0.378077	0.916104	-1.236378	0.411857
C	1.833092	1.146822	-1.571362	-0.381455
C	2.113135	0.918282	-3.075985	-0.465906
C	1.332560	-1.749573	0.710488	-0.368810
C	2.364605	-0.768556	1.217236	0.152559
C	1.983960	0.335216	1.993018	-0.194433
C	2.936906	1.253072	2.440218	-0.129868
C	4.283365	1.077333	2.117226	-0.128107
C	4.675272	-0.025676	1.354105	-0.125456
C	3.722599	-0.943260	0.909918	-0.194231
O	0.203617	-3.771158	-1.368262	-0.475447
C	-2.569110	-2.889457	-1.572541	-0.339586
C	-4.032020	1.943956	2.357512	-0.535080
C	-0.583085	1.996793	-1.346465	-0.185785
C	-0.286242	3.224255	-1.833529	-0.054219
C	-1.265828	4.340004	-1.946431	-0.512683
H	-0.903105	5.216901	-1.393361	0.206232
H	2.101476	2.167236	-1.291630	0.191898
H	2.468872	0.499676	-0.968410	0.217723
H	1.654858	-1.462531	-1.436759	0.211997
H	-2.222827	-3.901358	-1.787729	0.226918
H	-3.042133	-2.468129	-2.466690	0.182256
H	-3.297517	-2.916088	-0.757052	0.188722
H	-1.591451	1.823396	-0.989619	0.197489
H	-2.256931	4.068895	-1.574226	0.187676
H	-1.354730	4.660200	-2.993466	0.207610
H	0.720564	3.445448	-2.181975	0.183117
H	0.469566	-1.773688	1.382498	0.174376
H	1.746104	-2.764171	0.679982	0.210959
H	4.037806	-1.810560	0.333154	0.148054
H	5.724198	-0.179741	1.117683	0.159947
H	5.026287	1.786145	2.471041	0.158637
H	2.629082	2.096820	3.051516	0.151462
H	0.939160	0.465390	2.267104	0.135932
H	3.170257	1.115263	-3.275039	0.199250
H	1.901086	-0.112184	-3.379651	0.176306
H	1.516266	1.582678	-3.707380	0.172185
H	-2.024946	-0.146684	-1.601773	0.201774
H	-2.024417	-2.313483	1.718332	0.178025
H	-3.450618	-0.812373	3.494265	0.176186
H	-4.847997	2.190939	1.668223	0.190514
H	-4.457912	1.800751	3.353386	0.194960
H	-3.354595	2.805414	2.395946	0.181533

14(Z)-b1Φ

B3LYP/6-31G(d) energy= -1114.3189356000
 Zero-point correction (ZPC)= 0.452668
 Number of Imaginary Frequencies=0

O	-3.416349	-0.371749	0.640920	-0.477041
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C	-2.064665	-0.193543	0.523822	0.358374
C	-1.496447	-0.100567	1.760582	-0.203740
C	-2.566393	-0.242371	2.702602	-0.214440
C	-3.713437	-0.408878	1.983236	0.361680
C	-1.565194	-0.125059	-0.891547	0.064976
N	-0.097816	0.178896	-0.950747	-0.446160
C	0.644389	-1.067931	-1.297131	-0.097976
C	-0.450109	-1.934438	-1.934159	0.619617
N	-1.655627	-1.363689	-1.648781	-0.446182
C	0.360661	1.416989	-0.932640	0.416684
C	1.813138	1.718200	-1.206839	-0.369981
C	2.556197	2.367721	-0.019161	-0.458089
C	1.262922	-1.855410	-0.112737	-0.377796
C	2.532298	-1.303773	0.498449	0.169022
C	2.566378	-0.916877	1.844480	-0.208428
C	3.752456	-0.464613	2.429878	-0.127037
C	4.920770	-0.388903	1.671489	-0.126529
C	4.901265	-0.778604	0.329172	-0.128048
C	3.718256	-1.238059	-0.249667	-0.198635
O	-0.243482	-2.961631	-2.545481	-0.476680
C	-2.928334	-1.908912	-2.103736	-0.337468
C	-5.140650	-0.613973	2.346948	-0.533659
C	-0.561575	2.504787	-0.649101	-0.179575
C	-0.327028	3.797860	-0.968572	-0.053381
C	-1.273095	4.915193	-0.696732	-0.512668
H	-0.777759	5.687794	-0.093278	0.208383
H	2.349159	0.817228	-1.498904	0.194565
H	1.838142	2.395908	-2.070204	0.196871
H	1.398739	-0.845933	-2.051977	0.211981
H	-2.698991	-2.780682	-2.718044	0.224120
H	-3.467629	-1.168091	-2.704774	0.177789
H	-3.551892	-2.207681	-1.257534	0.196925
H	-1.491450	2.258549	-0.147512	0.189068
H	-2.176437	4.584795	-0.177839	0.188978
H	-1.560666	5.405135	-1.636727	0.208613
H	0.595077	4.072987	-1.477275	0.183970
H	0.493558	-1.993017	0.654082	0.175918
H	1.458662	-2.847935	-0.538161	0.222397
H	3.725911	-1.576522	-1.284493	0.144716
H	5.812750	-0.744852	-0.260792	0.159362
H	5.845100	-0.043964	2.125341	0.160515
H	3.763610	-0.183667	3.479165	0.156798
H	1.667737	-1.003497	2.451427	0.140993
H	3.594700	2.544226	-0.310919	0.191652
H	2.112268	3.322865	0.270589	0.163542
H	2.559708	1.704257	0.848347	0.191744
H	-2.107583	0.656035	-1.440715	0.196182
H	-0.451589	0.061047	1.984847	0.156893
H	-2.488352	-0.222332	3.780401	0.170637
H	-5.512682	-1.576175	1.975670	0.191624
H	-5.250401	-0.601723	3.433964	0.190447
H	-5.777769	0.172812	1.926678	0.188097

14(Z)-b2Φ

B3LYP/6-31G(d) energy= -1114.3211176000

Zero-point correction (ZPC)= 0.452722

Number of Imaginary Frequencies=0

O	-3.495462	-0.266219	0.444517	-0.477814
C	-2.133215	-0.133725	0.460173	0.356310
C	-1.693442	0.013465	1.742608	-0.199676
C	-2.858756	-0.042871	2.573695	-0.216138
C	-3.930613	-0.217411	1.748075	0.361202
C	-1.493038	-0.164910	-0.898405	0.068175
N	-0.021359	0.110777	-0.839601	-0.451480

C	0.730848	-1.157218	-1.056825	-0.098147
C	-0.320540	-2.054733	-1.719313	0.619174
N	-1.536148	-1.450364	-1.579323	-0.448577
C	0.480828	1.332179	-0.807956	0.418919
C	1.953605	1.539560	-1.058941	-0.385394
C	2.243559	1.764881	-2.562789	-0.464894
C	1.254639	-1.861816	0.226501	-0.373742
C	2.489275	-1.260800	0.861553	0.149947
C	2.413326	-0.540400	2.060174	-0.201234
C	3.558955	0.017011	2.633620	-0.127210
C	4.798490	-0.141045	2.013548	-0.128459
C	4.890115	-0.870551	0.824707	-0.124098
C	3.745409	-1.429232	0.256519	-0.197459
O	-0.083030	-3.125637	-2.237764	-0.478109
C	-2.773896	-2.014548	-2.102183	-0.337089
C	-5.394079	-0.360465	1.969758	-0.533598
C	-0.403216	2.461409	-0.601048	-0.173723
C	-0.007289	3.754974	-0.658505	-0.052169
C	-0.910506	4.918113	-0.444294	-0.513570
H	-0.532429	5.541228	0.377514	0.209558
H	2.295115	2.400048	-0.480374	0.192391
H	2.524442	0.687981	-0.691055	0.221860
H	1.545938	-0.985044	-1.760778	0.211214
H	-2.505725	-2.926314	-2.637636	0.223805
H	-3.252214	-1.310435	-2.792325	0.177673
H	-3.469357	-2.253021	-1.293700	0.196644
H	-1.439864	2.258502	-0.357109	0.185197
H	-1.937601	4.619108	-0.220829	0.190100
H	-0.912279	5.562724	-1.333878	0.209721
H	1.030497	3.997594	-0.877663	0.185480
H	0.433136	-1.925642	0.947547	0.176788
H	1.464938	-2.886136	-0.104090	0.219163
H	3.830473	-2.016580	-0.655918	0.148487
H	5.855641	-1.018849	0.349658	0.160271
H	5.691139	0.286091	2.460886	0.160001
H	3.483045	0.562815	3.569803	0.154376
H	1.457836	-0.441558	2.570374	0.142425
H	3.317995	1.916371	-2.698203	0.200702
H	1.946533	0.902618	-3.168458	0.177391
H	1.721008	2.643820	-2.950820	0.172887
H	-1.965547	0.584950	-1.547618	0.194227
H	-0.672778	0.159682	2.065108	0.157937
H	-2.891138	0.036405	3.651101	0.170578
H	-5.757904	-1.332343	1.615884	0.191548
H	-5.616330	-0.280456	3.036539	0.190310
H	-5.956838	0.417195	1.440450	0.187762

14(Z)-c1α

B3LYP/6-31G(d) energy= -1114.32355670

Zero-point correction (ZPC)= 0.452552

Number of Imaginary Frequencies=0

O	-1.694855	-1.492786	1.103019	-0.482194
C	-2.411315	-0.939306	0.075194	0.377269
C	-3.746376	-0.988084	0.355153	-0.197108
C	-3.862852	-1.606208	1.639905	-0.213673
C	-2.595252	-1.896298	2.058599	0.364272
C	-1.640033	-0.496960	-1.121396	0.029132
N	-0.506647	0.446287	-0.782264	-0.443367
C	0.797493	-0.260342	-0.894121	-0.086167
C	0.426412	-1.531684	-1.658946	0.614154
N	-0.930395	-1.562278	-1.805548	-0.434899
C	-0.668130	1.728683	-0.533889	0.418843
C	0.531359	2.598532	-0.240436	-0.381014
C	0.564904	3.104675	1.219753	-0.458144

C	1.496390	-0.572095	0.468188	-0.365938
C	2.983530	-0.271623	0.453596	0.145941
C	3.539881	0.585017	1.412131	-0.200968
C	4.909658	0.857834	1.415107	-0.126408
C	5.737752	0.279118	0.453530	-0.124583
C	5.191653	-0.578076	-0.505089	-0.129427
C	3.824928	-0.856156	-0.505554	-0.196782
O	1.221747	-2.360664	-2.053899	-0.477072
C	-1.640566	-2.668633	-2.431433	-0.341128
C	-2.035793	-2.531956	3.280987	-0.534147
C	-2.004845	2.296312	-0.512265	-0.173855
C	-2.263524	3.620705	-0.600198	-0.052979
C	-3.629682	4.213470	-0.595913	-0.512010
H	-3.719179	4.945561	0.217918	0.208435
H	1.460466	2.068919	-0.451353	0.208478
H	0.500135	3.456839	-0.921523	0.199522
H	1.461062	0.330701	-1.528893	0.225150
H	-0.886284	-3.345304	-2.834938	0.227302
H	-2.276994	-2.304125	-3.245083	0.180152
H	-2.257078	-3.202054	-1.700748	0.190869
H	-2.841147	1.613051	-0.417238	0.176924
H	-4.414457	3.461163	-0.483352	0.186008
H	-3.802781	4.772682	-1.525229	0.208973
H	-1.442695	4.328564	-0.701289	0.182675
H	1.004836	0.004139	1.257469	0.162725
H	1.319374	-1.626354	0.706891	0.206577
H	3.407579	-1.536609	-1.243688	0.176567
H	5.832913	-1.039379	-1.250738	0.155269
H	6.803251	0.489669	0.453417	0.154242
H	5.326728	1.519066	2.169453	0.148649
H	2.903539	1.029326	2.174800	0.123668
H	1.473165	3.694952	1.367539	0.198646
H	-0.298203	3.731771	1.455114	0.171760
H	0.583520	2.273439	1.930514	0.179301
H	-2.322564	0.008419	-1.813709	0.194291
H	-4.553502	-0.643605	-0.278330	0.168474
H	-4.774825	-1.814855	2.181077	0.174872
H	-1.370433	-1.847438	3.820340	0.184636
H	-2.847550	-2.820509	3.952860	0.193097
H	-1.458283	-3.430044	3.033027	0.194879

14(Z)-c2a

B3LYP/6-31G(d) energy= -1114.32503070

Zero-point correction (ZPC)= 0.45248

Number of Imaginary Frequencies=0

O	1.771725	-1.633022	-0.905872	-0.481827
C	2.447990	-0.896655	0.030046	0.378438
C	3.789962	-0.948042	-0.213504	-0.197059
C	3.953889	-1.762874	-1.377509	-0.214345
C	2.705151	-2.157588	-1.766153	0.364754
C	1.642604	-0.286520	1.125518	0.030311
N	0.494816	0.565363	0.632821	-0.443955
C	-0.792548	-0.150414	0.825785	-0.085038
C	-0.414894	-1.257502	1.809742	0.613075
N	0.941961	-1.242039	1.965784	-0.435555
C	0.615882	1.794179	0.176377	0.418678
C	-0.634231	2.586901	-0.127471	-0.385697
C	-1.094616	3.422678	1.091738	-0.461831
C	-1.408743	-0.726737	-0.493316	-0.365390
C	-2.898353	-0.469745	-0.612315	0.144439
C	-3.407580	0.236835	-1.709551	-0.197514
C	-4.779177	0.472419	-1.830483	-0.127444
C	-5.655441	0.005009	-0.851216	-0.124896
C	-5.155997	-0.702561	0.245338	-0.129353

C	-3.787318	-0.941830	0.365635	-0.195245
O	-1.201425	-2.019010	2.336151	-0.478162
C	1.663509	-2.214424	2.773991	-0.340758
C	2.192738	-3.000544	-2.878906	-0.534062
C	1.929766	2.382871	0.016936	-0.169007
C	2.146008	3.667868	-0.348825	-0.052133
C	3.493295	4.278894	-0.513444	-0.512521
H	3.603916	4.677284	-1.531005	0.209814
H	-0.436910	3.246819	-0.975071	0.191717
H	-1.443099	1.924088	-0.439594	0.214098
H	-1.503824	0.518172	1.313523	0.221462
H	0.916561	-2.820409	3.288361	0.226925
H	2.293504	-1.706706	3.512357	0.179402
H	2.288396	-2.858823	2.147272	0.191237
H	2.792509	1.747375	0.177607	0.173339
H	4.303543	3.571931	-0.318480	0.186858
H	3.601808	5.139622	0.160400	0.209510
H	1.302965	4.329241	-0.538485	0.184841
H	-0.881276	-0.291195	-1.347497	0.165094
H	-1.200398	-1.801436	-0.523503	0.206096
H	-3.404321	-1.501837	1.215389	0.175365
H	-5.835017	-1.076400	1.006383	0.155566
H	-6.722485	0.185338	-0.943625	0.154383
H	-5.159876	1.015620	-2.690789	0.149359
H	-2.731351	0.590056	-2.486051	0.124258
H	-2.001720	3.971645	0.825065	0.203101
H	-1.326735	2.789880	1.954133	0.179786
H	-0.332153	4.144272	1.398401	0.172721
H	2.304575	0.337509	1.737004	0.192931
H	4.571994	-0.478749	0.369310	0.167456
H	4.883706	-2.027279	-1.860847	0.174287
H	1.514520	-2.436034	-3.529609	0.185227
H	3.027498	-3.361114	-3.484538	0.192631
H	1.642453	-3.869188	-2.499062	0.194453

14(Z)-c1δ

B3LYP/6-31G(d) energy= -1114.32250120

Zero-point correction (ZPC)= 0.452684

Number of Imaginary Frequencies=0

O	-3.315512	-0.523676	0.519397	-0.486708
C	-2.133475	-1.189356	0.309152	0.374909
C	-1.896913	-2.052880	1.339835	-0.199294
C	-2.995802	-1.909625	2.242417	-0.209684
C	-3.835154	-0.973543	1.708427	0.364375
C	-1.395539	-0.855831	-0.946097	0.038815
N	-0.310011	0.191990	-0.755062	-0.441012
C	1.019838	-0.470699	-0.713577	-0.091046
C	0.722918	-1.851763	-1.301720	0.609404
N	-0.629552	-1.968448	-1.460834	-0.445678
C	-0.523981	1.490922	-0.757058	0.407901
C	0.634010	2.445464	-0.577686	-0.378741
C	0.589167	3.188595	0.777126	-0.458014
C	1.678803	-0.546370	0.701277	-0.370559
C	3.151985	-0.182412	0.691868	0.147070
C	3.632346	0.839117	1.521024	-0.199905
C	4.988790	1.171697	1.528023	-0.126401
C	5.878812	0.486816	0.700947	-0.124105
C	5.408353	-0.535233	-0.127394	-0.129339
C	4.054938	-0.871992	-0.131984	-0.196568
O	1.562545	-2.687226	-1.570270	-0.475444
C	-1.271722	-3.155038	-2.012593	-0.340127
C	-5.136464	-0.394468	2.136204	-0.534853
C	-1.875468	2.005245	-0.897389	-0.187228
C	-2.160117	3.285201	-1.230060	-0.054769

C	-3.539372	3.819950	-1.403824	-0.512399
H	-3.697011	4.678235	-0.736837	0.205984
H	1.588692	1.926189	-0.662757	0.206144
H	0.602242	3.174794	-1.394646	0.199336
H	1.687353	0.043768	-1.407510	0.227485
H	-0.476622	-3.844399	-2.299804	0.227063
H	-1.863977	-2.892166	-2.895768	0.183611
H	-1.919211	-3.629984	-1.269747	0.190429
H	-2.702365	1.325461	-0.728414	0.200763
H	-4.308853	3.069574	-1.205594	0.187835
H	-3.670966	4.203220	-2.424681	0.208263
H	-1.354324	3.994556	-1.408990	0.180963
H	1.133474	0.116615	1.379800	0.166347
H	1.544504	-1.562993	1.089085	0.199461
H	3.696923	-1.677843	-0.768111	0.175747
H	6.098331	-1.078634	-0.766597	0.156028
H	6.934240	0.743030	0.705185	0.155141
H	5.347451	1.961791	2.181635	0.149822
H	2.947567	1.367369	2.181296	0.125815
H	1.468058	3.834080	0.855642	0.198303
H	-0.305893	3.807714	0.873400	0.172188
H	0.608839	2.488308	1.617354	0.178347
H	-2.094272	-0.480209	-1.701609	0.203511
H	-1.055644	-2.724754	1.441985	0.176241
H	-3.149955	-2.447528	3.167152	0.176180
H	-5.921618	-0.587757	1.395876	0.192311
H	-5.444338	-0.839971	3.085071	0.194930
H	-5.067672	0.691188	2.274338	0.181076

14(Z)-c2δ

B3LYP/6-31G(d) energy= -1114.32413180

Zero-point correction (ZPC)= 0.452761

Number of Imaginary Frequencies=0

O	-3.360883	-0.548000	0.450983	-0.487044
C	-2.174829	-1.183677	0.180666	0.375675
C	-1.968311	-2.186360	1.083652	-0.199257
C	-3.091291	-2.166504	1.967584	-0.208995
C	-3.913730	-1.159160	1.549356	0.363700
C	-1.407049	-0.681466	-0.998177	0.041280
N	-0.309780	0.308741	-0.647696	-0.440792
C	1.006580	-0.375120	-0.675026	-0.089947
C	0.707441	-1.637516	-1.485456	0.608777
N	-0.646330	-1.717590	-1.662875	-0.446710
C	-0.489398	1.597035	-0.443370	0.408477
C	0.723828	2.478977	-0.250799	-0.384205
C	1.224400	3.074685	-1.588457	-0.461858
C	1.592373	-0.701690	0.739370	-0.370294
C	3.063957	-0.357736	0.868209	0.145536
C	3.498509	0.525305	1.864914	-0.196521
C	4.853482	0.838816	1.995536	-0.127234
C	5.786745	0.273626	1.126632	-0.124575
C	5.361297	-0.609383	0.130757	-0.129415
C	4.009485	-0.926882	0.001382	-0.195403
O	1.542126	-2.426861	-1.879411	-0.476310
C	-1.295293	-2.801765	-2.389278	-0.340156
C	-5.225322	-0.639636	2.020128	-0.534676
C	-1.825565	2.156786	-0.447070	-0.182568
C	-2.089304	3.481187	-0.352688	-0.054504
C	-3.458530	4.065635	-0.364080	-0.513112
H	-3.622925	4.657497	0.546484	0.207148
H	0.467159	3.285698	0.439247	0.191840
H	1.531910	1.919326	0.224433	0.211828
H	1.713370	0.232297	-1.242136	0.223608
H	-0.504853	-3.455508	-2.760306	0.226806

H	-1.869145	-2.406396	-3.234580	0.183370
H	-1.961516	-3.366960	-1.731119	0.190398
H	-2.665911	1.475465	-0.508515	0.196193
H	-4.239785	3.305394	-0.441376	0.188776
H	-3.561930	4.768125	-1.202274	0.208796
H	-1.273600	4.196365	-0.267554	0.183185
H	1.013067	-0.159944	1.493902	0.168720
H	1.436857	-1.768692	0.936741	0.199270
H	3.684806	-1.623654	-0.767885	0.174194
H	6.085003	-1.059053	-0.543039	0.156264
H	6.840961	0.514542	1.227445	0.155311
H	5.176833	1.519509	2.777929	0.150683
H	2.777872	0.957632	2.556729	0.126907
H	2.097225	3.703731	-1.394083	0.202591
H	1.524043	2.294961	-2.295788	0.179355
H	0.456907	3.687930	-2.068889	0.173488
H	-2.088991	-0.188856	-1.700401	0.203175
H	-1.131151	-2.870403	1.111361	0.175301
H	-3.271661	-2.828759	2.802556	0.175762
H	-5.990590	-0.722199	1.239442	0.192180
H	-5.559087	-1.213300	2.887944	0.194735
H	-5.158887	0.415141	2.312438	0.180224

TS13 (E)-a1-endo

B3LYP/6-31G(d) energy= -1118.884433

Zero-point correction (ZPC)= 0.526944

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5252500000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy= -1111.5902480000

Number of Imaginary Frequencies=1

C	-3.628822	-0.770079	-1.038202	-0.193669
C	-2.327070	-1.287774	-0.952812	0.156308
C	-2.083910	-2.346040	-0.066214	-0.193421
C	-3.106493	-2.865460	0.730602	-0.133420
C	-4.393655	-2.331201	0.649026	-0.128220
C	-4.651832	-1.285853	-0.240577	-0.133695
C	-1.206571	-0.729149	-1.804684	-0.377132
C	-0.571579	0.592549	-1.284438	-0.058941
N	-0.104471	0.584187	0.117184	-0.513321
C	-0.847400	1.618115	0.949010	0.353880
N	-1.725513	2.215953	-0.066611	-0.460843
C	-1.596620	1.713032	-1.322664	0.623677
C	0.981896	-0.124924	0.495971	0.417358
C	1.301620	-0.337795	1.962696	-0.366182
C	0.701317	-1.651068	2.514152	-0.462320
O	-2.204853	2.059602	-2.320513	-0.511766
C	-2.692516	3.266273	0.224260	-0.345718
C	-1.696837	0.988517	2.063768	-0.469389
C	0.107396	2.713635	1.464828	-0.460837
C	1.781749	-0.779529	-0.464908	-0.190759
C	2.869616	-1.664169	-0.197480	-0.150705
C	3.097820	-2.792926	-1.195573	-0.464519
C	4.557371	-0.664274	-0.380039	-0.176949
C	4.650769	0.130704	0.785174	-0.073759
C	4.044070	1.388032	0.561288	-0.098107
C	3.681884	1.472230	-0.766233	-0.097751
C	4.249534	0.307955	-1.510700	-0.327839
H	3.878960	2.149310	1.315137	0.178701
H	5.064877	-0.202512	1.731739	0.189064
H	5.242575	-1.493144	-0.531045	0.188542
H	3.183146	2.312090	-1.237648	0.189037
H	3.640978	-0.067771	-2.334705	0.185523
H	5.212749	0.621251	-1.948518	0.225589
H	2.982283	-1.996474	0.830305	0.178274

H	3.121566	-2.430303	-2.228396	0.171806
H	4.024359	-3.338031	-0.996931	0.178188
H	2.270895	-3.508905	-1.116883	0.192128
H	1.516788	-0.673029	-1.508388	0.157061
H	0.950063	0.489196	2.573410	0.173222
H	2.389214	-0.357743	2.082635	0.166735
H	0.945322	-1.744816	3.576999	0.180842
H	-0.386314	-1.666879	2.407351	0.187441
H	1.097444	-2.528973	1.996111	0.165992
H	-2.208207	4.160564	0.628247	0.175913
H	-3.458404	2.920655	0.925106	0.182991
H	-3.167523	3.519533	-0.724652	0.224214
H	-1.086270	0.562149	2.860797	0.166809
H	-2.322560	1.760579	2.521176	0.176496
H	-2.345493	0.211031	1.653437	0.203801
H	-0.478523	3.524447	1.906451	0.185776
H	0.791842	2.362095	2.238119	0.168106
H	0.688922	3.126604	0.635156	0.165151
H	0.252401	0.875956	-1.952076	0.179497
H	-0.427521	-1.486599	-1.927507	0.157369
H	-1.573262	-0.479118	-2.806474	0.204941
H	-1.088877	-2.783072	-0.014172	0.119567
H	-2.901790	-3.694846	1.402202	0.144883
H	-5.193447	-2.737634	1.261376	0.152814
H	-5.655862	-0.879636	-0.325706	0.153513
H	-3.842045	0.031414	-1.740049	0.167869

TS13 (E)-a1-exo

B3LYP/6-31G(d) energy= -1118.882975

Zero-point correction (ZPC)= 0.52697

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5236600000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5867580000

Number of Imaginary Frequencies=1

C	-3.515628	-0.647303	-1.316790	-0.193502
C	-2.238203	-1.200541	-1.137464	0.155283
C	-2.106790	-2.331758	-0.319988	-0.193661
C	-3.216134	-2.887820	0.320809	-0.133282
C	-4.478879	-2.317934	0.149168	-0.128220
C	-4.625245	-1.199900	-0.675085	-0.134062
C	-1.024599	-0.603425	-1.818789	-0.376532
C	-0.436690	0.667652	-1.138058	-0.060379
N	-0.117302	0.547869	0.298872	-0.509073
C	-0.953967	1.511100	1.128235	0.353724
N	-1.723364	2.189850	0.075749	-0.459522
C	-1.448359	1.798815	-1.196396	0.622000
C	0.942033	-0.175312	0.729663	0.400694
C	1.096664	-0.502452	2.205864	-0.365971
C	0.473225	-1.870099	2.564737	-0.461055
O	-1.939285	2.235540	-2.223286	-0.512809
C	-2.722255	3.215592	0.345797	-0.345759
C	-1.912956	0.793793	2.091202	-0.469862
C	-0.068256	2.562124	1.828488	-0.462059
C	1.834080	-0.754383	-0.196289	-0.180594
C	2.949546	-1.588155	0.107373	-0.148031
C	3.241134	-2.763753	-0.810832	-0.461343
C	4.605575	-0.495646	-0.003505	-0.196561
C	4.229458	0.800886	0.695366	-0.335625
C	3.678388	1.614157	-0.429916	-0.095694
C	4.080396	1.069858	-1.629094	-0.100493
C	4.720986	-0.165796	-1.371622	-0.050647
H	-3.562092	2.812902	0.920187	0.183405
H	-2.292289	4.067355	0.881493	0.175702
H	-3.085957	3.555145	-0.625084	0.223808

H	-2.508393	0.052973	1.552519	0.204469
H	-2.589683	1.526716	2.540239	0.176367
H	-1.388499	0.302542	2.911692	0.167613
H	-0.704919	3.330864	2.275027	0.186294
H	0.539998	2.149946	2.634430	0.170479
H	0.455471	0.987202	-1.691633	0.179720
H	-1.275309	-0.277217	-2.834412	0.204047
H	-0.244641	-1.364425	-1.909254	0.157654
H	-3.641125	0.212298	-1.969229	0.167822
H	-5.608220	-0.764482	-0.831652	0.153315
H	-5.345248	-2.752317	0.639616	0.152840
H	-3.096853	-3.772785	0.940000	0.145392
H	-1.130352	-2.796772	-0.201562	0.120998
H	-0.587154	-1.907246	2.301737	0.186837
H	0.976426	-2.689105	2.042963	0.164859
H	0.568172	-2.043045	3.641348	0.181834
H	2.158310	-0.519571	2.465514	0.169286
H	0.650765	0.262293	2.834507	0.174580
H	0.587704	3.046388	1.098605	0.164412
H	2.531941	-3.571743	-0.592275	0.187887
H	4.248846	-3.163883	-0.662655	0.173489
H	3.121652	-2.496025	-1.864850	0.170144
H	3.922280	1.502243	-2.610519	0.187000
H	5.163901	-0.802549	-2.129997	0.193235
H	3.087190	-1.838320	1.157729	0.178825
H	5.292844	-1.200282	0.457629	0.189831
H	1.633251	-0.621780	-1.250276	0.159011
H	3.148777	2.551916	-0.303082	0.186608
H	5.165926	1.274067	1.036640	0.224203
H	3.585076	0.720141	1.571298	0.180759

TS13 (E)-a2-endo

B3LYP/6-31G(d) energy= -1118.878289

Zero-point correction (ZPC)= 0.526985

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5172010000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5823640000

Number of Imaginary Frequencies=1

C	-2.751085	-2.052045	-1.464869	-0.101645
C	-3.943456	-1.325883	-1.226665	-0.073711
C	-4.194573	-1.237986	0.162999	-0.178408
C	-3.477807	0.460954	0.753873	-0.153963
C	-2.046224	0.453150	0.805627	-0.188253
C	-2.304709	-2.565482	-0.269186	-0.085529
C	-3.305364	-2.295175	0.804087	-0.338208
C	-1.179207	1.039118	-0.138005	0.412214
C	-1.788190	1.602205	-1.411945	-0.376108
C	-2.510271	2.962535	-1.271791	-0.458560
C	-4.182003	0.622716	2.099178	-0.462509
N	0.155270	1.107344	0.095244	-0.519223
C	0.739866	0.579378	1.348641	-0.068767
C	2.113338	1.219973	1.414934	0.627855
N	2.324697	1.887113	0.249987	-0.461928
C	1.203623	1.876513	-0.702880	0.358449
O	2.885771	1.105394	2.350755	-0.510412
C	3.605243	2.526478	-0.022544	-0.344554
C	0.872257	-0.965414	1.489613	-0.371349
C	1.842844	-1.665299	0.558782	0.154208
C	1.422602	-2.172274	-0.679469	-0.211325
C	2.309601	-2.849195	-1.519390	-0.128835
C	3.637747	-3.029369	-1.129708	-0.126911
C	4.069635	-2.527946	0.099691	-0.129657
C	3.180536	-1.853379	0.937607	-0.179654
C	0.804704	3.332821	-0.993799	-0.466676

C	1.607178	1.132466	-1.987760	-0.470149
H	0.153060	0.950313	2.196436	0.193098
H	1.195816	-1.113568	2.525364	0.196646
H	-0.119159	-1.416692	1.398646	0.147190
H	0.391557	-2.028746	-0.993909	0.107928
H	1.963428	-3.240323	-2.472421	0.140446
H	4.328941	-3.561892	-1.776517	0.153757
H	5.100133	-2.668823	0.413056	0.156416
H	3.524092	-1.465515	1.891983	0.170240
H	4.046848	2.148209	-0.949198	0.178952
H	4.259464	2.276625	0.813962	0.223355
H	3.512707	3.615512	-0.082382	0.179413
H	1.697372	3.880909	-1.306248	0.184803
H	0.407889	3.817229	-0.097141	0.175532
H	0.088003	3.420616	-1.808904	0.172446
H	1.976394	0.132497	-1.755088	0.202446
H	2.397901	1.689968	-2.499060	0.175648
H	0.772603	1.045283	-2.687535	0.162397
H	-2.513534	0.860044	-1.769848	0.169051
H	-1.037176	1.672929	-2.196541	0.177846
H	-1.847754	3.742989	-0.894972	0.178972
H	-2.878068	3.276665	-2.253748	0.181153
H	-3.366116	2.912561	-0.595439	0.169007
H	-3.969394	1.624008	2.491059	0.193542
H	-3.928382	1.079628	-0.014116	0.175767
H	-3.825200	-0.101606	2.838730	0.172268
H	-5.267165	0.524331	2.011346	0.176043
H	-4.551910	-0.859724	-1.995721	0.190922
H	-5.215798	-1.102341	0.507714	0.190481
H	-3.912651	-3.205023	0.947739	0.226285
H	-2.879021	-2.053899	1.780352	0.191344
H	-1.407008	-3.156516	-0.127339	0.201606
H	-2.276340	-2.182029	-2.430706	0.182939
H	-1.625176	0.068878	1.725674	0.155655

TS13 (E)-a2-exo

B3LYP/6-31G(d) energy= -1118.876893

Zero-point correction (ZPC)= 0.526794

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5169800000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -

1111.5822790000

Number of Imaginary Frequencies=1

C	-2.088604	2.790093	-1.790903	-0.129804
C	-1.224821	2.125766	-0.917461	-0.208408
C	-1.625788	1.792244	0.384634	0.155476
C	-2.922210	2.140562	0.791631	-0.181662
C	-3.789045	2.802641	-0.079198	-0.129546
C	-3.375613	3.131421	-1.371615	-0.127481
C	-0.677108	1.101498	1.342918	-0.376384
C	-0.690657	-0.452733	1.339067	-0.066124
N	-0.277839	-1.132665	0.091379	-0.518537
C	-1.452373	-1.894090	-0.517901	0.357585
N	-2.471322	-1.718974	0.529377	-0.462266
C	-2.099538	-0.954774	1.589332	0.627970
C	1.027253	-1.178745	-0.284106	0.404637
C	1.438720	-1.889295	-1.567310	-0.379428
C	2.106099	-3.269667	-1.371942	-0.456543
O	-2.769638	-0.673116	2.568053	-0.512051
C	-3.819740	-2.263959	0.440519	-0.345065
C	-1.940630	-1.257019	-1.831186	-0.470959
C	-1.181350	-3.399322	-0.680202	-0.465318
C	2.027250	-0.616824	0.531720	-0.185263
C	2.500554	2.549606	-0.448983	-0.082113
C	3.291036	1.592100	-1.278294	-0.346345
C	4.233574	0.966132	-0.259707	-0.200119

C	3.438512	-0.716032	0.310355	-0.149209
C	4.201843	1.826332	0.861076	-0.046118
C	3.098679	2.712867	0.776453	-0.103323
C	4.297904	-1.124731	1.499420	-0.460115
H	1.619743	3.076444	-0.797546	0.200640
H	1.738527	-0.206284	1.491530	0.154703
H	3.901673	2.166395	-1.995183	0.223159
H	2.684724	0.903384	-1.870935	0.188995
H	5.183202	0.546851	-0.583972	0.193384
H	2.788352	3.404395	1.551161	0.190962
H	4.890751	1.779123	1.698034	0.196648
H	3.728623	-1.235221	-0.599572	0.177631
H	4.158269	-2.196458	1.685173	0.189327
H	4.007575	-0.594114	2.411051	0.171171
H	5.364361	-0.957286	1.318497	0.170610
H	2.141872	-1.238311	-2.099425	0.173451
H	0.586882	-1.992064	-2.235056	0.178093
H	2.279253	-3.729544	-2.350086	0.181934
H	3.070708	-3.193980	-0.864739	0.165666
H	-0.060005	-0.803568	2.164199	0.192215
H	-4.351723	-1.913885	1.326309	0.223409
H	-4.337138	-1.902068	-0.453180	0.179629
H	-3.817240	-3.358317	0.440829	0.178699
H	-2.824762	-1.795089	-2.186256	0.175611
H	-2.203837	-0.209320	-1.677623	0.202772
H	-1.191579	-1.317346	-2.623738	0.165403
H	-2.133829	-3.908293	-0.849291	0.183623
H	-0.731911	-3.815589	0.225811	0.174721
H	-0.552906	-3.627700	-1.539820	0.173072
H	-0.227473	1.854583	-1.256526	0.105018
H	0.344448	1.448156	1.171102	0.152164
H	-0.939174	1.370122	2.371769	0.195180
H	-1.756474	3.044319	-2.793988	0.141476
H	-4.048498	3.654268	-2.045058	0.153762
H	-4.787153	3.068785	0.256904	0.156193
H	-3.251853	1.887742	1.795197	0.169663
H	1.484149	-3.948167	-0.785176	0.177570

TS13 (E)-c1-endo

B3LYP/6-31G(d) energy= -1118.883265

Zero-point correction (ZPC)= 0.526479

HF/6-31G(d)//B3LYP/6-31G(d) energy= -1111.5236240000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -

1111.5836300000

Number of Imaginary Frequencies=1

C	1.166813	2.787001	-1.880562	-0.331055
C	-0.125752	2.207013	-2.354201	-0.097173
C	-1.161680	3.048753	-2.007883	-0.099904
C	-0.656755	4.060366	-1.158892	-0.072832
C	0.693914	3.793301	-0.840903	-0.177996
C	0.628890	2.715285	0.813982	-0.153998
C	2.049423	2.899941	1.332207	-0.466460
C	0.233534	1.387922	0.468264	-0.195314
C	-1.064262	0.850303	0.592357	0.406725
C	-2.155238	1.725154	1.176810	-0.366635
C	-2.089466	1.796215	2.719238	-0.456443
N	-1.291974	-0.452210	0.306247	-0.521672
C	-2.636866	-1.127266	0.115255	0.351094
N	-2.218966	-2.445549	-0.380707	-0.461453
C	-0.883067	-2.590883	-0.597278	0.601177
C	-0.182776	-1.334862	-0.110052	-0.056271
C	-3.407880	-1.293499	1.433939	-0.459725
C	-3.468981	-0.433619	-0.982793	-0.459421
C	0.838791	-1.672509	1.025366	-0.367428

C	2.290195	-1.609689	0.585678	0.144171
C	3.214712	-0.844930	1.310066	-0.201067
C	4.556345	-0.790367	0.924870	-0.131996
C	4.988857	-1.498698	-0.196687	-0.127930
C	4.075762	-2.267108	-0.922821	-0.132445
C	2.736772	-2.327012	-0.534951	-0.198050
O	-0.321766	-3.568658	-1.061242	-0.495562
C	-3.152844	-3.514586	-0.711541	-0.346413
H	-2.194997	2.947201	-2.319597	0.177173
H	1.607399	3.358900	-2.715333	0.224509
H	-1.238087	4.883514	-0.755122	0.187891
H	1.345146	4.594637	-0.505540	0.188130
H	-0.090650	3.310872	1.368152	0.175558
H	2.785572	2.380922	0.710975	0.181284
H	2.327849	3.954447	1.405829	0.174450
H	2.113268	2.472593	2.340371	0.189081
H	-0.202864	1.330751	-2.988768	0.188802
H	1.920925	2.063905	-1.566068	0.196106
H	1.036813	0.731232	0.160575	0.177195
H	-2.879582	-0.344591	-1.900270	0.167330
H	2.887292	-0.303510	2.195540	0.124989
H	4.408917	-2.832880	-1.788472	0.151967
H	6.032020	-1.461167	-0.497256	0.150675
H	5.261864	-0.202230	1.505504	0.144486
H	2.034574	-2.946446	-1.087218	0.178020
H	0.342769	-0.884151	-0.961330	0.186516
H	0.609412	-2.677064	1.399555	0.200180
H	0.675726	-0.984182	1.860199	0.161583
H	-2.551803	-4.346304	-1.081928	0.226817
H	-3.856138	-3.210821	-1.493433	0.177203
H	-3.711013	-3.843210	0.170075	0.182092
H	-2.898867	2.431299	3.092486	0.183648
H	-2.200835	0.805464	3.168950	0.176043
H	-1.140709	2.212802	3.067734	0.169900
H	-2.049020	2.732948	0.762275	0.169243
H	-3.145050	1.386926	0.883034	0.171746
H	-4.353818	-1.037183	-1.203430	0.186048
H	-3.825237	0.556051	-0.693586	0.170299
H	-4.285138	-1.924715	1.265582	0.182491
H	-3.769893	-0.344115	1.829900	0.172924
H	-2.775785	-1.775687	2.184959	0.179966

TS13 (E)-c1-exo

B3LYP/6-31G(d) energy= -1118.882084

Zero-point correction (ZPC)= 0.526418

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5225730000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5820940000

Number of Imaginary Frequencies=1

C	2.970507	-0.130384	-0.005058	0.350606
N	1.491317	0.092919	-0.258315	-0.518126
C	0.700558	-1.106451	0.084651	-0.057151
C	1.735745	-2.085588	0.608126	0.599847
N	2.966716	-1.525144	0.457084	-0.461027
C	0.875262	1.266980	-0.533075	0.390198
C	1.668530	2.455796	-1.048307	-0.366652
C	1.639680	2.546154	-2.590509	-0.454740
C	-0.090642	-1.730228	-1.112869	-0.368861
C	-1.512734	-2.132177	-0.766380	0.145609
C	-1.779178	-2.964095	0.332164	-0.198746
C	-3.090249	-3.332769	0.636440	-0.134552
C	-4.152149	-2.885306	-0.153244	-0.129025
C	-3.895904	-2.067717	-1.254613	-0.133349
C	-2.584231	-1.692894	-1.555863	-0.199795

O	1.488594	-3.198129	1.041694	-0.496600
C	4.173885	-2.252431	0.828637	-0.346065
C	3.812505	-0.013816	-1.285439	-0.459951
C	3.491447	0.759937	1.141905	-0.459744
C	-0.530844	1.350016	-0.490581	-0.185671
C	-1.316039	2.503088	-0.776134	-0.149327
C	-1.911946	3.293616	0.966727	-0.197561
C	-0.665263	3.229757	1.833387	-0.334929
C	-0.790193	1.878848	2.461430	-0.097684
C	-2.083916	1.428899	2.330455	-0.096176
C	-2.792261	2.328378	1.496233	-0.048205
C	-2.616495	2.322953	-1.540188	-0.467655
H	-0.774676	3.990849	2.624560	0.223122
H	0.288315	3.428532	1.341787	0.178270
H	-0.772714	3.396196	-1.079861	0.175737
H	-2.283149	4.241176	0.585619	0.188846
H	-3.155608	1.427630	-1.218292	0.180519
H	-3.276980	3.190407	-1.445239	0.170954
H	-2.385310	2.204237	-2.606506	0.184773
H	-3.842034	2.235558	1.239670	0.193217
H	-2.493744	0.526164	2.768499	0.190056
H	-1.095554	0.447310	-0.301462	0.179734
H	-0.003856	1.396188	3.031356	0.184339
H	2.701879	2.428750	-0.714429	0.173184
H	1.246378	3.375152	-0.632369	0.172668
H	2.041192	1.639592	-3.052470	0.175390
H	0.622579	2.688944	-2.965242	0.168975
H	2.247806	3.394088	-2.920706	0.184330
H	0.009186	-0.862132	0.900915	0.187824
H	0.464521	-2.607348	-1.465161	0.200738
H	-3.280760	-3.983697	1.485312	0.151619
H	-0.953130	-3.337679	0.932339	0.177831
H	-2.390068	-1.068210	-2.425584	0.127346
H	-4.713108	-1.728868	-1.885687	0.144892
H	-5.170436	-3.182181	0.081243	0.150382
H	3.851879	-3.246920	1.140843	0.226316
H	4.856597	-2.348209	-0.020661	0.181735
H	4.697087	-1.772687	1.662009	0.177657
H	3.864598	1.008611	-1.661217	0.173985
H	3.403542	-0.660076	-2.067233	0.179768
H	4.838609	-0.331021	-1.078387	0.182365
H	4.516487	0.469991	1.389149	0.186527
H	3.514128	1.821022	0.891032	0.172483
H	2.873847	0.619960	2.034195	0.167108
H	-0.098927	-1.014126	-1.940311	0.162587

TS13 (E)-c2-endo

B3LYP/6-31G(d) energy= -1118.87978

Zero-point correction (ZPC)= 0.527203

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5190240000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5812830000

Number of Imaginary Frequencies=1

C	2.700487	1.897125	-0.943249	-0.206388
C	1.454480	2.246916	-0.403442	0.156055
C	1.398618	3.280985	0.542905	-0.195169
C	2.566105	3.928588	0.950473	-0.130792
C	3.803014	3.563783	0.415390	-0.125896
C	3.867493	2.549815	-0.540879	-0.130183
C	0.197489	1.538485	-0.878928	-0.374012
C	-0.812092	1.183809	0.260797	-0.071200
N	-1.460978	-0.140521	0.136496	-0.520306
C	-2.895522	0.011829	-0.332680	0.351981
N	-3.082207	1.462303	-0.178959	-0.458083

C	-1.981952	2.151568	0.227967	0.604879
C	-0.782553	-1.276851	0.422306	0.409750
C	-1.465038	-2.631587	0.410083	-0.372844
C	-1.960038	-3.112946	1.792963	-0.457610
C	-3.017711	-0.392644	-1.813618	-0.449581
C	-3.938036	-0.696963	0.547032	-0.469175
C	-4.351269	2.141244	-0.408741	-0.345265
O	-1.914222	3.346143	0.460978	-0.493788
C	0.575516	-1.215067	0.792901	-0.198820
C	1.348185	-2.293851	1.330719	-0.153773
C	2.392248	-1.904522	2.373218	-0.465155
C	2.473702	-3.088153	-0.045317	-0.177408
C	2.867220	-1.914397	-0.931337	-0.339025
C	1.793985	-1.934061	-1.968952	-0.093071
C	1.146547	-3.148227	-1.947394	-0.099631
C	1.614421	-3.887935	-0.835118	-0.076303
H	0.396671	-3.482944	-2.655074	0.179986
H	1.312402	-4.901531	-0.589362	0.190109
H	1.636014	-1.146564	-2.697466	0.189665
H	3.821968	-2.173190	-1.420728	0.222121
H	3.020491	-0.951675	-0.440450	0.199919
H	3.209596	-3.564588	0.595966	0.189559
H	0.798106	-3.184116	1.618960	0.175754
H	3.040645	-1.095713	2.021299	0.180012
H	1.877302	-1.545184	3.271790	0.192590
H	3.016885	-2.752437	2.666698	0.174701
H	1.073059	-0.252475	0.780704	0.174711
H	2.756808	1.126803	-1.710198	0.113566
H	4.822251	2.270391	-0.977994	0.143715
H	4.707972	4.073862	0.732419	0.152693
H	2.505338	4.729886	1.681464	0.155043
H	0.437015	3.598327	0.937371	0.180074
H	-0.321882	2.164969	-1.615190	0.195917
H	0.472128	0.616526	-1.400036	0.148942
H	-0.320728	1.247305	1.235805	0.202915
H	-4.930627	-0.338781	0.261021	0.186434
H	-3.949810	-1.777851	0.417325	0.173710
H	-3.782684	-0.454237	1.601698	0.181147
H	-2.308982	0.174117	-2.423745	0.173886
H	-4.028589	-0.186260	-2.177769	0.181806
H	-2.830420	-1.460261	-1.956906	0.164751
H	-4.775907	1.859596	-1.376822	0.175312
H	-5.078176	1.928459	0.381794	0.183900
H	-4.138729	3.211336	-0.407001	0.224374
H	-2.289655	-2.644621	-0.301588	0.173743
H	-0.740701	-3.359078	0.028632	0.170045
H	-2.433600	-4.094263	1.688670	0.181373
H	-2.691403	-2.429505	2.228202	0.177767
H	-1.138485	-3.209596	2.507331	0.170562

TS13 (E)-c2-exo

B3LYP/6-31G(d) energy= -1118.875654

Zero-point correction (ZPC)= 0.526898

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5157510000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5798670000

Number of Imaginary Frequencies=1

C	1.412538	3.018564	0.874440	-0.191873
C	1.427741	2.217605	-0.274793	0.159590
C	2.608634	2.154815	-1.030886	-0.198082
C	3.750678	2.854470	-0.642965	-0.132991
C	3.732589	3.628031	0.519879	-0.126124
C	2.560548	3.710620	1.270363	-0.133763
C	0.207785	1.454213	-0.767931	-0.364844

C	-0.823407	1.048936	0.325170	-0.082419
N	-1.546787	-0.210503	0.034254	-0.515330
C	-2.946159	0.093415	-0.475048	0.351399
N	-3.052920	1.522307	-0.143418	-0.457680
C	-1.935752	2.080850	0.398289	0.607339
C	-0.956332	-1.415704	0.219673	0.401616
C	-1.739857	-2.701794	0.008164	-0.377278
C	-2.350028	-3.294744	1.297944	-0.455743
O	-1.818457	3.221940	0.808879	-0.489896
C	-4.271401	2.303650	-0.314362	-0.345114
C	-4.079677	-0.644054	0.256441	-0.470663
C	-3.011767	-0.114441	-1.999595	-0.450214
C	0.369294	-1.492158	0.692541	-0.191239
C	1.012430	-2.681193	1.154180	-0.147666
C	1.812039	-2.590911	2.444989	-0.462296
C	2.126007	-1.828074	-1.938644	-0.095331
C	3.175753	-1.420871	-1.151504	-0.090727
C	3.369994	-2.381897	-0.127370	-0.049306
C	2.340763	-3.344421	-0.158572	-0.199433
C	1.679197	-3.189362	-1.519192	-0.340477
H	0.418076	-3.590557	1.101985	0.177939
H	2.463595	-3.458268	2.590167	0.171343
H	1.114880	-2.557571	3.291213	0.188292
H	2.419442	-1.682136	2.484045	0.176079
H	2.490663	-4.328573	0.277863	0.189735
H	2.134259	-3.932421	-2.195832	0.223282
H	0.910439	-0.570338	0.871060	0.169819
H	1.728994	-1.296384	-2.796455	0.186762
H	3.748885	-0.509613	-1.266952	0.188628
H	4.156836	-2.337074	0.618041	0.194659
H	0.601359	-3.351518	-1.567752	0.183172
H	-2.241573	0.478672	-2.500022	0.174871
H	-3.969322	-0.546099	1.339681	0.181129
H	-4.159332	-1.696188	-0.011163	0.174823
H	-5.027733	-0.180089	-0.028285	0.187161
H	-3.988967	0.197769	-2.380354	0.181760
H	-2.876686	-1.165265	-2.270526	0.166441
H	-5.034662	2.040459	0.425126	0.183367
H	-4.681787	2.174578	-1.320188	0.175279
H	-3.995178	3.349184	-0.170318	0.224211
H	-0.341486	0.966581	1.302871	0.197816
H	-0.315999	2.049885	-1.527853	0.188040
H	2.624823	1.572996	-1.950904	0.114566
H	0.542685	0.543393	-1.274536	0.152741
H	0.494289	3.143710	1.439618	0.171144
H	2.528471	4.328547	2.163282	0.152603
H	4.620167	4.172994	0.827916	0.151152
H	4.650684	2.801264	-1.249778	0.143400
H	-3.013835	-2.590584	1.802376	0.177677
H	-2.929597	-4.189525	1.049751	0.183000
H	-1.574796	-3.583328	2.012496	0.168225
H	-1.064019	-3.446482	-0.420436	0.173291
H	-2.517633	-2.559428	-0.740294	0.176291

TS13 (Z)-a1-endo

B3LYP/6-31G(d) energy= -1118.878187

Zero-point correction (ZPC)= 0.526845

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5167980000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5837480000

Number of Imaginary Frequencies=1

C	-4.190606	1.002896	1.335627	-0.098551
C	-3.980037	1.631724	0.129933	-0.088404
C	-4.525068	0.792935	-0.978746	-0.332745

C	-4.675111	-0.566852	-0.306435	-0.176226
C	-4.695782	-0.294581	1.084201	-0.076681
C	-3.013023	-1.479890	-0.661794	-0.150800
C	-3.311640	-2.136385	-2.007605	-0.464048
C	-1.906349	-0.568953	-0.651489	-0.186235
C	-1.007566	-0.367135	0.413234	0.414833
C	-1.294843	-1.089227	1.722993	-0.371841
C	-0.950932	-2.595061	1.768996	-0.466950
N	0.086923	0.427366	0.329984	-0.517122
C	1.038549	0.634629	1.451133	-0.065054
C	1.864575	1.830239	1.007431	0.621436
N	1.547609	2.113444	-0.282450	-0.457826
C	0.435017	1.335803	-0.842555	0.359162
C	2.007923	-0.527443	1.817607	-0.383643
C	2.926555	-1.011418	0.712469	0.153150
C	2.592419	-2.120922	-0.077263	-0.200919
C	3.446556	-2.567284	-1.087804	-0.129503
C	4.653848	-1.908129	-1.324135	-0.127991
C	5.003226	-0.807585	-0.538994	-0.132607
C	4.149573	-0.365132	0.472187	-0.188053
C	0.908947	0.533815	-2.065653	-0.470174
C	-0.697987	2.324193	-1.178398	-0.460353
C	2.272977	3.135744	-1.024820	-0.344753
O	2.704460	2.381525	1.697539	-0.510743
H	0.490574	0.921994	2.354154	0.192262
H	2.732525	2.718169	-1.925578	0.182041
H	1.627998	3.975735	-1.301592	0.175071
H	3.056826	3.500930	-0.359784	0.223673
H	-1.033144	2.834638	-0.270639	0.165431
H	-0.309426	3.077996	-1.868062	0.183740
H	-1.553917	1.860471	-1.665549	0.158452
H	1.768789	-0.085371	-1.802980	0.207560
H	0.124745	-0.113135	-2.463639	0.163298
H	1.199372	1.223155	-2.864056	0.173213
H	2.605210	-0.117444	2.639650	0.203668
H	1.438733	-1.360184	2.234360	0.162484
H	1.661942	-2.653977	0.101308	0.121564
H	5.949017	-0.299106	-0.703882	0.152953
H	5.323810	-2.258468	-2.104076	0.151779
H	3.173990	-3.435845	-1.681156	0.144121
H	4.433845	0.485453	1.085065	0.168493
H	-1.275434	-3.006354	2.729953	0.183193
H	-1.444086	-3.161630	0.975452	0.167754
H	0.121008	-2.775583	1.676954	0.190964
H	-2.369900	-0.978405	1.908938	0.169767
H	-0.801123	-0.589813	2.557362	0.182782
H	-3.054071	-2.195010	0.152375	0.178088
H	-5.364408	-1.302333	-0.711971	0.189810
H	-4.999265	-1.003569	1.848521	0.192353
H	-3.996706	1.423672	2.315681	0.184809
H	-1.702205	-0.091633	-1.598217	0.143312
H	-3.581778	2.631015	-0.002372	0.190804
H	-2.482027	-2.802922	-2.270345	0.191942
H	-4.223487	-2.738657	-1.978662	0.177050
H	-3.408218	-1.398304	-2.810876	0.169491
H	-5.537659	1.158892	-1.219831	0.225058
H	-3.956254	0.821856	-1.910279	0.185716

TS13 (Z)-a1-exo

B3LYP/6-31G(d) energy= -1118.875875

Zero-point correction (ZPC)= 0.52694

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5148710000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5822800000

Number of Imaginary Frequencies=1

C	-4.555880	1.477582	-0.893604	-0.103356
C	-4.142275	1.591590	0.413710	-0.082436
C	-4.441686	0.329556	1.148300	-0.341751
C	-4.705752	-0.654743	0.016048	-0.198041
C	-4.986382	0.147835	-1.115793	-0.047648
C	-1.923586	-0.607261	-0.373025	-0.182260
C	-3.019177	-1.530489	-0.334188	-0.147524
C	-3.289415	-2.332058	-1.601305	-0.460707
C	-0.949876	-0.438160	0.628370	0.403758
C	-1.083692	-1.248017	1.917061	-0.375876
C	-0.723678	-2.745669	1.807175	-0.466500
N	0.127130	0.376240	0.492870	-0.514038
C	1.172046	0.538015	1.535985	-0.067863
C	1.926267	1.783118	1.102854	0.621397
N	1.499250	2.129505	-0.138508	-0.456514
C	0.367591	1.348743	-0.655744	0.358707
C	2.196856	-0.617738	1.738956	-0.382588
C	3.036592	-0.996195	0.534120	0.151922
C	4.205770	-0.280985	0.228806	-0.188496
C	4.985905	-0.627456	-0.874905	-0.132913
C	4.617181	-1.699852	-1.689645	-0.128103
C	3.464777	-2.427707	-1.389882	-0.128971
C	2.683685	-2.076790	-0.286796	-0.201805
C	0.770178	0.616617	-1.946625	-0.469250
C	-0.808605	2.319388	-0.864619	-0.462000
C	2.129682	3.219787	-0.870732	-0.344362
O	2.802635	2.320773	1.757780	-0.511486
H	-3.692818	0.044007	1.888199	0.187868
H	-5.387829	0.463361	1.699912	0.225345
H	-5.298972	-1.547850	0.199017	0.192145
H	-3.737764	2.484332	0.877470	0.192451
H	-5.406200	-0.217994	-2.046975	0.195065
H	-4.553596	2.268343	-1.635028	0.186180
H	-3.072738	-2.150282	0.557424	0.179421
H	-2.519232	-3.105476	-1.706251	0.188324
H	-4.260842	-2.835580	-1.573721	0.171574
H	-3.246839	-1.702723	-2.495490	0.167510
H	-1.774260	-0.117109	-1.324035	0.143971
H	-0.496834	-0.800859	2.718884	0.185556
H	-2.124595	-1.176458	2.247935	0.173191
H	-1.345876	-3.267798	1.076078	0.165377
H	-0.873502	-3.223370	2.780475	0.185018
H	0.317169	-2.899783	1.518294	0.190223
H	1.442330	4.056530	-1.030945	0.175020
H	2.515053	2.876148	-1.835255	0.181111
H	2.961559	3.564108	-0.254699	0.223111
H	-0.027995	-0.028536	-2.319055	0.162258
H	0.989060	1.349491	-2.729056	0.171970
H	-1.083110	2.790424	0.084418	0.162945
H	-1.690333	1.851058	-1.295656	0.163216
H	-0.491077	3.105773	-1.554288	0.180459
H	0.701806	0.751564	2.500741	0.194021
H	1.682102	-1.495141	2.134942	0.163213
H	2.847985	-0.250471	2.540175	0.203466
H	1.658587	0.005715	-1.776810	0.207803
H	4.506620	0.547690	0.863436	0.169199
H	5.891118	-0.066420	-1.089661	0.152656
H	5.230985	-1.975315	-2.542455	0.151533
H	3.178813	-3.275399	-2.006618	0.144188
H	1.796314	-2.663041	-0.061310	0.123420

TS13 (Z)-a2-endo

B3LYP/6-31G(d) energy= -1118.883369

Zero-point correction (ZPC)= 0.526477
HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5167980000
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -
1111.5852280000

Number of Imaginary Frequencies=1

C	3.309185	1.743594	-1.360780	-0.330167
C	2.199985	2.237043	-0.489725	-0.097770
C	2.630920	2.277102	0.818211	-0.103033
C	3.894628	1.645323	0.898802	-0.074815
C	4.228000	1.076646	-0.348033	-0.176700
C	2.072299	-0.710164	-0.471936	-0.187458
C	3.482777	-0.772387	-0.269198	-0.145975
C	4.306719	-1.441133	-1.362223	-0.465303
C	1.087941	-0.824457	0.529317	0.414772
C	1.522801	-0.843101	1.984147	-0.373530
C	1.792763	-2.278244	2.489174	-0.459141
N	-0.221179	-1.024491	0.262863	-0.513136
C	-1.267470	-1.024722	1.313930	-0.063102
C	-2.457857	-1.680937	0.632269	0.621828
N	-2.149476	-1.872588	-0.677092	-0.457876
C	-0.791198	-1.474443	-1.072058	0.355724
C	-1.696965	0.349137	1.906775	-0.381019
C	-2.172718	1.401183	0.925568	0.157160
C	-3.446521	1.330696	0.339760	-0.194334
C	-3.872231	2.314329	-0.554665	-0.133058
C	-3.041005	3.391749	-0.868922	-0.127776
C	-1.782115	3.486681	-0.273137	-0.137270
C	-1.356256	2.497091	0.615521	-0.195837
C	-0.856114	-0.328918	-2.097073	-0.467936
C	-0.060152	-2.719047	-1.610603	-0.460231
C	-3.127571	-2.422043	-1.606848	-0.345609
O	-3.513459	-1.937895	1.185364	-0.511523
H	1.250795	2.609109	-0.858294	0.192450
H	2.087242	2.698282	1.656167	0.180571
H	4.487634	1.549634	1.803101	0.188415
H	5.260657	0.847661	-0.592317	0.186492
H	3.843182	2.621446	-1.763048	0.224446
H	3.003649	1.145784	-2.221043	0.181457
H	1.751258	-0.684369	-1.503062	0.145024
H	4.062108	-1.054485	-2.357070	0.170010
H	5.381031	-1.324239	-1.198092	0.179728
H	4.090217	-2.516444	-1.363079	0.191241
H	3.818355	-1.047835	0.726303	0.178766
H	2.589042	-2.762476	1.915928	0.168533
H	0.901747	-2.909637	2.415018	0.176250
H	2.096959	-2.248750	3.539710	0.188149
H	2.429177	-0.243288	2.092440	0.168122
H	0.777158	-0.368975	2.621713	0.186349
H	-0.596595	-3.094366	-2.486120	0.182367
H	-0.047931	-3.506872	-0.851781	0.175324
H	0.963222	-2.516297	-1.924433	0.166071
H	0.136179	0.013325	-2.397874	0.157206
H	-1.362361	-0.677991	-3.002072	0.176626
H	-1.412543	0.517790	-1.689672	0.201215
H	-2.795718	-3.377187	-2.025106	0.180134
H	-3.336741	-1.721824	-2.421319	0.178819
H	-4.041247	-2.586701	-1.033913	0.223784
H	-0.962702	-1.669503	2.143390	0.196563
H	-1.143506	4.340960	-0.483167	0.140779
H	-0.387328	2.589376	1.101439	0.115037
H	-0.880647	0.760195	2.508662	0.158914
H	-2.502950	0.092810	2.604383	0.209455
H	-3.380532	4.162312	-1.554933	0.154543
H	-4.864236	2.247816	-0.992531	0.156276

H -4.111392 0.511575 0.597720 0.173859

TS13 (Z)-a2-exo

B3LYP/6-31G(d) energy= -1118.882117

Zero-point correction (ZPC)= 0.526916

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5224980000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -
1111.5836240000

Number of Imaginary Frequencies=1

C	2.929437	2.138194	-1.466851	-0.106869
C	2.174826	2.270694	-0.324481	-0.093693
C	2.998193	1.884950	0.861305	-0.341084
C	4.139137	1.111558	0.220652	-0.197994
C	4.156604	1.514527	-1.129523	-0.050951
C	2.065264	-0.739509	-0.224616	-0.179255
C	3.444087	-0.770511	0.134630	-0.142939
C	4.416524	-1.467276	-0.802034	-0.462394
C	0.982685	-0.933003	0.654401	0.402879
C	1.252660	-1.130714	2.138990	-0.374299
C	1.463004	-2.620947	2.488000	-0.457328
N	-0.295176	-1.086331	0.237723	-0.512924
C	-1.444909	-1.189221	1.170453	-0.060116
C	-2.574732	-1.699179	0.288549	0.621854
N	-2.130713	-1.748203	-0.994032	-0.458461
C	-0.728113	-1.360241	-1.192834	0.355157
C	-1.906253	0.101158	1.911167	-0.387145
C	-2.195731	1.319854	1.060159	0.162954
C	-3.363211	1.409279	0.285699	-0.196100
C	-3.624193	2.548023	-0.478775	-0.132446
C	-2.733526	3.623581	-0.470804	-0.128256
C	-1.582742	3.558107	0.316832	-0.136178
C	-1.318864	2.413418	1.072866	-0.197185
C	-0.652430	-0.099900	-2.071814	-0.470729
C	0.023087	-2.563679	-1.794726	-0.459616
C	-3.015754	-2.147152	-2.080605	-0.345598
O	-3.693607	-1.969513	0.690446	-0.512244
H	1.170892	2.675709	-0.266540	0.193112
H	3.662214	-0.975797	1.180519	0.180580
H	4.315457	-2.552560	-0.676257	0.187513
H	5.457116	-1.208483	-0.583354	0.174715
H	5.063147	0.918887	0.759372	0.187772
H	4.958636	1.307583	-1.830120	0.191066
H	2.633940	2.440412	-2.465106	0.181685
H	2.451806	1.388485	1.663869	0.182259
H	1.862486	-0.672128	-1.282556	0.147769
H	4.210821	-1.235081	-1.851172	0.167905
H	3.429570	2.802752	1.296315	0.222225
H	-2.814183	-0.215076	2.438291	0.212070
H	-1.176451	0.367467	2.681099	0.163179
H	-0.438755	2.382951	1.713109	0.118550
H	-0.905622	4.407486	0.362162	0.142235
H	-2.947126	4.514764	-1.053751	0.154660
H	-4.079764	0.593001	0.298505	0.172849
H	-4.536874	2.602575	-1.065510	0.156611
H	-1.246248	-1.955253	1.926422	0.197399
H	-3.080084	-1.367347	-2.845379	0.177701
H	-2.690740	-3.083711	-2.544260	0.181053
H	-4.001632	-2.297263	-1.638234	0.223558
H	-0.439838	-2.827752	-2.749269	0.181985
H	1.075398	-2.364560	-1.993925	0.166831
H	-0.052654	-3.426719	-1.126875	0.175318
H	0.368277	0.272172	-2.173707	0.160846
H	-1.273135	0.693306	-1.648931	0.197359
H	-1.017404	-0.331856	-3.076821	0.174443

H 2.317347 -3.038387 1.946873 0.167780
H 2.143628 -0.571338 2.429868 0.168684
H 0.442365 -0.726963 2.743567 0.186572
H 0.585084 -3.226554 2.241942 0.175705
H 1.652104 -2.724938 3.560629 0.189063

TS13 (Z)-b2-endo

B3LYP/6-31G(d) energy= -1118.881591

Zero-point correction (ZPC)= 0.526317

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5216980000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -
1111.5817330000

Number of Imaginary Frequencies=1

C 0.012273 3.575211 0.763719 -0.196019
C -0.123113 2.793353 -0.395108 0.165720
C 0.899552 2.836025 -1.350224 -0.197284
C 2.034978 3.627965 -1.152629 -0.140535
C 2.168044 4.380887 0.014862 -0.130955
C 1.150795 4.353153 0.972815 -0.124841
C -1.387817 1.999266 -0.645977 -0.368393
C -1.769842 0.876564 0.364610 -0.074330
N -1.152740 -0.455868 0.146942 -0.512289
C -2.150377 -1.403534 -0.495270 0.351688
N -3.399184 -0.646255 -0.333116 -0.458146
C -3.258813 0.601578 0.191846 0.606319
C 0.069490 -0.803606 0.612815 0.414207
C 0.697251 0.079402 1.672649 -0.381603
C 0.137157 -0.216339 3.081351 -0.460560
C -1.851752 -1.621035 -1.990022 -0.455518
C -2.288020 -2.726772 0.279613 -0.463951
C -4.713028 -1.170201 -0.683887 -0.345146
O -4.144356 1.401942 0.430088 -0.496204
C 0.719016 -1.993386 0.232617 -0.189128
C 1.833720 -2.586814 0.894873 -0.143475
C 1.892430 -4.108284 0.917407 -0.466328
C 3.499640 -2.191055 -0.147213 -0.176714
C 3.802386 -0.856332 0.187248 -0.078434
C 3.170376 0.027365 -0.721144 -0.093860
C 2.574061 -0.718313 -1.712327 -0.104544
C 2.981881 -2.149852 -1.576830 -0.327376
H -1.600855 1.216824 1.387517 0.196105
H -1.368820 1.569621 -1.653578 0.157472
H -2.241825 2.687515 -0.616486 0.218573
H 0.792048 2.270386 -2.273698 0.128058
H 2.805172 3.669058 -1.918533 0.149890
H 3.045972 5.001490 0.168639 0.156605
H -0.789869 3.593409 1.499171 0.149305
H 1.234258 4.955534 1.872918 0.157621
H -1.422064 -3.379634 0.183457 0.166972
H -3.147753 -3.274609 -0.115040 0.184047
H -2.465918 -2.526812 1.340190 0.177346
H -0.898507 -2.130543 -2.149783 0.162613
H -2.632111 -2.241847 -2.440284 0.181318
H -1.829183 -0.664051 -2.518185 0.175959
H -5.032732 -1.961352 0.001953 0.182315
H -4.723745 -1.553892 -1.708512 0.174773
H -5.412042 -0.336077 -0.606300 0.225106
H 0.621019 0.437029 3.813617 0.185715
H 1.776649 -0.081390 1.673975 0.164612
H 0.559483 1.132663 1.427279 0.205316
H 0.320744 -1.254024 3.377688 0.165199
H -0.942286 -0.042773 3.139279 0.173270
H 2.120873 -2.146616 1.845309 0.180481
H 4.125666 -3.006700 0.200670 0.185396

H 4.374865 -0.549869 1.057351 0.187531
H 2.221926 -2.885044 -1.848092 0.178997
H 3.841568 -2.328012 -2.244985 0.223059
H 0.284037 -2.579120 -0.565068 0.142795
H 3.129934 1.106005 -0.628189 0.189883
H 1.996004 -0.325075 -2.541003 0.181109
H 1.750578 -4.540253 -0.078831 0.169508
H 1.087089 -4.485606 1.559662 0.190726
H 2.836410 -4.478389 1.325647 0.179871

TS13 (Z)-b2-exo

B3LYP/6-31G(d) energy= -1118.880178

Zero-point correction (ZPC)= 0.52615

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5212650000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -
1111.5815470000

Number of Imaginary Frequencies=1

C 0.108589 2.750467 -1.312006 -0.197959
C -0.988600 2.628224 -0.450299 0.166452
C -1.129898 3.563223 0.587625 -0.196172
C -0.184743 4.572313 0.773730 -0.123796
C 0.912687 4.674137 -0.085401 -0.130203
C 1.053067 3.765095 -1.134816 -0.137118
C -2.026744 1.550236 -0.664811 -0.369101
C -2.076046 0.366935 0.349283 -0.078180
N -1.021090 -0.667138 0.214915 -0.509335
C -1.573729 -1.900018 -0.477440 0.352616
N -3.015293 -1.617673 -0.444846 -0.458796
C -3.359370 -0.402883 0.064660 0.611205
C 0.211757 -0.560370 0.767668 0.403794
C 0.395910 0.491050 1.848809 -0.381458
C -0.128400 0.000426 3.216267 -0.458761
C -1.082482 -2.000112 -1.933196 -0.458144
C -1.322038 -3.189889 0.325474 -0.463121
C -4.032189 -2.555704 -0.902324 -0.344737
O -4.483126 0.041508 0.209738 -0.496769
C 1.255913 -1.456547 0.476761 -0.180118
C 2.477579 -1.574539 1.201534 -0.142975
C 3.010572 -2.968160 1.489620 -0.462073
C 3.959560 -0.718827 0.156687 -0.199249
C 3.335967 0.549635 -0.400773 -0.341984
C 2.774778 0.079498 -1.701360 -0.090431
C 3.332449 -1.131671 -2.035500 -0.104594
C 4.121602 -1.580223 -0.946043 -0.051248
H 2.106603 0.666841 -2.319313 0.182942
H 1.092954 -2.205158 -0.284830 0.144513
H 3.189462 -1.666623 -2.967449 0.180895
H 4.159696 1.252326 -0.614647 0.220473
H 4.705402 -2.494563 -0.941226 0.190730
H 2.631588 1.087460 0.233969 0.198367
H 4.701051 -0.680733 0.950249 0.188309
H 2.592299 -0.906518 2.052741 0.183209
H 4.059120 -2.953571 1.802626 0.174650
H 2.911703 -3.631699 0.625424 0.167140
H 2.429982 -3.405599 2.311533 0.187699
H 0.025397 0.778484 3.970076 0.186549
H 0.397666 -0.901684 3.544083 0.163804
H -1.198022 -0.231169 3.186773 0.173167
H 1.454319 0.737428 1.944205 0.163708
H -0.092533 1.423778 1.570751 0.206849
H -1.912416 -3.996683 -0.116867 0.183351
H -0.283013 -3.514796 0.317390 0.166522
H -1.644972 -3.058614 1.362231 0.177563
H 0.003130 -2.106293 -1.992700 0.164332

H	-1.527293	-2.873134	-2.420242	0.179634
H	-1.374207	-1.108518	-2.494923	0.174366
H	-4.123900	-3.417166	-0.232959	0.181971
H	-3.816505	-2.906679	-1.916032	0.174239
H	-4.978661	-2.012882	-0.904640	0.224753
H	-2.118943	0.748550	1.370635	0.195974
H	0.199899	2.066913	-2.153727	0.125522
H	1.884154	3.860014	-1.828931	0.142500
H	1.639530	5.469732	0.049936	0.155721
H	-0.315487	5.291841	1.576952	0.158581
H	-1.996405	3.512293	1.244176	0.149905
H	-3.028877	1.991448	-0.605028	0.214046
H	-1.930176	1.132816	-1.673510	0.160311

TS13 (Z)-c2-endo

B3LYP/6-31G(d) energy= -1118.882772

Zero-point correction (ZPC)= 0.526119

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5239650000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5855110000

Number of Imaginary Frequencies=1

C	-2.841375	-3.008324	-0.368268	-0.074653
C	-3.917651	-2.097558	-0.272428	-0.177333
C	-3.892328	-1.301993	-1.570635	-0.328691
C	-2.484054	-1.503866	-2.027299	-0.097650
C	-1.943403	-2.592677	-1.378889	-0.098306
C	-2.417996	0.126601	0.475186	-0.188674
C	-3.361508	-0.767419	1.068154	-0.148357
C	-1.020049	0.070289	0.625419	0.408175
C	-0.399070	-1.101048	1.364944	-0.377533
C	-0.227402	-0.802112	2.871166	-0.456819
C	-4.709356	-0.173946	0.460572	-0.465133
N	-0.186718	1.054585	1.224030	-0.513137
C	1.283969	0.878365	0.194470	-0.069327
C	1.800404	2.292803	-0.016587	0.606710
N	0.732978	3.105126	-0.252444	-0.460820
C	-0.578613	2.445888	-0.218178	0.354019
C	1.791127	-0.079644	-0.935157	-0.370250
C	2.902594	-1.015036	-0.496228	0.151576
C	2.764616	-2.399618	-0.659699	-0.196802
C	3.783660	-3.271958	-0.271564	-0.127005
C	4.955492	-2.766049	0.290642	-0.125591
C	5.103192	-1.386825	0.456934	-0.130170
C	4.087482	-0.514719	0.065297	-0.195550
C	-1.463601	3.150749	0.824525	-0.462791
C	-1.194237	2.446105	-1.630306	-0.454654
C	0.912711	4.524146	-0.530967	-0.345542
O	2.974862	2.618793	-0.010788	-0.494171
H	-2.843498	0.963366	-0.060335	0.143169
H	-2.975141	-1.441353	1.827568	0.181589
H	-4.859164	-2.412690	0.167558	0.188702
H	-4.559154	-1.813640	-2.285548	0.225380
H	-0.982140	-3.046928	-1.590366	0.185255
H	-2.020150	-0.951521	-2.837067	0.188661
H	-5.160811	0.398417	0.643393	0.169282
H	-5.419309	-0.940776	1.781187	0.179511
H	-4.563525	0.512084	2.303594	0.192141
H	-4.228528	-0.264994	-1.520609	0.181888
H	-2.692036	-3.862525	0.284863	0.190920
H	-1.352327	3.475236	-1.965513	0.183249
H	-2.162492	1.942704	-1.664377	0.160586
H	-0.517724	1.956040	-2.336647	0.173408
H	0.493534	5.147499	0.265040	0.182152
H	0.457871	4.802971	-1.486395	0.175576

H	1.988657	4.696341	-0.584805	0.226191
H	-2.443612	2.687357	0.935687	0.167317
H	-0.964380	3.154534	1.797640	0.179938
H	-1.627112	4.187055	0.516226	0.183160
H	1.642426	0.527160	1.164949	0.208058
H	0.940571	-0.666484	-1.299090	0.144677
H	2.128808	0.531815	-1.781027	0.193504
H	4.211627	0.558352	0.185387	0.182121
H	6.016668	-0.986152	0.887293	0.153499
H	5.750981	-3.440929	0.593099	0.151418
H	3.662284	-4.342518	-0.411732	0.143238
H	1.858433	-2.801283	-1.110970	0.109357
H	0.215264	-1.669141	3.370087	0.189322
H	-1.187433	-0.582995	3.348724	0.165476
H	-1.036832	-1.979278	1.243064	0.163108
H	0.566459	-1.374117	0.936423	0.201290
H	0.431455	0.055145	3.041273	0.175193

TS13 (Z)-c2-exo

B3LYP/6-31G(d) energy= -1118.881124

Zero-point correction (ZPC)= 0.526369

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1111.5222230000

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1111.5836610000

Number of Imaginary Frequencies=1

C	-2.604461	-2.577888	-0.965696	-0.338451
C	-2.588661	-1.518611	-2.017565	-0.093358
C	-3.832451	-0.935046	-2.099631	-0.102673
C	-4.632883	-1.425484	-1.039076	-0.050167
C	-3.855257	-2.226144	-0.175829	-0.197713
C	-3.202274	-0.959875	1.210620	-0.146282
C	-4.481544	-0.418452	1.828032	-0.461589
C	-2.301784	-0.029192	0.612165	-0.179140
C	-0.898987	-0.050914	0.707769	0.393377
C	-0.199449	-1.190478	1.433530	-0.378515
C	0.060606	-0.846639	2.917271	-0.455728
N	-0.111171	0.962100	0.280703	-0.509634
C	1.361472	0.828153	0.186068	-0.068310
C	1.829063	2.256324	-0.042892	0.606051
N	0.730527	3.040604	-0.222761	-0.460249
C	-0.559563	2.344969	-0.135533	0.353484
C	1.846644	-0.112808	-0.968306	-0.367857
C	2.993901	-1.025282	-0.576512	0.150456
C	4.192897	-0.498696	-0.071737	-0.195282
C	5.241295	-1.348910	0.279625	-0.130374
C	5.111914	-2.731834	0.129046	-0.125608
C	3.925888	-3.263403	-0.376835	-0.126909
C	2.873956	-2.413288	-0.725086	-0.194168
C	-1.235929	2.335287	-1.519179	-0.456631
C	-1.415662	3.021686	0.949531	-0.462436
C	0.860045	4.462934	-0.511915	-0.345742
O	2.993636	2.612885	-0.092191	-0.494569
H	-2.767903	0.818204	0.130573	0.144953
H	-1.752847	-1.331376	-2.682586	0.188524
H	-4.150287	-0.212011	-2.842176	0.183258
H	-5.671645	-1.159695	-0.874191	0.192481
H	-5.214959	-1.207826	2.019421	0.174943
H	-4.241488	0.046210	2.792362	0.189021
H	-4.946408	0.346342	1.198793	0.167230
H	-4.324291	-2.953272	0.481889	0.190425
H	-2.747693	-1.738147	1.820819	0.183477
H	-2.789535	-3.548465	-1.457044	0.225031
H	-1.677592	-2.688613	-0.402605	0.186360
H	-1.609283	4.057783	0.658640	0.182595

H	-2.382726	2.540963	1.094611	0.167040
H	-0.878530	3.025497	1.902226	0.179749
H	-1.461414	3.360241	-1.827821	0.181200
H	-0.565448	1.893254	-2.262161	0.172460
H	-2.174691	1.778341	-1.521990	0.163541
H	0.370450	4.724725	-1.455197	0.175541
H	0.446058	5.077401	0.293542	0.181676
H	1.928563	4.665844	-0.597596	0.226186
H	1.774285	0.485718	1.137520	0.208288
H	2.139054	0.510824	-1.821985	0.193740
H	1.956268	-2.834855	-1.132214	0.110058
H	3.818387	-4.337006	-0.504287	0.143811
H	5.932597	-3.389691	0.400128	0.151131
H	6.165397	-0.928409	0.666191	0.153132
H	4.301519	0.577340	0.036598	0.181285
H	0.996256	-0.716442	-1.304251	0.143096
H	0.694802	0.038271	3.028117	0.175154
H	-0.876425	-0.654528	3.449146	0.164680
H	0.567083	-1.684922	3.404478	0.190760
H	0.741534	-1.452965	0.946970	0.203181
H	-0.816330	-2.089213	1.388816	0.163974

TS14 (E)-b1a-endo

B3LYP/6-31G(d) energy= -1308.4124887000
 Zero-point correction (ZPC)= 0.548544
 HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.977972
 CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1300.038286
 Number of Imaginary Frequencies=1

C	0.074059	2.924251	-0.310522	-0.184886
C	0.294649	2.477334	0.999449	0.161010
C	1.406577	2.970092	1.698955	-0.196592
C	2.280904	3.879531	1.101504	-0.130486
C	2.051843	4.315496	-0.206018	-0.132977
C	0.944995	3.836371	-0.910461	-0.135866
C	-0.665200	1.515531	1.662643	-0.375016
C	-0.293695	0.006934	1.625389	-0.074555
C	-1.296532	-0.746538	2.502250	0.609316
N	-2.053113	-1.531101	1.682056	-0.437018
C	-1.684337	-1.471232	0.275488	0.039324
N	-0.420959	-0.668000	0.318529	-0.470990
C	-2.749761	-0.920322	-0.615046	0.385859
C	-3.516074	-1.493425	-1.586989	-0.203716
C	-4.428789	-0.483561	-2.030091	-0.215665
C	-4.163850	0.638157	-1.298475	0.362804
O	-3.134727	0.381221	-0.425133	-0.484781
C	-4.745678	2.006757	-1.264837	-0.535218
C	-3.173349	-2.330870	2.147955	-0.337228
O	-1.407678	-0.620528	3.706331	-0.492984
C	0.582797	-0.803116	-0.575879	0.405480
C	0.326178	-1.559636	-1.861916	-0.356848
C	-0.097150	-0.629480	-3.019915	-0.454858
C	1.831086	-0.188427	-0.372493	-0.179737
C	2.948937	-2.505339	1.079406	-0.100519
C	4.074452	-1.558835	0.813668	-0.325927
C	4.180203	-1.620645	-0.704183	-0.177095
C	2.931523	-0.221463	-1.282243	-0.154293
C	3.578257	-2.846327	-1.073299	-0.075003
C	2.771948	-3.324717	-0.016120	-0.099083
C	3.842442	0.999026	-1.298166	-0.462780
H	3.973076	-0.568576	1.260091	0.186067
H	2.722031	-0.590195	-2.282379	0.175084
H	5.078784	-1.281615	-1.211365	0.186224
H	3.665768	-3.310755	-2.050601	0.185619

H	2.454670	-2.611747	2.039003	0.190280
H	4.996469	-2.001293	1.228084	0.221785
H	2.111684	-4.183100	-0.067262	0.175030
H	4.176062	1.274418	-0.292875	0.170985
H	3.281186	1.852161	-1.695049	0.196774
H	4.720496	0.846054	-1.931446	0.169481
H	1.949264	0.456035	0.488940	0.169443
H	1.243112	-2.090719	-2.135572	0.168285
H	-0.436929	-2.327958	-1.729322	0.168296
H	-0.231673	-1.217802	-3.932772	0.178026
H	-1.043451	-0.130735	-2.796214	0.185371
H	0.656929	0.138872	-3.212938	0.167938
H	-5.152132	2.242409	-0.274318	0.191734
H	-3.995739	2.769927	-1.505178	0.181904
H	-5.555649	2.082443	-1.994358	0.189172
H	-5.189048	-0.581390	-2.792159	0.168179
H	-3.449772	-2.513160	-1.942955	0.161014
H	-1.464269	-2.486318	-0.076182	0.175148
H	-3.231918	-2.200321	3.229540	0.221030
H	-3.017549	-3.391321	1.917165	0.169482
H	-4.109694	-1.999242	1.687735	0.187950
H	0.711968	-0.152603	2.025355	0.177411
H	-0.750425	1.751024	2.729709	0.201696
H	-1.664654	1.619947	1.229994	0.184553
H	-0.797811	2.568480	-0.854727	0.134405
H	0.748615	4.187603	-1.919985	0.146741
H	2.720456	5.038230	-0.665146	0.151898
H	3.126387	4.265752	1.664204	0.151475
H	1.572891	2.660353	2.728956	0.141814

TS14 (E)-b1a-exo

B3LYP/6-31G(d) energy= -1308.4111642000
 Zero-point correction (ZPC)= 0.548431
 HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.976625
 CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1300.034786
 Number of Imaginary Frequencies=1

C	4.638830	-1.279068	0.120171	-0.049513
C	4.085191	-1.671176	-1.118056	-0.196015
C	3.178817	-2.850258	-0.801391	-0.333392
C	2.923043	-2.661669	0.659244	-0.098751
C	3.875221	-1.815493	1.183612	-0.099253
C	2.809272	-0.223877	-1.577793	-0.152705
C	3.677939	1.020420	-1.643247	-0.458053
C	1.741257	-0.251414	-0.634934	-0.169220
C	0.464413	-0.801299	-0.847171	0.386300
C	0.075736	-1.327826	-2.216062	-0.355884
C	-0.402033	-0.199793	-3.156765	-0.453218
N	-0.475288	-0.768323	0.124952	-0.464879
C	-0.226835	-0.321671	1.510472	-0.077740
C	-1.193283	-1.182251	2.327909	0.608497
N	-2.045234	-1.788976	1.452748	-0.435702
C	-1.778660	-1.503588	0.050492	0.036891
C	-3.161486	-2.622220	1.866728	-0.337375
O	-1.206178	-1.261533	3.541172	-0.493968
C	-0.535106	1.169483	1.825433	-0.375173
C	0.403107	2.203648	1.245750	0.159067
C	0.104840	2.847318	0.036823	-0.184443
C	0.961951	3.817053	-0.486958	-0.134099
C	2.132718	4.158598	0.193769	-0.131111
C	2.438574	3.528090	1.402420	-0.133106
C	1.577892	2.560572	1.924346	-0.194322
C	-2.878915	-0.771057	-0.645305	0.386539
O	-3.187106	0.490818	-0.208238	-0.485182

C	-4.265785	0.927978	-0.938626	0.362592
C	-4.636665	-0.042042	-1.824635	-0.215182
C	-3.741958	-1.143068	-1.633792	-0.203498
C	-4.779275	2.288717	-0.626314	-0.535289
H	3.127266	1.807801	-2.171346	0.187141
H	3.912063	1.405282	-0.647087	0.174497
H	4.610766	0.842657	-2.187507	0.165028
H	5.474161	-0.597658	0.240305	0.189693
H	2.586066	-0.626770	-2.564421	0.174608
H	2.288924	-2.966902	-1.421124	0.176917
H	4.684705	-1.654984	-2.024619	0.186658
H	4.009305	-1.580684	2.233389	0.183938
H	3.776401	-3.768668	-0.930301	0.220751
H	2.181520	-3.213140	1.226919	0.186808
H	1.909160	0.297129	0.282267	0.173054
H	-0.701682	-2.090237	-2.147605	0.169934
H	0.939629	-1.822107	-2.667807	0.170682
H	-0.662817	-0.621914	-4.132126	0.179092
H	-1.286815	0.301609	-2.757084	0.185110
H	0.381328	0.549430	-3.303811	0.167008
H	0.798565	-0.574150	1.795874	0.179133
H	-1.561754	1.369251	1.504749	0.185166
H	-0.522894	1.226060	2.919894	0.200556
H	3.334224	3.807049	1.950888	0.150144
H	2.792362	4.924352	-0.204486	0.151496
H	0.707036	4.318697	-1.416664	0.146477
H	-0.815011	2.596794	-0.486576	0.134898
H	1.807167	2.096137	2.881516	0.140252
H	-1.638033	-2.451360	-0.481787	0.176638
H	-5.103117	2.361991	0.418555	0.191602
H	-4.013220	3.056072	-0.790161	0.182069
H	-5.634626	2.517462	-1.266642	0.189206
H	-3.750205	-2.088057	-2.160919	0.161786
H	-5.455562	0.017762	-2.527558	0.168295
H	-4.113821	-2.189496	1.543833	0.187997
H	-3.068816	-3.632608	1.451202	0.170070
H	-3.135154	-2.674645	2.956163	0.220764

TS14 (E)-b2 α -endo

B3LYP/6-31G(d) energy= -1308.4115486000

Zero-point correction (ZPC)= 0.548794

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.976908

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ϵ =78.39) energy= -1300.030494

Number of Imaginary Frequencies=1

C	3.281443	1.509650	0.757599	-0.335590
C	1.972449	1.745424	1.435676	-0.086513
C	1.468541	2.968596	1.055330	-0.099952
C	2.275504	3.484073	0.012363	-0.077316
C	3.234505	2.524397	-0.374229	-0.178282
C	2.352089	1.496295	-1.834827	-0.147428
C	3.569432	0.894263	-2.524627	-0.465268
C	1.424332	0.576532	-1.262766	-0.194626
C	0.033612	0.753954	-1.195135	0.402347
C	-0.590904	2.085147	-1.563642	-0.383923
C	-0.976192	2.177000	-3.056606	-0.458323
N	-0.780809	-0.277437	-0.883207	-0.468723
C	-0.391666	-1.705559	-0.878244	-0.080306
C	-1.661627	-2.390969	-1.410237	0.605481
N	-2.672428	-1.472366	-1.388477	-0.442337
C	-2.275785	-0.179660	-0.869566	0.045850
C	-0.016845	-2.351734	0.482467	-0.370888
C	1.420085	-2.239079	0.951681	0.168901
C	2.480334	-2.702466	0.156751	-0.201207

C	3.795431	-2.666168	0.624907	-0.134037
C	4.072069	-2.179838	1.905735	-0.136974
C	3.024279	-1.733178	2.712979	-0.133495
C	1.710990	-1.760010	2.235742	-0.203666
O	-1.734897	-3.553980	-1.753118	-0.488087
C	-4.031616	-1.762257	-1.819416	-0.337790
C	-2.853653	0.098551	0.487037	0.382681
C	-3.353789	-0.683092	1.486384	-0.208684
C	-3.770419	0.210790	2.525106	-0.216114
C	-3.503124	1.477252	2.093991	0.360460
O	-2.939227	1.421121	0.841334	-0.488332
C	-3.709930	2.829804	2.677936	-0.532326
H	4.137733	2.828627	-0.894174	0.183268
H	1.930538	2.330349	-2.389323	0.175222
H	1.828429	-0.377110	-0.943328	0.170246
H	0.585435	3.448178	1.461635	0.173098
H	2.133558	4.447468	-0.467991	0.184492
H	3.488696	0.471592	0.494758	0.202889
H	1.556510	1.084663	2.186090	0.182589
H	4.083666	1.822561	1.448050	0.216512
H	4.068058	0.150975	-1.894503	0.174370
H	3.243567	0.386033	-3.440185	0.189710
H	4.298247	1.656112	-2.813448	0.174985
H	-3.434896	-1.761403	1.482998	0.171037
H	-4.227045	-0.056997	3.467643	0.167819
H	-4.167984	2.739658	3.665923	0.190334
H	-4.369176	3.440504	2.049717	0.189378
H	-2.763007	3.372265	2.789370	0.169280
H	-2.589817	0.611615	-1.554754	0.188476
H	-4.742572	-1.606107	-1.002642	0.183973
H	-4.053289	-2.808213	-2.129260	0.221490
H	-4.312940	-1.126500	-2.666898	0.176049
H	0.405941	-1.859500	-1.609694	0.194478
H	-0.102109	2.044940	-3.701537	0.170536
H	-1.410939	3.158827	-3.266918	0.184601
H	-1.709551	1.416616	-3.344411	0.170855
H	-1.458867	2.283880	-0.930353	0.199491
H	0.897234	-1.432915	2.879924	0.138743
H	0.126269	2.877006	-1.335068	0.168079
H	5.092450	-2.170209	2.277989	0.155408
H	3.225675	-1.378028	3.720107	0.151572
H	2.277331	-3.125660	-0.825209	0.148716
H	4.600309	-3.042709	-0.000378	0.155571
H	-0.694532	-1.965017	1.249904	0.166354
H	-0.254537	-3.416324	0.357701	0.214440

TS14 (E)-b2 α -exo

B3LYP/6-31G(d) energy= -1308.4067458000

Zero-point correction (ZPC)= 0.548663

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.97196

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ϵ =78.39) energy= -1300.025784

Number of Imaginary Frequencies=1

C	2.248877	2.182041	2.161573	-0.339218
C	2.245502	0.690278	2.237511	-0.097299
C	3.394107	0.196646	1.670163	-0.085313
C	4.100708	1.272735	1.074659	-0.054791
C	3.331588	2.447954	1.129382	-0.198544
C	2.343050	2.405742	-0.638263	-0.143556
C	1.381339	1.355253	-0.641024	-0.185528
C	-0.000895	1.537371	-0.481821	0.394340
C	-0.575623	2.890707	-0.098255	-0.377876
C	-0.905598	3.775799	-1.320720	-0.458351
C	3.461656	2.350692	-1.663800	-0.463851

N	-0.874950	0.546736	-0.768216	-0.472980
C	-2.360359	0.733219	-0.716727	0.037550
N	-2.815324	-0.157907	-1.769758	-0.431139
C	-1.852031	-0.987937	-2.259699	0.599722
C	-0.548554	-0.701558	-1.498565	-0.068904
C	-2.973577	0.469638	0.621428	0.385760
C	-3.784054	1.224366	1.418731	-0.204118
C	-4.117233	0.407432	2.545932	-0.216468
C	-3.494357	-0.793028	2.361365	0.360883
O	-2.789742	-0.766313	1.182502	-0.480720
C	-3.444340	-2.057443	3.143380	-0.533051
C	-0.198911	-1.960253	-0.658140	-0.378657
C	1.257574	-2.307373	-0.411409	0.168069
C	1.631427	-2.848151	0.826843	-0.193212
C	2.925303	-3.327051	1.043615	-0.142754
C	3.879860	-3.250755	0.026653	-0.136880
C	3.523548	-2.706131	-1.209133	-0.131659
C	2.221513	-2.251087	-1.429050	-0.197899
O	-1.983823	-1.839983	-3.116219	-0.490083
C	-4.204939	-0.205356	-2.192283	-0.337456
H	1.737929	0.370212	-0.922008	0.170095
H	2.607886	2.582517	3.124838	0.219611
H	1.272775	2.635395	1.987117	0.181077
H	1.484985	0.106903	2.743840	0.180001
H	3.696531	-0.842250	1.641529	0.188469
H	5.060513	1.179706	0.577766	0.187325
H	3.786987	3.429020	1.025625	0.183688
H	3.062320	2.651261	-2.640651	0.185795
H	1.952216	3.412021	-0.499879	0.177350
H	3.864966	1.339489	-1.769228	0.174085
H	4.280641	3.034604	-1.420533	0.171560
H	-1.331804	4.726260	-0.985621	0.185518
H	-0.004030	3.991755	-1.901602	0.171414
H	-1.623434	3.305505	-2.000050	0.173958
H	0.145250	3.424222	0.523284	0.171295
H	-1.459053	2.755238	0.530713	0.183699
H	-0.742336	-1.905098	0.289222	0.178178
H	-0.636067	-2.798981	-1.215878	0.219091
H	0.232334	-0.485510	-2.232437	0.191975
H	4.251004	-2.663568	-2.015137	0.152044
H	1.951060	-1.886830	-2.417811	0.145084
H	4.884925	-3.629824	0.188291	0.154101
H	3.183620	-3.768328	2.002717	0.151564
H	0.890457	-2.926784	1.619614	0.132349
H	-4.521100	0.762377	-2.598592	0.172319
H	-4.858954	-0.473503	-1.356115	0.185582
H	-4.277488	-0.966141	-2.970796	0.221578
H	-2.615315	1.761813	-0.984188	0.178245
H	-4.120419	2.234304	1.223701	0.162564
H	-4.748063	0.675488	3.381710	0.167613
H	-2.417972	-2.310446	3.435552	0.174533
H	-4.042568	-1.954905	4.051991	0.189207
H	-3.840863	-2.899855	2.564513	0.192697

TS14 (E)-b2δ-endo

B3LYP/6-31G(d) energy= -1308.4104266000

Zero-point correction (ZPC)= 0.548962

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.97614

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy= -1300.02956

Number of Imaginary Frequencies=1

C	-3.957375	-1.900867	0.376029	-0.055133
C	-3.066303	-2.902697	-0.045811	-0.198131
C	-1.996585	-2.980080	1.030472	-0.339525

C	-2.149960	-1.664849	1.721961	-0.097376
C	-3.356733	-1.103890	1.383969	-0.086354
C	-2.128934	-2.023390	-1.609491	-0.142925
C	-3.268903	-1.663776	-2.546397	-0.463502
C	-1.284942	-0.973316	-1.148581	-0.186583
C	0.112160	-1.057641	-1.040126	0.390570
C	0.837727	-2.380326	-1.224857	-0.387718
C	1.284932	-2.625347	-2.683285	-0.457527
N	0.863035	0.053559	-0.872633	-0.465238
C	0.399492	1.444342	-1.077530	-0.078044
C	1.631543	2.105106	-1.719284	0.599642
N	2.693439	1.263751	-1.545143	-0.441245
C	2.362507	0.045148	-0.836809	0.046052
C	0.004365	2.261922	0.182763	-0.372705
C	-1.452786	2.293607	0.603723	0.168344
C	-1.787198	2.176206	1.959485	-0.193684
C	-3.103016	2.355043	2.393387	-0.141820
C	-4.113433	2.633226	1.470150	-0.138345
C	-3.795224	2.740423	0.113875	-0.130822
C	-2.475246	2.583033	-0.312698	-0.197078
O	1.641332	3.198056	-2.249080	-0.487236
C	4.037833	1.555263	-2.019147	-0.337851
C	2.935415	0.005095	0.548894	0.382804
O	3.079406	-1.244492	1.097014	-0.487998
C	3.630919	-1.086398	2.346276	0.361224
C	3.833809	0.241627	2.584334	-0.216662
C	3.387050	0.949993	1.422336	-0.207828
C	3.892624	-2.325648	3.126586	-0.532185
H	-1.750268	-0.004635	-0.999637	0.168479
H	-1.445725	-1.268894	2.444685	0.180595
H	-3.768336	-0.186434	1.784738	0.187380
H	-4.932115	-1.711262	-0.060756	0.186872
H	-3.417323	-3.792802	-0.560783	0.183631
H	-1.628576	-2.946461	-1.895933	0.178325
H	-2.291832	-3.781429	1.728851	0.218873
H	-4.006436	-2.467988	-2.629069	0.171588
H	-0.981861	-3.213712	0.707420	0.181704
H	-3.778031	-0.747990	-2.232543	0.173111
H	-2.860851	-1.488238	-3.549732	0.186043
H	4.266326	0.668372	3.478420	0.167562
H	3.416734	2.018467	1.259008	0.170613
H	4.589358	-2.989473	2.601080	0.188878
H	4.331368	-2.067703	4.093534	0.189496
H	2.970500	-2.890737	3.308982	0.172690
H	4.357332	0.812604	-2.759462	0.175702
H	4.006466	2.540791	-2.486354	0.221460
H	4.751280	1.564086	-1.189782	0.184217
H	-0.405671	1.446524	-1.815940	0.194034
H	2.730619	-0.819904	-1.392492	0.188437
H	0.629511	1.935060	1.019219	0.167607
H	0.300881	3.294497	-0.044901	0.215556
H	-1.003744	1.978707	2.687974	0.136666
H	-2.238531	2.728850	-1.364734	0.146156
H	-4.569930	2.978185	-0.609906	0.152839
H	-5.135607	2.784337	1.805498	0.154517
H	-3.335180	2.289155	3.453102	0.152283
H	1.813813	-3.580819	-2.751144	0.186234
H	1.954736	-1.843594	-3.055705	0.171787
H	1.689958	-2.439440	-0.543431	0.203086
H	0.173617	-3.195321	-0.933197	0.168466
H	0.423847	-2.663344	-3.357394	0.169930

TS14 (E)-b2δ-exo

B3LYP/6-31G(d) energy= -1308.4060915000

Zero-point correction (ZPC)= 0.548694
HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.97614
CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -
1300.025388

Number of Imaginary Frequencies=1

C	-3.957375	-1.900867	0.376029	-0.055133
C	-3.066303	-2.902697	-0.045811	-0.198131
C	-1.996585	-2.980080	1.030472	-0.339525
C	-2.149960	-1.664849	1.721961	-0.097376
C	-3.356733	-1.103890	1.383969	-0.086354
C	-2.128934	-2.023390	-1.609491	-0.142925
C	-3.268903	-1.663776	-2.546397	-0.463502
C	-1.284942	-0.973316	-1.148581	-0.186583
C	0.112160	-1.057641	-1.040126	0.390570
C	0.837727	-2.380326	-1.224857	-0.387718
C	1.284932	-2.625347	-2.683285	-0.457527
N	0.863035	0.053559	-0.872633	-0.465238
C	0.399492	1.444342	-1.077530	-0.078044
C	1.631543	2.105106	-1.719284	0.599642
N	2.693439	1.263751	-1.545143	-0.441245
C	2.362507	0.045148	-0.836809	0.046052
C	0.004365	2.261922	0.182763	-0.372705
C	-1.452786	2.293607	0.603723	0.168344
C	-1.787198	2.176206	1.959485	-0.193684
C	-3.103016	2.355043	2.393387	-0.141820
C	-4.113433	2.633226	1.470150	-0.138345
C	-3.795224	2.740423	0.113875	-0.130822
C	-2.475246	2.583033	-0.312698	-0.197078
O	1.641332	3.198056	-2.249080	-0.487236
C	4.037833	1.555263	-2.019147	-0.337851
C	2.935415	0.005095	0.548894	0.382804
O	3.079406	-1.244492	1.097014	-0.487998
C	3.630919	-1.086398	2.346276	0.361224
C	3.833809	0.241627	2.584334	-0.216662
C	3.387050	0.949993	1.422336	-0.207828
C	3.892624	-2.325648	3.126586	-0.532185
H	-1.750268	-0.004635	-0.999637	0.168479
H	-1.445725	-1.268894	2.444685	0.180595
H	-3.768336	-0.186434	1.784738	0.187380
H	-4.932115	-1.711262	-0.060756	0.186872
H	-3.417323	-3.792802	-0.560783	0.183631
H	-1.628576	-2.946461	-1.895933	0.178325
H	-2.291832	-3.781429	1.728851	0.218873
H	-4.006436	-2.467988	-2.629069	0.171588
H	-0.981861	-3.213712	0.707420	0.181704
H	-3.778031	-0.747990	-2.232543	0.173111
H	-2.860851	-1.488238	-3.549732	0.186043
H	4.266326	0.668372	3.478420	0.167562
H	3.416734	2.018467	1.259008	0.170613
H	4.589358	-2.989473	2.601080	0.188878
H	4.331368	-2.067703	4.093534	0.189496
H	2.970500	-2.890737	3.308982	0.172690
H	4.357332	0.812604	-2.759462	0.175702
H	4.006466	2.540791	-2.486354	0.221460
H	4.751280	1.564086	-1.189782	0.184217
H	-0.405671	1.446524	-1.815940	0.194034
H	2.730619	-0.819904	-1.392492	0.188437
H	0.629511	1.935060	1.019219	0.167607
H	0.300881	3.294497	-0.044901	0.215556
H	-1.003744	1.978707	2.687974	0.136666
H	-2.238531	2.728850	-1.364734	0.146156
H	-4.569930	2.978185	-0.609906	0.152839
H	-5.135607	2.784337	1.805498	0.154517
H	-3.335180	2.289155	3.453102	0.152283

H	1.813813	-3.580819	-2.751144	0.186234
H	1.954736	-1.843594	-3.055705	0.171787
H	1.689958	-2.439440	-0.543431	0.203086
H	0.173617	-3.195321	-0.933197	0.168466
H	0.423847	-2.663344	-3.357394	0.169930

TS14 (E)-c1a-endo

B3LYP/6-31G(d) energy= -1308.4131157000

Zero-point correction (ZPC)= 0.548553

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.979571

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -
1300.03787

Number of Imaginary Frequencies=1

C	2.101012	-3.174319	1.902318	-0.099677
C	2.635348	-1.903344	1.943010	-0.098006
C	3.693429	-1.774493	0.896179	-0.330427
C	3.365619	-2.942686	-0.022834	-0.178602
C	2.605378	-3.839815	0.761781	-0.072738
C	2.076108	-2.155699	-1.288497	-0.151761
C	3.012840	-1.622379	-2.365554	-0.465902
C	1.288369	-1.193529	-0.588837	-0.201182
C	-0.012447	-1.401376	-0.091638	0.410585
C	-0.704306	-2.731501	-0.295848	-0.358760
C	-1.322577	-2.886828	-1.702576	-0.456561
N	-0.673855	-0.396543	0.513178	-0.478211
C	-2.032811	-0.494182	1.123864	0.038897
N	-2.026646	0.639521	2.038165	-0.437847
C	-0.976667	1.494192	1.872634	0.605165
C	-0.060956	0.910410	0.799311	-0.062618
C	-3.147977	-0.455442	0.131486	0.383220
O	-3.146729	0.584643	-0.759912	-0.484970
C	-4.278254	0.466869	-1.528964	0.361596
C	-4.987588	-0.629626	-1.129014	-0.215851
C	-4.257952	-1.226405	-0.051246	-0.202712
C	-4.487218	1.502204	-2.576468	-0.532964
C	0.074564	1.860126	-0.434698	-0.362875
C	1.427343	2.539864	-0.523210	0.143493
C	2.218159	2.401231	-1.671816	-0.202475
C	3.464357	3.026747	-1.762486	-0.132616
C	3.936313	3.797249	-0.699596	-0.128508
C	3.153839	3.943943	0.448737	-0.132276
C	1.907761	3.322979	0.538140	-0.197453
O	-0.789989	2.543455	2.461398	-0.492174
C	-3.141557	0.909595	2.931247	-0.338384
H	2.430219	-1.151641	2.697438	0.191116
H	1.399974	-3.592252	2.615914	0.176785
H	2.383267	-4.867075	0.489835	0.186542
H	4.102119	-3.320980	-0.725344	0.186503
H	4.666774	-1.990802	1.369179	0.222899
H	3.782363	-0.789761	0.434863	0.196291
H	1.569340	-3.065779	-1.596897	0.175481
H	1.707335	-0.196279	-0.523856	0.176326
H	3.696050	-2.391077	-2.736194	0.174255
H	2.411908	-1.278142	-3.215987	0.188600
H	3.599558	-0.768739	-2.011989	0.178572
H	0.925272	0.743192	1.247622	0.186738
H	1.847977	1.815700	-2.511348	0.124979
H	4.059022	2.918556	-2.665557	0.143624
H	4.902770	4.288433	-0.768153	0.149795
H	3.510320	4.552936	1.274901	0.151593
H	1.294992	3.451451	1.427307	0.176846
H	-0.113326	1.278538	-1.342195	0.165805
H	-0.722054	2.610126	-0.378826	0.200342
H	-4.071100	1.045553	2.368920	0.188128

H	-3.271615	0.089255	3.646154	0.172079
H	-2.904578	1.827532	3.470943	0.221075
H	-2.089901	-2.130426	-1.883177	0.188697
H	-1.791726	-3.871709	-1.788675	0.179084
H	-0.565416	-2.799517	-2.487053	0.164580
H	0.033275	-3.524979	-0.132465	0.168630
H	-1.482544	-2.885730	0.454266	0.169933
H	-2.123635	-1.424545	1.697726	0.177472
H	-4.531998	-2.108681	0.512068	0.161608
H	-5.923760	-0.969687	-1.548880	0.167667
H	-3.662625	1.514236	-3.299027	0.181067
H	-4.557370	2.504341	-2.137456	0.191102
H	-5.414421	1.299610	-3.117892	0.188307

TS14 (E)-c1 α -exo

B3LYP/6-31G(d) energy= -1308.4120726000

Zero-point correction (ZPC)= 0.548572

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.978372

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ϵ =78.39) energy= -1300.034695

Number of Imaginary Frequencies=1

C	2.622038	-2.878820	1.611446	-0.333975
C	2.714614	-1.451291	2.046937	-0.098820
C	3.706594	-0.815617	1.334644	-0.095027
C	4.171022	-1.694589	0.326635	-0.049769
C	3.371966	-2.856810	0.289678	-0.196725
C	1.955741	-2.434990	-1.046590	-0.148867
C	2.740461	-2.146656	-2.315723	-0.464877
C	1.136461	-1.400466	-0.512331	-0.189294
C	-0.145362	-1.556303	0.046280	0.390998
C	-0.859662	-2.892081	-0.005401	-0.358237
C	-1.502831	-3.176880	-1.379724	-0.454963
N	-0.784979	-0.484259	0.556106	-0.470561
C	-2.147852	-0.485102	1.165813	0.029407
N	-2.081006	0.683553	2.033694	-0.434049
C	-1.001205	1.486548	1.811626	0.603390
C	-0.128588	0.817229	0.752929	-0.065383
C	-3.256957	-0.425181	0.167451	0.387283
O	-3.214834	0.599044	-0.741444	-0.484002
C	-4.346117	0.508581	-1.514236	0.362580
C	-5.095961	-0.554882	-1.099670	-0.216144
C	-4.393166	-1.158910	-0.008085	-0.203510
C	-4.513298	1.532772	-2.579966	-0.532957
C	0.015963	1.704179	-0.526529	-0.363406
C	1.406643	2.287705	-0.690781	0.145055
C	1.992667	3.038314	0.340906	-0.198697
C	3.275707	3.566118	0.189828	-0.138067
C	3.989842	3.358203	-0.993489	-0.131243
C	3.411237	2.622855	-2.028503	-0.133885
C	2.128548	2.089814	-1.875192	-0.200245
O	-0.759580	2.553383	2.346955	-0.494041
C	-3.175357	1.042407	2.920970	-0.338322
H	1.613674	-3.296510	1.597813	0.177940
H	2.160603	-1.031054	2.879287	0.187823
H	3.546226	-2.869364	-2.477174	0.170326
H	3.165211	-1.138658	-2.306551	0.176334
H	2.062490	-2.213512	-3.175769	0.184582
H	3.208186	-3.494775	2.314328	0.221385
H	4.971166	-1.466837	-0.369355	0.191306
H	4.056151	0.198305	1.491796	0.192107
H	1.531784	-3.438260	-1.034783	0.175217
H	3.743035	-3.774788	-0.158759	0.187257
H	1.517909	-0.393389	-0.629156	0.178516
H	0.862057	0.635881	1.185999	0.187881

H	3.712539	4.154104	0.992458	0.151936
H	1.677451	1.529206	-2.691695	0.129025
H	3.951833	2.470989	-2.958886	0.145125
H	4.984729	3.778118	-1.111838	0.150196
H	1.430621	3.220546	1.254181	0.175506
H	-0.724579	2.509522	-0.470629	0.202118
H	-2.290580	-1.384299	1.775725	0.179613
H	-3.331721	0.264033	3.676313	0.172869
H	-2.896751	1.975229	3.413216	0.220519
H	-4.103907	1.188688	2.359444	0.187966
H	-4.701725	-2.020591	0.569037	0.162208
H	-6.041861	-0.868296	-1.518452	0.167764
H	-3.688842	1.499152	-3.302088	0.180981
H	-5.447665	1.357682	-3.118631	0.188402
H	-4.543596	2.544486	-2.158703	0.190608
H	-1.988480	-4.157356	-1.361361	0.179582
H	-0.751047	-3.182008	-2.174244	0.164118
H	-2.259399	-2.428326	-1.627194	0.186619
H	-1.622103	-2.960108	0.773028	0.170121
H	-0.135673	-3.682047	0.217695	0.172572
H	-0.249417	1.102884	-1.401262	0.167700

TS14 (E)-c2 α -endo

B3LYP/6-31G(d) energy= -1308.4125508000

Zero-point correction (ZPC)= 0.548823

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.979057

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ϵ =78.39) energy= -1300.035042

Number of Imaginary Frequencies=1

C	2.541403	2.411248	1.449513	-0.335326
C	1.145094	2.227711	1.947863	-0.094665
C	0.391181	3.335828	1.630143	-0.098037
C	1.153857	4.170221	0.779946	-0.075605
C	2.364308	3.529241	0.431140	-0.178071
C	1.970823	2.555819	-1.230762	-0.150536
C	3.374982	2.351982	-1.787344	-0.464392
C	1.231870	1.372515	-0.922871	-0.202466
C	-0.158415	1.223051	-1.065871	0.412017
C	-1.037697	2.403619	-1.417544	-0.371073
C	-1.210548	2.592550	-2.940595	-0.458358
N	-0.729993	0.007803	-0.977234	-0.477077
C	-2.189258	-0.259036	-1.133704	0.037559
N	-2.188230	-1.657350	-1.534937	-0.434004
C	-0.990021	-2.289470	-1.364749	0.610044
C	0.022182	-1.254656	-0.870922	-0.068189
C	-2.990736	0.011507	0.100070	0.383258
C	-4.114278	0.749988	0.332169	-0.204081
C	-4.450879	0.548872	1.709392	-0.218028
C	-3.515550	-0.301509	2.225100	0.358779
O	-2.613136	-0.637696	1.245771	-0.482244
C	-3.305865	-0.908988	3.566860	-0.531801
C	0.546431	-1.597568	0.559106	-0.366013
C	1.965208	-2.134490	0.573918	0.153697
C	2.345423	-3.194491	-0.263384	-0.195694
C	3.651034	-3.685480	-0.231989	-0.129961
C	4.594448	-3.133560	0.637779	-0.126551
C	4.223567	-2.087690	1.482975	-0.129182
C	2.917903	-1.592355	1.447046	-0.207590
O	-0.756380	-3.469309	-1.550532	-0.489387
C	-3.409191	-2.350526	-1.912152	-0.338165
H	1.427386	3.335965	-1.757397	0.176024
H	3.299277	1.910109	-2.787898	0.192574
H	3.963656	1.666595	-1.169368	0.178145
H	3.920197	3.294600	-1.883207	0.175101

H	-0.624241	3.529158	1.956531	0.180272
H	0.827717	5.130681	0.392735	0.187389
H	3.214968	4.116312	0.097798	0.187224
H	0.823070	1.400220	2.570025	0.187731
H	3.039890	1.502286	1.108161	0.195179
H	1.815764	0.495246	-0.664130	0.174016
H	3.149760	2.813564	2.277724	0.221165
H	-2.600267	0.358336	-1.939544	0.180007
H	4.945784	-1.661200	2.173906	0.141298
H	1.610086	-3.644534	-0.925964	0.179412
H	3.929036	-4.509192	-0.883484	0.153783
H	5.608386	-3.522222	0.662352	0.150961
H	2.629745	-0.793260	2.128080	0.110711
H	-0.137870	-2.323007	1.013207	0.199922
H	0.858218	-1.224920	-1.576654	0.203334
H	0.483629	-0.695322	1.174819	0.151002
H	-3.136866	-3.384106	-2.130269	0.221651
H	-3.851935	-1.894365	-2.804627	0.174111
H	-4.141207	-2.330407	-1.097844	0.185332
H	-4.085785	-0.570268	4.253114	0.188966
H	-3.343025	-2.003573	3.518191	0.193750
H	-2.332688	-0.630550	3.988861	0.173181
H	-5.288695	0.973793	2.244142	0.167540
H	-4.650637	1.352353	-0.389333	0.163744
H	-1.856182	3.453933	-3.136293	0.184347
H	-2.012383	2.297132	-0.934209	0.180278
H	-0.592587	3.308032	-0.995055	0.168179
H	-0.248534	2.768520	-3.431322	0.172385
H	-1.663637	1.716967	-3.416562	0.172305

TS14 (E)-c2a-exo

B3LYP/6-31G(d) energy= -1308.4095108000

Zero-point correction (ZPC)= 0.548867

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.976059

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1300.032288

Number of Imaginary Frequencies=1

C	-1.479877	-3.333082	1.531950	-0.337800
C	-2.660158	-3.447862	0.580922	-0.198537
C	-3.592060	-2.484480	1.015863	-0.049548
C	-2.961460	-1.548102	1.872253	-0.092858
C	-1.676293	-1.971937	2.114803	-0.095976
C	-1.975989	-2.699550	-1.133463	-0.146256
C	-3.224791	-2.557580	-1.987864	-0.462009
C	-1.200988	-1.529264	-0.881494	-0.193140
C	0.202254	-1.465363	-0.931655	0.401854
C	1.051317	-2.708583	-1.121974	-0.374776
C	1.318732	-3.030495	-2.608550	-0.457598
N	0.835300	-0.275637	-0.919853	-0.474672
C	2.314552	-0.099768	-1.028278	0.039597
N	2.408540	1.241007	-1.582914	-0.434081
C	1.236682	1.940905	-1.570618	0.612728
C	0.153972	1.031455	-0.984241	-0.079154
C	3.047617	-0.273614	0.263889	0.382549
O	2.669903	0.518753	1.315439	-0.481656
C	3.513113	0.241287	2.363219	0.359931
C	4.412308	-0.713151	1.983159	-0.216776
C	4.114623	-1.044959	0.622721	-0.203231
C	3.291877	1.003676	3.621379	-0.532029
C	-0.362768	1.554315	0.387839	-0.358071
C	-1.669271	2.326926	0.323326	0.155169
C	-1.964882	3.209736	-0.725199	-0.197332
C	-3.170505	3.914500	-0.737357	-0.132478
C	-4.091529	3.761511	0.299661	-0.126946

C	-3.797406	2.901760	1.359284	-0.130249
C	-2.597589	2.189695	1.365441	-0.201347
O	1.074689	3.089606	-1.938377	-0.486012
C	3.679570	1.817225	-1.989637	-0.337828
H	-3.417531	-0.638552	2.242874	0.185182
H	-4.622035	-2.419050	0.681848	0.192817
H	-2.988829	-4.414882	0.209455	0.187688
H	-1.407784	-3.596047	-1.376257	0.178215
H	-1.751064	-0.599079	-0.784683	0.171180
H	-0.938492	-1.458396	2.721140	0.185382
H	-3.879995	-3.430858	-1.910692	0.171640
H	-0.488959	-3.516475	1.115354	0.183631
H	-1.626230	-4.079402	2.331134	0.221609
H	-2.925840	-2.462828	-3.039041	0.187857
H	-3.797354	-1.662702	-1.727255	0.175952
H	2.728712	-0.821212	-1.739969	0.179676
H	-0.671211	0.964139	-1.699455	0.198888
H	3.473817	2.826049	-2.350075	0.221814
H	4.376756	1.865492	-1.146526	0.185728
H	4.130801	1.227493	-2.795534	0.173342
H	1.949965	-3.920772	-2.686771	0.185859
H	0.547163	-3.564952	-0.669139	0.170317
H	1.993105	-2.598607	-0.578171	0.183664
H	1.825726	-2.211066	-3.127794	0.172987
H	0.384354	-3.226607	-3.143098	0.171311
H	-1.238669	3.371999	-1.516785	0.177283
H	0.423051	2.169747	0.841629	0.196925
H	-0.487362	0.691708	1.050483	0.151188
H	-2.365164	1.537520	2.205374	0.110878
H	-4.499059	2.788502	2.181481	0.139713
H	-5.025529	4.315892	0.288745	0.149309
H	-3.382515	4.595486	-1.556884	0.151500
H	2.286489	0.833279	4.024837	0.173947
H	3.403469	2.082096	3.458388	0.193195
H	4.020091	0.694375	4.375025	0.188951
H	5.201493	-1.124678	2.596517	0.167746
H	4.638693	-1.753286	-0.005559	0.163629

TS14 (E)-c2δ-endo

B3LYP/6-31G(d) energy= -1308.4109190000

Zero-point correction (ZPC)= 0.548751

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.976618

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) ($\epsilon=78.39$) energy= -1300.031972

Number of Imaginary Frequencies=1

C	-3.259359	-2.531729	-0.109354	-0.195372
C	-2.580173	-1.561076	-0.861311	0.153797
C	-3.324819	-0.692118	-1.670032	-0.206079
C	-4.717921	-0.780293	-1.724347	-0.129684
C	-5.384761	-1.740483	-0.963180	-0.126205
C	-4.651145	-2.615911	-0.158992	-0.129869
C	-1.066239	-1.467602	-0.825773	-0.369544
C	-0.474132	-1.417003	0.618399	-0.073480
N	0.589037	-0.420959	0.831973	-0.476206
C	1.923872	-1.094703	0.901081	0.053499
N	1.544737	-2.465904	1.182300	-0.444756
C	0.215722	-2.727795	1.000659	0.605232
C	0.361952	0.880943	1.086770	0.406177
C	1.515629	1.735455	1.566734	-0.383926
C	1.711336	1.664839	3.097441	-0.456991
C	2.738659	-0.973178	-0.353422	0.376025
C	2.770445	-1.658915	-1.532136	-0.207061
C	3.787211	-1.042802	-2.329070	-0.213493
C	4.315098	-0.025382	-1.587671	0.356262

O	3.678097	0.027871	-0.371945	-0.485205
C	2.520067	-3.484375	1.541140	-0.337907
O	-0.334588	-3.808091	1.103446	-0.488097
C	5.402476	0.963165	-1.820409	-0.531530
C	-0.940530	1.404046	0.999134	-0.201654
C	-1.352996	2.685592	1.474607	-0.149740
C	-2.765962	2.778641	2.038473	-0.464436
C	-1.477763	3.929898	-0.046480	-0.178127
C	-1.925963	3.026604	-1.186972	-0.335312
C	-0.618335	2.555434	-1.734961	-0.096662
C	0.389869	3.389804	-1.304833	-0.096788
C	-0.141548	4.280460	-0.343156	-0.074789
H	0.415810	5.070999	0.149883	0.186767
H	1.423600	3.357007	-1.629074	0.177115
H	-1.728916	0.749015	0.642906	0.172496
H	-0.512370	1.756632	-2.460436	0.188305
H	-2.403878	3.668162	-1.947207	0.220753
H	-2.153658	4.666115	0.378355	0.186738
H	-2.643782	2.240593	-0.945546	0.194586
H	-3.051379	3.809507	2.264438	0.175038
H	-2.812633	2.209269	2.974256	0.192207
H	-3.507000	2.350511	1.355943	0.177753
H	-0.630542	3.228313	2.078490	0.176551
H	-2.809742	0.042748	-2.286418	0.113839
H	-0.735864	-0.575668	-1.367232	0.154901
H	-2.693027	-3.232232	0.499942	0.177625
H	-5.163057	-3.375133	0.425530	0.154856
H	-5.278604	-0.104892	-2.364857	0.142942
H	-0.630938	-2.326500	-1.351074	0.193921
H	-6.467743	-1.812969	-1.002935	0.152122
H	3.273908	-3.597702	0.756067	0.185156
H	3.016697	-3.226452	2.483274	0.177475
H	1.975017	-4.421536	1.663220	0.221464
H	2.496898	-0.676248	1.735014	0.190267
H	2.160442	-2.510745	-1.799792	0.169404
H	4.099659	-1.333848	-3.322212	0.167955
H	5.822310	0.822892	-2.819457	0.189658
H	5.036007	1.994131	-1.744469	0.170726
H	6.211658	0.846106	-1.089860	0.191997
H	-1.275399	-1.233320	1.340367	0.205977
H	1.926096	0.646504	3.437554	0.170959
H	2.551270	2.300950	3.392221	0.184880
H	0.819391	2.006280	3.631513	0.170216
H	2.438069	1.449860	1.056449	0.201199
H	1.323069	2.772365	1.279202	0.165821

TS14 (E)-c2δ-exo

B3LYP/6-31G(d) energy= -1308.4081612000

Zero-point correction (ZPC)= 0.548624

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.974156

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy= -1300.030201

Number of Imaginary Frequencies=1

C	-3.131738	-1.329323	-1.739728	-0.200847
C	-2.319709	-1.848064	-0.720895	0.155387
C	-2.887223	-2.736565	0.203392	-0.198290
C	-4.239477	-3.075206	0.118777	-0.132522
C	-5.040597	-2.545616	-0.893549	-0.126582
C	-4.480150	-1.675946	-1.830696	-0.130193
C	-0.848915	-1.469445	-0.679182	-0.359610
C	-0.261726	-1.278004	0.750131	-0.085733
N	0.752750	-0.212940	0.856004	-0.471250
C	2.121885	-0.819860	0.895233	0.052247
N	1.829172	-2.175347	1.315208	-0.445379

C	0.506234	-2.510971	1.237991	0.610426
C	0.474005	1.089639	1.059117	0.395904
C	1.623234	2.008289	1.431896	-0.387995
C	1.926731	1.995439	2.946492	-0.456105
C	2.848244	-0.775047	-0.416862	0.378014
C	2.918986	-1.615467	-1.488781	-0.205951
C	3.800756	-0.993751	-2.429750	-0.215310
C	4.214662	0.182149	-1.874283	0.359585
O	3.635877	0.327435	-0.636511	-0.486745
C	2.867986	-3.101159	1.741237	-0.337817
O	0.018171	-3.595273	1.495116	-0.483734
C	5.134560	1.264412	-2.316712	-0.532116
C	-0.856936	1.543524	1.040237	-0.192068
C	-1.294527	2.827129	1.477212	-0.145484
C	-2.561220	2.902312	2.313862	-0.461738
C	-1.710962	3.974473	-0.104557	-0.197791
C	-0.571607	3.688452	-1.069475	-0.337494
C	-1.096563	2.520724	-1.838691	-0.097943
C	-2.455236	2.421125	-1.652852	-0.093961
C	-2.847181	3.360931	-0.667091	-0.050496
H	-3.868645	3.521834	-0.339430	0.191942
H	-3.120199	1.724233	-2.147879	0.184144
H	-0.499564	1.921942	-2.517617	0.185962
H	-1.636421	0.825139	0.809582	0.169017
H	-1.786329	4.928961	0.409595	0.187204
H	-0.496130	4.550522	-1.753883	0.221014
H	-0.514679	3.493614	1.842194	0.178834
H	-2.953781	3.921769	2.378638	0.171744
H	-3.345178	2.246366	1.924407	0.175120
H	-2.331973	2.572784	3.334771	0.187798
H	0.420263	3.549376	-0.637710	0.183131
H	-1.065270	-1.073722	1.463120	0.201742
H	2.721754	-0.306905	1.653165	0.189594
H	-4.663027	-3.766626	0.841824	0.152340
H	-2.696763	-0.667136	-2.486252	0.114036
H	-6.090392	-2.816564	-0.959008	0.150288
H	-2.266014	-3.188571	0.971768	0.177573
H	-5.090439	-1.271006	-2.633551	0.141393
H	2.377434	-4.045836	1.980366	0.221746
H	3.601774	-3.259449	0.945204	0.184960
H	3.380075	-2.721351	2.632612	0.176969
H	-0.703961	-0.534594	-1.230209	0.155578
H	-0.252207	-2.225835	-1.205058	0.187384
H	1.061011	2.328290	3.527016	0.169312
H	2.516774	1.744211	0.862399	0.205686
H	1.376492	3.030784	1.138306	0.167708
H	2.762053	2.668714	3.160821	0.186418
H	2.198298	0.998079	3.307108	0.171166
H	4.622398	2.232629	-2.373366	0.173058
H	2.422430	-2.570136	-1.594078	0.170522
H	4.102214	-1.382947	-3.392171	0.168108
H	5.531356	1.030020	-3.307474	0.189692
H	5.979713	1.377083	-1.627385	0.190442

TS14 (Z)-b2a-endo

B3LYP/6-31G(d) energy= -1308.4136277000

Zero-point correction (ZPC)= 0.548659

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.980265

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy= -1300.036486

Number of Imaginary Frequencies=1

C	2.610416	-2.289507	0.851624	-0.209827
C	2.219766	-1.064475	0.395078	0.382935
O	2.239032	-0.158880	1.422834	-0.481842

C	2.650491	-0.823250	2.553357	0.358069
C	2.884582	-2.133272	2.248780	-0.220994
C	1.877287	-0.568317	-0.975543	0.049710
N	0.582007	0.165192	-1.078515	-0.473938
C	0.830928	1.610956	-1.280897	-0.080584
C	2.290690	1.634784	-1.748437	0.611682
N	2.820166	0.398144	-1.514487	-0.437749
C	-0.591635	-0.478867	-1.242227	0.415585
C	-1.790815	0.322885	-1.695679	-0.380665
C	-1.875636	0.435653	-3.234231	-0.460590
C	0.731909	2.522328	-0.025856	-0.375960
C	-0.649577	2.822686	0.511668	0.164556
C	-1.505499	3.708410	-0.162258	-0.194367
C	-2.767716	4.011744	0.348869	-0.125179
C	-3.190605	3.446382	1.554740	-0.131434
C	-2.341652	2.578948	2.244518	-0.141771
C	-1.083686	2.266071	1.721437	-0.194365
O	2.867799	2.607409	-2.192512	-0.489534
C	4.208914	0.058480	-1.773782	-0.337539
C	2.769867	-0.018941	3.799664	-0.536216
C	-0.677715	-1.877197	-1.101696	-0.189225
C	-1.797012	-2.681684	-1.458651	-0.142933
C	-1.508232	-4.081382	-1.982264	-0.463859
C	-2.809667	-3.126978	0.215090	-0.177770
C	-1.693597	-3.201085	1.246483	-0.328298
C	-1.585788	-1.775006	1.679714	-0.101930
C	-2.732479	-1.098706	1.326817	-0.096377
C	-3.516779	-1.942669	0.504236	-0.077806
H	-4.487155	-1.683581	0.091980	0.185630
H	-2.973786	-0.076291	1.592353	0.185484
H	-0.771531	-1.382464	2.278246	0.185521
H	0.203838	-2.409023	-0.765765	0.148562
H	-2.418334	-4.677013	-2.090632	0.178012
H	-3.330473	-4.019659	-0.117194	0.183443
H	-2.071121	-3.792513	2.097967	0.219589
H	-2.593364	-2.188077	-2.008249	0.178525
H	-0.810404	-4.624987	-1.336976	0.167473
H	-1.047464	-4.001911	-2.974429	0.190556
H	-0.757443	-3.666665	0.934195	0.182969
H	1.836007	-1.446509	-1.633576	0.176799
H	4.281404	-0.746330	-2.514845	0.172840
H	1.354782	2.084604	0.759256	0.181587
H	1.216714	3.456509	-0.334290	0.206932
H	0.197658	1.995065	-2.082127	0.195283
H	4.690058	0.955568	-2.166221	0.222274
H	4.713696	-0.254914	-0.854176	0.183941
H	2.713831	-3.192441	0.263860	0.161426
H	1.813257	0.435043	4.085431	0.177119
H	3.496622	0.793062	3.679834	0.196264
H	3.103637	-0.657338	4.621326	0.189761
H	3.228679	-2.894332	2.935066	0.167778
H	-2.649428	2.162259	3.200423	0.145272
H	-1.172776	4.181020	-1.084488	0.146980
H	-4.165132	3.697765	1.963207	0.154504
H	-0.416763	1.604102	2.269785	0.130000
H	-3.412624	4.705795	-0.182611	0.156416
H	-2.760981	1.015824	-3.510987	0.185402
H	-1.774443	1.316941	-1.246439	0.205235
H	-1.000132	0.938383	-3.657435	0.174485
H	-1.950177	-0.548363	-3.707388	0.165818
H	-2.697070	-0.159056	-1.319986	0.166513

TS14 (Z)-b2 α -exo

B3LYP/6-31G(d) energy= -1308.4117545000

Zero-point correction (ZPC)= 0.548548

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.978832

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ϵ =78.39) energy= -1300.035767

Number of Imaginary Frequencies=1

C	-3.163944	1.012522	0.853893	-0.341946
C	-4.122688	0.280926	-0.071072	-0.198276
C	-4.274270	-1.006654	0.479949	-0.053595
C	-3.230354	-1.266146	1.402299	-0.097193
C	-2.491824	-0.117150	1.561198	-0.089456
C	-3.012422	-0.052607	-1.714849	-0.140876
C	-3.848097	-1.033136	-2.518917	-0.461158
C	-1.705783	-0.447772	-1.311072	-0.181422
C	-0.566209	0.376170	-1.312629	0.402851
C	-0.651137	1.832253	-1.726091	-0.380291
C	-0.456499	2.010871	-3.248230	-0.459175
N	0.661797	-0.135992	-1.079425	-0.471286
C	0.920182	-1.604430	-1.052798	0.051328
N	2.313751	-1.676954	-1.465443	-0.438028
C	2.942170	-0.467568	-1.551530	0.612753
C	1.942363	0.605024	-1.109966	-0.081653
C	0.633363	-2.284535	0.250583	0.383991
O	1.191046	-1.764875	1.389460	-0.481914
C	0.878589	-2.610061	2.427074	0.357883
C	0.130357	-3.649708	1.954487	-0.224137
C	-0.025703	-3.441697	0.545642	-0.207204
C	1.405086	-2.248083	3.770949	-0.535726
C	2.438558	1.180976	0.246703	-0.371735
C	1.642269	2.326766	0.827109	0.160218
C	0.701731	2.100299	1.841014	-0.198963
C	-0.036079	3.155168	2.383673	-0.138441
C	0.155826	4.456255	1.915088	-0.130195
C	1.097953	4.696957	0.912064	0.124796
C	1.838079	3.641448	0.377226	-0.194246
O	4.097667	-0.261889	-1.865939	-0.489680
C	2.969456	-2.941928	-1.749084	-0.337716
H	-1.579188	-1.494506	-1.062653	0.150924
H	-1.609305	-0.007537	2.179417	0.182910
H	-3.111112	0.970269	-2.073574	0.181088
H	-3.491257	-1.036222	-3.556441	0.187312
H	-4.906512	-0.755755	-2.537951	0.173322
H	-4.957655	0.794080	-0.540655	0.185691
H	-5.029516	-1.726015	0.181453	0.187798
H	-3.030696	-2.220094	1.875618	0.178614
H	-2.488317	1.740384	0.404160	0.194788
H	-3.776044	1.566421	1.586174	0.218585
H	-3.759570	-2.054298	-2.136382	0.166214
H	2.586497	3.842339	-0.386730	0.147793
H	-0.409515	5.279946	2.341325	0.153406
H	-0.744738	2.965915	3.186070	0.137934
H	0.573392	1.089542	2.222094	0.131733
H	2.488599	0.356334	0.963560	0.181198
H	3.468979	1.497813	0.048148	0.203495
H	1.269321	5.709639	0.558231	0.156854
H	1.909940	1.390057	-1.866442	0.195947
H	0.288374	-2.086149	-1.811086	0.176524
H	-0.544196	-4.083023	-0.155112	0.161442
H	-0.248550	-4.477132	2.538167	0.166833
H	1.027323	-1.275634	4.109666	0.176671
H	2.499858	-2.191776	3.766083	0.196306
H	1.105283	-3.003500	4.501421	0.189586
H	2.476162	-3.458764	-2.580818	0.172424
H	3.999604	-2.713162	-2.026194	0.222229
H	2.963294	-3.592668	-0.868700	0.183454

H -0.518843 3.072845 -3.503939 0.186497
H 0.517262 1.641382 -3.585466 0.174233
H 0.080056 2.426973 -1.178354 0.207143
H -1.626949 2.235365 -1.447992 0.166583
H -1.226365 1.476723 -3.813465 0.164750

TS14 (Z)-b2δ-endo

B3LYP/6-31G(d) energy= -1308.4121532000

Zero-point correction (ZPC)= 0.548793

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.97826

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy= -1300.033808

Number of Imaginary Frequencies=1

C 1.701053 3.238384 -0.617996 -0.331876
C 0.595868 2.470522 -1.268658 -0.103124
C -0.616914 3.014314 -0.907195 -0.097195
C -0.394348 3.972522 0.110351 -0.078257
C 0.959960 3.953847 0.501975 -0.178058
C 1.023010 2.589304 1.965648 -0.143731
C 2.311137 2.997635 2.666583 -0.463623
C 0.990671 1.297360 1.366415 -0.201115
C -0.141606 0.466041 1.274802 0.408490
C -1.500845 0.967451 1.710300 -0.380384
C -1.774325 0.705105 3.208038 -0.460794
N -0.033156 -0.822147 0.890437 -0.467325
C 1.285597 -1.525267 0.784659 0.053296
N 0.938720 -2.878497 1.172762 -0.447663
C -0.406801 -3.115902 1.230059 0.610608
C -1.123660 -1.819017 0.833257 -0.087933
C 1.938119 -1.471111 -0.567482 0.377405
O 2.819944 -0.439606 -0.782438 -0.494109
C 3.341997 -0.598462 -2.045412 0.356600
C 2.798074 -1.708774 -2.621670 -0.213459
C 1.896075 -2.277850 -1.666526 -0.206582
C 4.355093 0.397526 -2.488632 -0.537677
C -1.792693 -2.030241 -0.552628 -0.367566
C -2.749353 -0.956246 -1.022115 0.167386
C -2.419551 -0.120898 -2.096695 -0.194731
C -3.320123 0.844745 -2.555905 -0.141270
C -4.562023 0.994972 -1.936462 -0.131270
C -4.905153 0.163705 -0.866865 -0.125642
C -4.009049 -0.807669 -0.419997 -0.195099
O -0.954475 -4.165136 1.503060 -0.487343
C 1.943957 -3.879278 1.495148 -0.337532
H 0.748334 1.685767 -2.000801 0.185153
H -1.584255 2.722648 -1.299124 0.185654
H -1.166527 4.576029 0.577485 0.185245
H 1.401381 4.800938 1.017966 0.183085
H 0.136580 2.892390 2.515595 0.177568
H 1.941568 0.906258 1.025757 0.171809
H 3.191978 2.820732 2.041022 0.169856
H 2.426841 2.397419 3.577172 0.190303
H 2.300775 4.049031 2.965663 0.176829
H 2.574840 2.649457 -0.335550 0.187170
H 2.050073 4.009656 -1.325715 0.216728
H 1.964665 -1.081885 1.523217 0.187751
H 2.541375 -3.564015 2.358591 0.176509
H 1.314944 -3.182582 -1.780688 0.173976
H 3.027640 -2.091628 -3.606253 0.170124
H 5.222114 0.411723 -1.817570 0.190388
H 4.706339 0.143327 -3.491690 0.193838
H 3.944807 1.414631 -2.522256 0.166374
H 2.608351 -4.054444 0.643700 0.183113
H 1.411998 -4.799921 1.739992 0.221962

H -1.880749 -1.600918 1.587508 0.198129
H -1.462128 -0.248501 -2.597470 0.132904
H -1.004036 -2.178584 -1.296907 0.163600
H -2.326322 -2.984124 -0.459056 0.207845
H -4.299650 -1.471778 0.391978 0.147187
H -5.878702 0.258041 -0.394276 0.156885
H -5.266681 1.738658 -2.297202 0.155211
H -1.751894 -0.362485 3.449514 0.174217
H -2.764636 1.087607 3.472558 0.185260
H -1.035430 1.201125 3.844903 0.166873
H -1.558031 2.041717 1.517521 0.167381
H -2.283838 0.515534 1.099307 0.203137
H -3.059428 1.464315 -3.410259 0.147592

TS14 (Z)-b2δ-exo

B3LYP/6-31G(d) energy= -1308.4089392000

Zero-point correction (ZPC)= 0.548361

HF/6-31G(d)// B3LYP/6-31G(d) energy= -1299.975016

CPCM:HF/6-31G(d)// B3LYP/6-31G(d) (ε=78.39) energy= -1300.032055

Number of Imaginary Frequencies=1

C 2.448024 -0.517835 -1.987906 -0.197156
C 3.009100 0.407602 -1.098225 0.165568
C 4.280456 0.140690 -0.567137 -0.194341
C 4.960745 -1.031558 -0.898843 -0.124558
C 4.384737 -1.952379 -1.777674 -0.129636
C 3.129151 -1.689414 -2.327838 -0.136730
C 2.273451 1.676326 -0.732708 -0.369676
C 1.575583 1.705905 0.656626 -0.082256
N 0.362576 0.874387 0.801930 -0.478207
C -0.863012 1.725956 0.710345 0.067034
N -0.318868 3.062854 0.867454 -0.449483
C 1.044759 3.124121 0.886447 0.612195
C 0.314277 -0.403846 1.239803 0.398100
C 1.607136 -1.027976 1.727012 -0.379830
C 1.888850 -0.684486 3.207047 -0.459057
C -1.694017 1.559590 -0.531550 0.372980
C -1.524588 1.831350 -1.857942 -0.216390
C -2.759009 1.497294 -2.501445 -0.214918
C -3.609069 1.054772 -1.528140 0.351081
O -2.965688 1.084908 -0.317685 -0.483314
C -1.174656 4.228064 1.019534 -0.337334
O 1.733561 4.118128 1.005833 -0.489828
C -5.032061 0.616740 -1.524281 -0.534336
C -0.913805 -1.074310 1.372369 -0.192722
C -1.096948 -2.351639 1.974785 -0.143458
C -2.328255 -2.571363 2.835924 -0.461785
C -1.277726 -3.730461 0.526512 -0.198444
C -2.510365 -3.412221 -0.077935 -0.053527
C -2.305617 -2.515781 -1.155513 -0.096991
C -0.952478 -2.360849 -1.345692 -0.090942
C -0.212875 -3.325622 -0.479531 -0.342724
H 0.736725 -2.959809 -0.088852 0.194260
H -0.482629 -1.715374 -2.077651 0.184914
H -3.085736 -2.016789 -1.717656 0.177637
H -3.480845 -3.739467 0.279982 0.186813
H -1.166278 -4.621434 1.138682 0.185986
H -0.205584 -2.813521 2.395143 0.180817
H 0.022789 -4.219887 -1.081730 0.219029
H -2.523583 -3.633182 3.014697 0.172066
H -2.167361 -2.098567 3.812821 0.187516
H -3.220151 -2.118311 2.393280 0.169643
H -1.817544 -0.558079 1.071906 0.171236
H 4.920538 -2.857951 -2.046944 0.154933

H	2.689992	-2.385601	-3.037675	0.141821
H	4.747877	0.863373	0.098761	0.148791
H	5.947928	-1.217680	-0.485538	0.158018
H	2.970842	2.521851	-0.706453	0.209327
H	1.483402	-0.299573	-2.441776	0.127980
H	1.526234	1.909675	-1.498734	0.161194
H	2.297620	1.471625	1.440428	0.197966
H	-1.511300	1.482134	1.562889	0.190703
H	-0.643233	2.245767	-2.327543	0.171131
H	-2.991900	1.599227	-3.552369	0.167839
H	-5.416897	0.596113	-2.546911	0.189499
H	-5.657454	1.301566	-0.939180	0.195818
H	-5.150424	-0.383662	-1.090741	0.166851
H	-1.809098	4.362244	0.137638	0.184160
H	-0.520528	5.093774	1.133615	0.221942
H	-1.808599	4.130847	1.908535	0.175827
H	2.827868	-1.151488	3.518871	0.186167
H	1.090912	-1.050240	3.860515	0.165616
H	1.980820	0.394160	3.369870	0.173425
H	2.443794	-0.715271	1.102413	0.206096
H	1.552128	-2.113474	1.624560	0.166097

13 (E)-a1-endo

B3LYP/6-31G(d) energy= -1118.914745

Zero-point correction (ZPC)= 0.531645

Number of Imaginary Frequencies=0

C	-4.041735	-0.160210	-1.687902	-0.272245
C	-4.479256	0.713507	-0.491523	-0.152159
C	-4.769746	-0.368420	0.534595	-0.098302
C	-3.895058	-1.365997	0.332060	-0.118389
C	-3.028135	-0.973435	-0.849589	-0.163775
C	-3.114042	1.382134	-0.059524	-0.094982
C	-2.833257	2.711434	-0.770169	-0.477674
C	-2.069577	0.267403	-0.425567	-0.235809
C	-1.044095	-0.197273	0.569974	0.445652
C	-1.368166	-0.068560	2.033513	-0.371212
C	-0.925623	1.313439	2.585492	-0.478893
N	0.075183	-0.737445	0.136867	-0.463908
C	0.524778	-0.655954	-1.287599	-0.075317
C	1.685006	-1.633626	-1.359674	0.626255
N	1.948072	-2.087947	-0.105899	-0.457321
C	1.021459	-1.654009	0.944729	0.337886
C	1.002617	0.747561	-1.764944	-0.390139
C	2.077121	1.400031	-0.919730	0.150157
C	3.425363	1.033622	-1.054377	-0.191222
C	4.406013	1.637565	-0.265914	-0.133596
C	4.057314	2.620901	0.662852	-0.127062
C	2.721991	3.006962	0.792096	-0.133993
C	1.741770	2.400022	0.003787	-0.204203
C	1.781325	-0.908866	2.049027	-0.474538
C	0.248573	-2.885680	1.454391	-0.464095
C	3.071673	-2.985493	0.142444	-0.349145
O	2.289293	-1.898680	-2.382359	-0.500317
H	-3.772685	-2.268995	0.920977	0.154725
H	-5.501581	-0.286944	1.331675	0.166513
H	-5.275791	1.439446	-0.664387	0.160126
H	-2.482262	-1.777049	-1.348683	0.152300
H	-3.589823	0.395895	-2.516444	0.152980
H	-4.849042	-0.789989	-2.069829	0.185893
H	-3.145932	1.569097	1.015375	0.153612
H	-2.844075	2.601275	-1.860662	0.164105
H	-3.592775	3.454092	-0.505105	0.181128
H	-1.857702	3.125003	-0.486806	0.160118
H	-1.575358	0.568210	-1.345770	0.183112
H	-0.899731	-0.844065	2.632931	0.180096
H	-2.449588	-0.178395	2.147103	0.205278
H	-1.212349	1.371368	3.639603	0.196805

H	0.156081	1.446824	2.511420	0.186404
H	-1.404152	2.143391	2.061021	0.184236
H	2.741959	-3.935957	0.572006	0.182942
H	3.810122	-2.521923	0.803148	0.187488
H	3.532567	-3.177094	-0.827447	0.229685
H	1.138089	-0.633341	2.885067	0.174512
H	2.552282	-1.573622	2.448835	0.187963
H	2.268262	-0.014774	1.653244	0.209116
H	0.960498	-3.592363	1.889067	0.194656
H	-0.479579	-2.652847	2.231488	0.180493
H	-0.260835	-3.384518	0.624784	0.180006
H	-0.270673	-1.015153	-1.944670	0.211559
H	0.146055	1.421299	-1.856201	0.175237
H	1.371029	0.564374	-2.780584	0.217876
H	0.707809	2.728696	0.089180	0.127860
H	2.446057	3.791108	1.491657	0.151924
H	4.823678	3.097280	1.267244	0.159206
H	5.446362	1.350514	-0.389496	0.159199
H	3.708081	0.284000	-1.788319	0.170972

14 (Z)-b2a-endo

B3LYP/6-31G(d) energy= -1308.4460984

Zero-point correction (ZPC)= 0.553650

Number of Imaginary Frequencies=0

C	-4.167666	-0.483443	0.861060	-0.103037
C	-3.880414	-1.888328	0.361223	-0.150828
C	-2.826665	-2.331228	1.399998	-0.272348
C	-1.963103	-1.060967	1.214685	-0.157243
C	-3.022253	0.015177	1.352519	-0.117301
C	-3.002574	-1.723580	-0.944170	-0.094734
C	-2.904665	-2.998559	-1.789510	-0.466712
C	-1.614207	-1.284867	-0.350951	-0.226604
C	-0.903425	-0.113796	-0.944588	0.445445
C	-1.689707	1.075775	-1.427182	-0.383633
C	-1.944759	1.005229	-2.955503	-0.476399
N	0.406627	-0.112220	-1.052629	-0.422726
C	1.279198	-1.347227	-0.901080	0.028939
N	2.424754	-0.986774	-1.717483	-0.439599
C	2.455740	0.314055	-2.135202	0.619365
C	1.244309	1.024585	-1.528553	-0.097768
C	1.602685	-1.741996	0.499070	0.384078
C	1.459145	-2.926017	1.163165	-0.197791
C	2.049685	-2.740016	2.452412	-0.214863
C	2.521409	-1.459034	2.492358	0.364215
O	2.253602	-0.837185	1.296124	-0.485269
C	3.234192	-0.655833	3.521313	-0.536978
C	1.757084	1.987581	-0.418738	-0.379340
C	0.717103	2.834613	0.278255	0.154526
C	0.269677	4.035277	-0.294346	-0.194133
C	-0.692673	4.815394	0.347842	-0.124398
C	-1.215032	4.411311	1.579340	-0.128709
C	-0.765149	3.227558	2.166761	-0.134621
C	0.192980	2.443972	1.518247	-0.199382
O	3.306696	0.847713	-2.815667	-0.478982
C	3.466147	-1.953467	-2.031798	-0.339398
H	-5.113698	0.034972	0.743078	0.163670
H	-2.836739	1.020086	1.715919	0.160328
H	-1.064469	-0.960469	1.824645	0.158618
H	-0.953817	-2.151282	-0.355720	0.165831
H	-3.891393	-3.280464	-2.171129	0.180924
H	-4.746804	-2.536150	0.214289	0.157224
H	-3.234685	-2.400717	2.411463	0.180734
H	-3.438852	-0.935602	-1.562564	0.156279
H	-2.520574	-3.844548	-1.207727	0.157370
H	-2.245848	-2.859774	-2.655352	0.151685

H	-2.306397	-3.263403	1.153305	0.144969
H	0.751048	-2.189176	-1.362160	0.196267
H	3.049163	-2.808844	-2.575517	0.177422
H	2.316271	1.395622	0.310683	0.192687
H	2.482162	2.623968	-0.939036	0.210891
H	0.713559	1.574440	-2.304580	0.208451
H	4.195312	-1.443485	-2.662859	0.226831
H	3.956493	-2.309818	-1.120429	0.190306
H	1.002944	-3.829710	0.780587	0.168391
H	2.653713	0.225414	3.819716	0.185905
H	4.203326	-0.304020	3.149115	0.195842
H	3.409273	-1.266260	4.410387	0.193686
H	2.123058	-3.469845	3.246203	0.175130
H	-1.145509	2.923303	3.138309	0.151028
H	0.690035	4.370052	-1.240667	0.148294
H	-1.954100	5.025414	2.085441	0.159157
H	0.557411	1.533583	1.988715	0.135660
H	-1.021690	5.746709	-0.104075	0.160391
H	-2.553678	1.865471	-3.247110	0.199797
H	-1.176846	2.005670	-1.180100	0.214341
H	-1.015740	1.040078	-3.532835	0.175188
H	-2.482687	0.098077	-3.243414	0.181056
H	-2.644673	1.086425	-0.899206	0.201642

Protonated amine 1

B3LYP/6-31G(d) energy= -691.3503907

Zero-point correction (ZPC)= 0.308285

Number of Imaginary Frequencies=0

N	0.820463	-0.848357	-1.047317
C	0.651394	0.610768	-1.417906
C	1.193924	1.315320	-0.166789
N	1.822038	0.383350	0.619044
C	1.911476	-0.954067	0.046644
C	-0.810399	0.965638	-1.754905
C	-1.798520	0.419930	-0.743303
C	-2.070013	1.111097	0.448729
C	-2.952300	0.576736	1.387385
C	-3.569323	-0.656636	1.157260
C	-3.308837	-1.353233	-0.022402
C	-2.428712	-0.817098	-0.968536
O	1.063463	2.499425	0.057474
C	2.509701	0.759109	1.851853
C	1.513737	-2.056452	1.026059
C	3.256965	-1.226662	-0.634737
H	1.311699	0.825754	-2.263423
H	2.121010	0.195124	2.704321
H	2.319184	1.822034	2.006815
H	3.589896	0.599926	1.768392
H	2.270569	-2.150908	1.809407
H	0.552577	-1.835174	1.501453
H	1.453238	-3.023398	0.515531
H	4.052101	-1.208170	0.115457
H	3.490797	-0.464886	-1.385466
H	3.273258	-2.217312	-1.102489
H	-0.840096	2.059678	-1.792306
H	-1.044458	0.600390	-2.760869
H	-2.277764	-1.338610	-1.913413
H	-3.802776	-2.300059	-0.219959
H	-4.261260	-1.063834	1.888349
H	-3.167007	1.129718	2.297143
H	-1.599689	2.073358	0.630953
H	-0.090866	-1.167882	-0.668490
H	1.049823	-1.442797	-1.849388

Protonated amine 2

B3LYP/6-31G(d) energy= -769.9661563

Zero-point correction (ZPC)= 0.365578

Number of Imaginary Frequencies=0

N	0.222048	-0.157746	-0.397001	-0.671699
C	-0.186896	1.301055	-0.359187	-0.087785
C	1.127814	1.985806	0.008398	0.632343
N	2.144426	1.052435	-0.067307	-0.461017
C	1.735591	-0.221639	-0.636831	0.187355
C	-1.352730	1.549017	0.606534	-0.390464
C	-2.517863	0.619261	0.330561	0.144717
C	-2.770865	-0.467739	1.179835	-0.222935
C	-3.810257	-1.360658	0.903813	-0.123556
C	-4.605008	-1.176501	-0.227580	-0.125133
C	-4.363407	-0.093986	-1.078462	-0.123922
C	-3.326353	0.796957	-0.802711	-0.195483
O	1.229026	3.152651	0.312174	-0.457984
C	3.535344	1.506929	-0.006870	-0.349259
C	2.325643	-1.538099	-0.054178	0.039270
C	3.782559	-1.707278	-0.540673	-0.466822
C	2.272319	-1.546934	1.485094	-0.474241
C	1.502777	-2.719144	-0.624710	-0.483742
H	-0.461107	1.576313	-1.382751	0.229530
H	4.075603	1.030279	0.813715	0.194980
H	3.503205	2.583389	0.168980	0.234564
H	4.051121	1.309637	-0.952097	0.188291
H	-0.996323	1.429119	1.636960	0.184521
H	-1.626000	2.603676	0.496087	0.228364
H	-3.161168	1.649280	-1.458986	0.148997
H	-4.991104	0.063030	-1.950692	0.168044
H	-5.418007	-1.864138	-0.440049	0.169092
H	-4.005543	-2.187759	1.580037	0.164884
H	-2.182403	-0.593561	2.087865	0.140083
H	1.859626	-0.229995	-1.730388	0.191951
H	-0.001464	-0.592069	0.507475	0.406814
H	-0.298728	-0.687772	-1.101056	0.418814
H	2.840815	-0.721189	1.921783	0.184514
H	1.248252	-1.495961	1.882268	0.137011
H	2.697488	-2.482513	1.860480	0.196531
H	0.475344	-2.759178	-0.239907	0.141264
H	1.465434	-2.700475	-1.721317	0.169490
H	1.973319	-3.663008	-0.336022	0.202848
H	3.853363	-1.643924	-1.632859	0.166556
H	4.463895	-0.972437	-0.108329	0.176095
H	4.144841	-2.697065	-0.246631	0.187018

Imidazolidinone 2 iminium intermediate

B3LYP/6-31G(d) energy= -1003.4177967

Zero-point correction (ZPC)= 0.487732

Number of Imaginary Frequencies=0

N	-0.700252	0.391095	-0.228572	-0.453736
C	-0.127375	-0.818540	-0.892847	-0.095020
C	-1.374062	-1.435548	-1.544613	0.613233
N	-2.472247	-0.759504	-1.094553	-0.452227
C	-2.185676	0.207020	-0.047983	0.165306
C	0.632106	-1.850880	-0.017600	-0.377733
C	2.099698	-1.564709	0.222458	0.140319
C	2.566127	-1.191006	1.489180	-0.185916
C	3.921691	-0.931895	1.702346	-0.128753
C	4.829461	-1.042554	0.647673	-0.132078
C	4.377082	-1.423168	-0.619186	-0.130692
C	3.022620	-1.686893	-0.828192	-0.193804
O	-1.344575	-2.346931	-2.345353	-0.478953
C	-3.799574	-0.972021	-1.656644	-0.341373

C	-2.664412	-0.211999	1.411089	0.079336
C	-4.066411	0.409577	1.610011	-0.472220
C	-0.084570	1.556251	-0.117103	0.404019
C	1.334577	1.640989	-0.382732	-0.165516
C	2.057577	2.785632	-0.333203	-0.061037
C	3.519922	2.856169	-0.602561	-0.515942
C	-0.866135	2.811640	0.202328	-0.376681
C	-1.300326	3.551715	-1.085342	-0.462197
C	-2.771877	-1.742191	1.570282	-0.475078
C	-1.728136	0.324624	2.514867	-0.476375
H	0.521069	-0.486833	-1.707141	0.213913
H	-4.468757	-1.478960	-0.955190	0.189119
H	-3.675958	-1.601221	-2.539626	0.226403
H	-4.244277	-0.013837	-1.947225	0.175964
H	4.037772	3.304706	0.255920	0.204637
H	3.714594	3.523905	-1.453330	0.205098
H	3.955338	1.875384	-0.807832	0.197278
H	1.579115	3.730483	-0.083004	0.178583
H	1.862825	0.723246	-0.609669	0.197334
H	0.112925	-1.979758	0.935107	0.176097
H	0.528435	-2.794699	-0.566973	0.220242
H	2.683655	-2.010381	-1.810624	0.151872
H	5.081350	-1.536191	-1.438534	0.160673
H	5.885551	-0.851307	0.814323	0.159684
H	4.268734	-0.654301	2.693562	0.156314
H	1.868027	-1.116476	2.320378	0.138592
H	-1.955072	2.933460	-1.708331	0.175470
H	-1.850035	4.456719	-0.811741	0.199346
H	-0.438730	3.843077	-1.691827	0.179739
H	-2.669857	1.151190	-0.304963	0.179023
H	-0.244321	3.468185	0.814458	0.195635
H	-1.742722	2.586854	0.807298	0.192540
H	-3.465681	-2.192551	0.856541	0.170029
H	-1.809659	-2.250424	1.464827	0.163172
H	-3.145080	-1.967750	2.574396	0.176804
H	-0.710513	-0.069751	2.426141	0.154156
H	-1.673218	1.417478	2.539388	0.153873
H	-2.115042	0.009697	3.489043	0.183568
H	-4.034962	1.505254	1.560720	0.151668
H	-4.784802	0.059383	0.861485	0.165402
H	-4.460449	0.136445	2.593762	0.181044

C	-3.260115	-2.089008	-0.121608
C	-2.013459	2.895249	1.968993
H	1.156120	-2.578399	-0.439369
H	-3.763011	-1.226686	0.326997
H	-3.302183	-2.933556	0.567550
H	-3.757844	-2.355866	-1.059286
H	0.446672	-0.323410	1.518306
H	1.473162	-1.722869	1.815765
H	3.738908	-1.874782	0.577747
H	5.627554	-0.600256	-0.379459
H	5.351144	1.797768	-0.969772
H	3.172054	2.925656	-0.571550
H	1.286765	1.664157	0.426822
H	-1.781446	-0.892253	-2.265540
H	-2.766429	1.646739	-2.551218
H	-3.093683	3.677117	-0.757605
H	-2.452773	3.895320	1.958065
H	-2.539530	2.295093	2.720231
H	-0.967736	2.983114	2.286664
H	0.594149	-0.001498	-1.173146
H	0.398742	-1.338150	-2.122754

Protonated amine 5

B3LYP/6-31G(d) energy= -880.8667656

Zero-point correction (ZPC)= 0.330463

Number of Imaginary Frequencies=0

O	-1.639890	1.006159	0.473463
C	-1.855470	0.637057	-0.832328
C	-2.464339	1.654228	-1.512137
C	-2.636619	2.715166	-0.573983
C	-2.125103	2.282752	0.618825
C	-1.449344	-0.724633	-1.234867
N	-1.848517	-1.803360	-0.358921
C	-0.845649	-2.396824	0.368624
C	0.493153	-1.796432	-0.064166
N	0.108535	-0.911178	-1.238635
C	1.182039	-0.990261	1.056283
C	2.367650	-0.205137	0.536680
C	2.223607	1.153039	0.208065
C	3.293064	1.872202	-0.336569
C	4.516490	1.240415	-0.555504
C	4.671129	-0.109494	-0.225062
C	3.604167	-0.828353	0.312308
O	-0.966107	-3.243066	1.225678