

Spirocyclization enhances the Diels–Alder reactivities of geminally substituted cyclopentadienes and 4*H*-pyrazoles

Brian J. Levandowski | Nile. S. Abularrage | Ronald T. Raines

Department of Chemistry, Massachusetts Institute of Technology

Cambridge, Massachusetts, United States

Table of Contents

Table of Contents	S1
S1. M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) Energetic Data	S2
S2. M06-2X/6-31G(d) Optimized Cartesian Coordinates	S3
S3. Distortion/Interaction Analysis	S28

S1. M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) Energetic Data

	ΔE	ΔG
Ethylene	-78.563592	-78.532717
3-Cp	-271.439285	-271.339578
4-Cp	-310.737377	-310.609945
5-Cp	-350.071528	-349.915325
6-Cp	-389.385273	-389.19942
7-Cp	-428.679295	-428.465868
8-Cp	-467.978084	-467.736049
DiMe-Cp	-272.668586	-272.54745
Cp	-194.059101	-193.991748
Cp-Dimer	-388.096272	-387.937654
4-Cp-Dimer	-621.457139	-621.177476
DiMe-Cp-Dimer	-545.308259	-545.040921
Cp-Dimer-Adduct	-388.158664	-387.993482
4-Cp-Dimer-Adduct	-621.522563	-621.237194
DiMe-Cp-Dimer-Adduct	-545.372915	-545.100701
3-Cp-TS	-349.973306	-349.821283
4-Cp-TS	-389.277044	-389.09628
5-Cp-TS	-428.606729	-428.396852
6-Cp-TS	-467.918354	-467.67909
7-Cp-TS	-507.210578	-506.943492
8-Cp-TS	-546.508517	-546.212818
DiMe-Cp-TS	-351.201347	-351.027096
Cp-TS	-272.597027	-272.476785
3-Cp-Adduct	-350.044824	-349.886906
4-Cp-Adduct	-389.353656	-389.167209
5-Cp-Adduct	-428.684355	-428.468402
6-Cp-Adduct	-467.995432	-467.750163
7-Cp-Adduct	-507.290091	-507.016517
8-Cp-Adduct	-546.586014	-546.284221
DiMe-Cp-Adduct	-351.279217	-351.099014
Cp-Adduct	-272.671003	-272.544297
3N	-303.508582	-303.432655
4N	-342.806547	-342.702953
5N	-382.140838	-382.008385
6N	-421.454673	-421.292753
DiMeN	-304.737587	-304.640499
N	-226.127535	-226.083986

3N-TS	-382.043678	-381.914975
4N-TS	-421.347734	-421.19052
5N-TS	-460.678764	-460.492395
6N-TS	-499.991363	-499.775577
DiMeN-TS	-383.273973	-383.123233
N-TS	-304.666829	-304.570122

S2. M06-2X/6-31G(d) Optimized Cartesian Coordinates

Ethylene

C	0.00000000	0.00000000	-0.66354000
H	0.00000000	-0.92386700	-1.23441200
H	0.00000000	0.92386700	-1.23441200
C	0.00000000	0.00000000	0.66354000
H	0.00000000	-0.92386700	1.23441200
H	0.00000000	0.92386700	1.23441200

DiMe-Cp

C	-0.40725200	-1.17197800	0.00012900
C	-0.40728200	1.17196200	-0.00017200
H	-0.06936200	2.20312800	-0.00034500
H	-0.06913100	-2.20307000	0.00034000
C	0.54549600	0.00006300	-0.00001700
C	1.42605000	0.00032400	1.26114200
H	2.06958800	-0.88571200	1.27963100
H	2.06965100	0.88632200	1.27918600
H	0.80860300	0.00057000	2.16373100
C	1.42616800	-0.00031300	-1.26107500
H	2.06972200	0.88571400	-1.27959500
H	2.06976000	-0.88631900	-1.27896000
H	0.80882200	-0.00065100	-2.16373300
C	-1.67648800	0.73665500	-0.00037200
H	-2.56954300	1.35150100	-0.00050900
C	-1.67645800	-0.73670200	0.00032700
H	-2.56952000	-1.35154900	0.00048100

DiMe-Cp-TS

C	0.06256400	0.37378300	1.14972700
C	0.06278000	0.37379300	-1.14982500
C	-1.83752600	-0.77293100	0.68841500
C	-1.83770700	-0.77303100	-0.68826800

H	-1.50588100	-1.63971600	1.25139200
H	-1.50622700	-1.63991900	-1.25122400
H	0.27283200	0.13073600	-2.18808000
H	0.27246700	0.13081400	2.18803300
H	-2.47837300	-0.09102900	-1.23420700
H	-2.47806500	-0.09088400	1.23444400
C	0.80683800	-0.28000100	0.00002500
C	2.25777600	0.28730500	0.00017700
H	2.79853200	-0.06568100	0.88451700
H	2.79902900	-0.06651500	-0.88351600
H	2.25585200	1.37803300	-0.00033900
C	0.95177800	-1.80130400	-0.00011400
H	1.51845000	-2.11932100	-0.88227100
H	1.51773900	-2.11966200	0.88238300
H	0.00388200	-2.33662000	-0.00057000
C	-0.38960000	1.60828200	-0.70419400
H	-0.79676100	2.39225000	-1.33275700
C	-0.38968200	1.60830200	0.70400300
H	-0.79680600	2.39233000	1.33251400

DiMe-Cp-Adduct

C	-0.23873100	0.09462000	1.12140800
C	-0.23891200	0.09468300	-1.12141900
C	-1.16739900	-1.11248100	0.77786500
C	-1.16769000	-1.11231600	-0.77782800
H	-0.77028100	-2.04767700	1.18297400
H	-0.77105800	-2.04754300	-1.18330200
H	0.13219700	0.10634300	-2.14968400
H	0.13258800	0.10621300	2.14958600
H	-2.16693700	-0.97137200	-1.19628800
H	-2.16655400	-0.97193100	1.19673200
C	0.83746200	-0.00610400	-0.00010900
C	-1.02140900	1.31409200	-0.66793000
H	-1.56664500	1.98137700	-1.32684300
C	-1.02118300	1.31410500	0.66817600
H	-1.56616900	1.98140900	1.32726800
C	1.63617400	-1.31252300	-0.00004800
H	2.28399100	-1.35338000	-0.88317100
H	2.28390500	-1.35353600	0.88312800
H	1.01979700	-2.21256000	-0.00016400

C	1.84828600	1.14346600	-0.00011000
H	2.49407400	1.07745200	0.88291000
H	2.49392100	1.07773500	-0.88325200
H	1.36758400	2.12221400	0.00007300

DiMe-Dimer

C	-1.97905400	-0.37190000	-0.16300600
C	-1.96690800	1.13444700	-0.27793700
C	-0.71938000	-0.57013300	0.68846800
C	0.53221200	0.61777600	-1.41759200
C	0.71859500	-0.57127800	-0.68578300
H	-0.04231700	0.73950100	-2.32596900
H	0.53876100	-1.54975200	-1.12887500
H	-0.53982500	-1.54757100	1.13397900
H	-2.61381400	1.68338100	-0.95540500
C	1.25907500	1.65580800	-0.76667600
H	1.19565100	2.70772100	-1.02448200
C	1.96912800	1.13537400	0.27375600
H	2.61740700	1.68571900	0.94876200
C	1.97938200	-0.37134200	0.16364400
C	-0.53395000	0.62067900	1.41768100
H	0.04079000	0.74483100	2.32560200
C	-1.25883200	1.65724700	0.76293700
H	-1.19525100	2.70980600	1.01803100
C	-2.09746400	-1.15886400	-1.46952800
H	-1.34051700	-0.89545700	-2.20772300
H	-2.02404100	-2.23476100	-1.27234900
H	-3.07913800	-0.97627300	-1.92022300
C	-3.19309100	-0.78066400	0.71367000
H	-4.13021000	-0.53281200	0.20442000
H	-3.18504300	-1.86200300	0.89274000
H	-3.16840600	-0.26404000	1.67539400
C	2.09832700	-1.15409400	1.47263400
H	2.02441600	-2.23060100	1.27900800
H	3.08030400	-0.97036600	1.92221100
H	1.34183600	-0.88800600	2.21033400
C	3.19198000	-0.78420700	-0.71305100
H	4.12995100	-0.53566000	-0.20570400
H	3.18262100	-1.86611000	-0.88863600
H	3.16670900	-0.27065300	-1.67641700

Cp

C	-1.17724900	-0.28120900	-0.00001200
C	1.17747500	-0.28020000	0.00000800
H	2.20960300	-0.60849500	0.00001600
H	-2.20906200	-0.61047700	0.00001200
C	0.00055800	-1.21457100	-0.00000900
C	0.73487300	0.98854800	-0.00003800
H	1.34832500	1.88231500	0.00003900
C	-0.73574200	0.98790200	0.00003000
H	-1.34993400	1.88117000	-0.00002000
H	0.00083100	-1.87360900	0.87922800
H	0.00074500	-1.87372600	-0.87914900

Cp-TS

C	0.46255600	1.15404200	0.36091000
C	0.46232200	-1.15419600	0.36051600
C	-1.61646200	0.68954600	-0.33443700
C	-1.61662800	-0.68924200	-0.33433100
H	-2.04941200	1.23833400	0.49646700
H	-2.04962100	-1.23774500	0.49674300
H	0.39497700	-2.19179500	0.66940700
H	0.39531500	2.19154500	0.67014400
H	-1.54417200	-1.24066000	-1.26421100
H	-1.54367700	1.24077100	-1.26440800
C	0.36735700	-0.00023700	1.32291400
C	1.17871500	-0.70322400	-0.74183900
H	1.55754600	-1.32917600	-1.54200700
C	1.17883000	0.70330100	-0.74160200
H	1.55786900	1.32947400	-1.54149900
H	-0.49857500	-0.00023500	1.98590700
H	1.27960900	-0.00045800	1.94067000

Cp-Adduct

C	-0.08477600	-1.12481700	0.32412800
C	-0.08527700	1.12467300	0.32444500
C	1.18099700	-0.77718800	-0.52075400
C	1.18055100	0.77779100	-0.52066200
H	2.08029700	-1.17206300	-0.03775600
H	2.07963900	1.17309700	-0.03760700

H	-0.11506100	2.15172400	0.69182600
H	-0.11404700	-2.15194500	0.69134500
H	1.12582600	1.20249300	-1.52583900
H	1.12657500	-1.20176500	-1.52601500
C	-0.03098600	-0.00020100	1.37618200
H	0.89570300	-0.00015000	1.96137700
H	-0.89733600	-0.00050000	2.04247400
C	-1.27588900	0.66803300	-0.50041000
H	-1.91802800	1.32527100	-1.07687700
C	-1.27562900	-0.66837700	-0.50054200
H	-1.91751400	-1.32564100	-1.07725300

Cp-Dimer

C	-1.83587400	-0.92953500	-0.31244800
C	-2.00447200	0.54802300	-0.53817600
C	-0.71311100	-0.95902400	0.71100800
C	0.79057400	-0.12300500	-1.40420500
C	0.90548900	-1.13618900	-0.43417300
H	0.33112800	-0.22893300	-2.37942100
H	0.84770800	-2.19094000	-0.69110000
H	-0.54908500	-1.85221900	1.30790500
H	-2.61476300	0.97422000	-1.32570200
C	1.26467700	1.08412900	-0.84714400
H	1.16681100	2.05924500	-1.31178000
C	1.73009900	0.85097100	0.42493400
H	2.16553200	1.59039200	1.08676600
C	1.89607700	-0.63216900	0.59742700
H	2.91032400	-0.91996300	0.27996900
H	1.73999000	-1.00809400	1.61134700
H	-1.64098900	-1.51064800	-1.21834600
H	-2.74991800	-1.33567400	0.14717100
C	-0.62793600	0.32680900	1.27921500
H	-0.20342300	0.56766400	2.24512900
C	-1.40131200	1.22844000	0.46444100
H	-1.42858600	2.30425700	0.60279300

3-Cp

C	-0.46324500	-1.17321200	0.00004900
C	-0.46362000	1.17334800	0.00007000
H	-0.11634300	2.20021700	0.00013700

H	-0.11557900	-2.19995200	0.00007600
C	0.43378800	0.00023300	-0.00002800
C	1.76611600	-0.00001200	0.74057900
C	1.76611700	0.00001600	-0.74061300
H	2.02801500	-0.91448600	1.26110000
H	2.02848000	0.91437700	1.26101900
H	2.02844400	0.91448500	-1.26093800
H	2.02808500	-0.91437700	-1.26123900
C	-1.73818500	0.73324300	-0.00004400
H	-2.62978800	1.34895400	-0.00004500
C	-1.73796000	-0.73356200	-0.00002200
H	-2.62938300	-1.34953800	-0.00005600

3-Cp-TS

C	0.11650200	-0.42694000	1.15154700
C	0.11650800	-0.42702400	-1.15151500
C	1.32132300	1.37775700	0.69176500
C	1.32157100	1.37760300	-0.69181600
H	0.63094100	2.01766500	1.23303400
H	0.63144600	2.01743200	-1.23350000
H	-0.18748300	-0.28678100	-2.18443600
H	-0.18749700	-0.28663200	2.18445600
H	2.20832600	1.08357200	-1.24118700
H	2.20790300	1.08395500	1.24154100
C	-0.75999800	-0.08764000	0.00000800
C	-2.22896200	-0.47335900	-0.00002000
C	-1.81615300	0.96802900	-0.00005900
H	-2.63539100	-0.89319600	0.91364900
H	-2.63532900	-0.89326100	-0.91368800
H	-1.95278600	1.53765500	-0.91484400
H	-1.95284200	1.53771100	0.91468500
C	1.00644700	-1.40280900	-0.70094200
H	1.68529400	-1.96770100	-1.32939700
C	1.00644500	-1.40275900	0.70105300
H	1.68531300	-1.96756700	1.32955800

3-Cp-Adduct

C	0.27353300	-0.09549200	1.12697900
C	0.27348800	-0.09624600	-1.12692500
C	1.06784500	1.20279000	0.77815800

C	1.06823100	1.20202500	-0.77882500
H	0.54227400	2.08009000	1.16759200
H	0.54315600	2.07917000	-1.16926700
H	-0.11123800	-0.13980500	-2.14825500
H	-0.11114400	-0.13868100	2.14834300
H	2.07475800	1.19044900	-1.20414700
H	2.07416600	1.19188600	1.20396200
C	1.14085000	-1.25610600	-0.66814700
H	1.73639900	-1.88154100	-1.32429300
C	1.14140300	-1.25526500	0.66880500
H	1.73737000	-1.88001900	1.32522700
C	-0.75510100	-0.07278300	0.00003400
C	-2.00571400	0.73777600	-0.00027900
C	-2.06307600	-0.77812100	0.00032700
H	-2.28576600	1.25427700	-0.91438300
H	-2.28577300	1.25506000	0.91337400
H	-2.38145500	-1.27079000	0.91405700
H	-2.38150100	-1.27156200	-0.91296500

4-Cp

C	-0.95062500	-1.17609600	0.00001900
C	-0.61763300	1.14551300	0.00002000
H	-0.13749500	2.11854700	0.00003200
H	-0.76048000	-2.24406500	0.00001900
C	0.14164600	-0.15258500	0.00002600
C	1.27876300	-0.21486700	1.06966300
C	1.27871400	-0.21486900	-1.06967300
C	2.26766500	0.29063400	-0.00002700
H	1.48590300	-1.25571600	1.33573600
H	1.13635900	0.36993300	1.98121700
H	1.48584000	-1.25572000	-1.33575000
H	1.13626400	0.36992700	-1.98122000
H	3.27836600	-0.12363800	-0.00005000
H	2.33324500	1.38238600	-0.00003000
C	-2.14635500	-0.56415900	-0.00000900
H	-3.11841500	-1.04460700	-0.00003600
C	-1.93660000	0.89512800	-0.00000200
H	-2.73303600	1.63075600	-0.00002000

4-Cp-TS

C	0.53825000	-0.48429100	1.16523700
C	0.27018700	-0.39110500	-1.11895500
C	1.66018900	1.39859900	0.63412900
C	1.57184300	1.40567800	-0.74003600
H	0.99619100	2.02071200	1.22803100
H	0.86590500	2.05597900	-1.24685500
H	-0.13749200	-0.20577300	-2.10894600
H	0.36663100	-0.38153000	2.23311100
H	2.40512200	1.07013600	-1.34621900
H	2.57062100	1.08344400	1.12936900
C	1.20237400	-1.37465500	-0.81809300
H	1.79941100	-1.91703400	-1.54263500
C	1.36619000	-1.43238000	0.58026200
H	2.10593600	-2.03052000	1.10037400
C	-0.49986100	-0.11306700	0.14788300
C	-1.83022100	-0.95300700	0.19278000
C	-1.38798800	1.14525000	0.22842700
C	-2.58560500	0.30760500	-0.26837400
H	-2.08266300	-1.20876100	1.22569500
H	-1.87021900	-1.85301500	-0.42369900
H	-1.52395200	1.44585600	1.27307800
H	-1.08935900	2.01859900	-0.35695300
H	-3.56445100	0.50447500	0.17397100
H	-2.67381900	0.34566200	-1.35789200

4-Cp-Adduct

C	0.68718900	-0.08681000	1.13124900
C	0.42171500	-0.09337500	-1.09939200
C	1.45681800	1.19379600	0.68671300
C	1.29405500	1.17673700	-0.85976500
H	0.98812700	2.08369400	1.12002800
H	0.77915700	2.07524400	-1.21346200
H	-0.07493600	-0.12944600	-2.07273100
H	0.42885400	-0.11725600	2.19277800
H	2.24909500	1.11216900	-1.38654200
H	2.50150300	1.17493800	1.00629100
C	1.30250300	-1.27672600	-0.74248000
H	1.79395000	-1.92476700	-1.46036000
C	1.46265500	-1.27090000	0.58508200

H	2.10877000	-1.91581100	1.17101400
C	-0.49126300	-0.05095600	0.14569400
C	-1.55317000	1.06985000	0.19957500
C	-1.62908000	-1.09059400	0.20047400
C	-2.60980900	0.02589900	-0.22773000
H	-1.40973200	1.94406600	-0.44314700
H	-1.71388000	1.41160500	1.22840300
H	-1.53639800	-1.96952800	-0.44253600
H	-1.81699900	-1.42051100	1.22766200
H	-2.76402100	0.03195200	-1.31029300
H	-3.58317300	0.06213100	0.26636700

4-Cp-Dimer

C	-1.85276200	1.26958000	-0.01381200
C	-0.62185400	-0.46729500	0.88156600
C	0.20284800	0.75015000	-1.43857300
C	0.56521700	-0.42306400	-0.75669200
H	-0.49291700	0.82259500	-2.26405800
H	0.30880500	-1.41030300	-1.13619300
H	-0.38818200	-1.45540200	1.27359000
H	-2.54300200	1.84022600	-0.62746100
C	1.09377700	1.80225900	-1.01395500
H	0.98555600	2.84525700	-1.29280700
C	2.01884500	1.30480500	-0.16117600
H	2.79958200	1.86560100	0.34315600
C	-0.33488100	0.71305000	1.58530300
H	0.37824400	0.81718100	2.39346900
C	-1.07111900	1.76867100	0.99881000
H	-0.95011400	2.81848200	1.24297900
C	1.93341600	-0.19671000	-0.14732100
C	2.44600000	-0.91898900	1.12287500
C	3.14640500	-0.84450800	-0.90133500
C	3.83698400	-1.03248200	0.46340000
H	1.97903200	-1.90499400	1.21983700
H	2.36449400	-0.38851400	2.07517400
H	2.85503500	-1.80828500	-1.33133300
H	3.63676100	-0.23817300	-1.66625800
H	4.40631300	-1.95019600	0.62646000
H	4.46810900	-0.17476900	0.71285200
C	-1.91469100	-0.22556500	0.13655700

C	-2.38963200	-1.06245300	-1.07305200
C	-3.23013900	-0.67904000	0.86208900
C	-3.83003700	-0.98858400	-0.52304500
H	-2.00031900	-2.08465600	-1.00899100
H	-2.19515100	-0.66879700	-2.07435600
H	-3.05404300	-1.59845800	1.42914500
H	-3.72229900	0.05527300	1.50301100
H	-4.45960000	-1.87563100	-0.62094300
H	-4.36655800	-0.12539500	-0.92710900

5-Cp

C	1.35234000	1.12961700	-0.00002600
C	0.74104100	-1.13407700	0.00007900
H	0.15260600	-2.04580100	0.00012500
H	1.29418800	2.21322200	-0.00007300
C	0.13535700	0.24863600	0.00002700
C	-0.82669500	0.46546600	1.19058700
C	-0.82662600	0.46534900	-1.19062100
C	-2.11524400	-0.26951500	0.77649700
H	-1.01741100	1.54099000	1.28977900
H	-0.40589600	0.11117400	2.13546100
C	-2.11520400	-0.26958300	-0.77653500
H	-0.40576600	0.11096400	-2.13543300
H	-1.01733100	1.54086500	-1.28992900
H	-2.10289700	-1.29528200	1.15797700
H	-3.00417900	0.21205800	1.19261500
H	-2.10284900	-1.29538300	-1.15792300
H	-3.00411200	0.21196500	-1.19274100
C	2.08053300	-1.04339300	0.00004800
H	2.78209900	-1.87022200	0.00006300
C	2.46515600	0.37853600	-0.00002900
H	3.48758700	0.73923700	-0.00007900

5-Cp-TS

C	0.91796700	-0.53062300	1.13968300
C	0.38100100	-0.33895300	-1.08916200
C	2.03883800	1.34142900	0.54835400
C	1.75845400	1.42463400	-0.79735500
H	1.49691100	1.94808600	1.26766200
H	1.00892800	2.11385200	-1.17378000

H	-0.13378800	-0.11347000	-2.01929900
H	0.87894900	-0.47799000	2.22450100
H	2.49016600	1.10276700	-1.52893900
H	2.99847600	0.97006700	0.88711600
C	-0.25041800	-0.13042800	0.27475500
C	-1.01507200	1.17288500	0.53667700
C	-1.41902800	-1.15388600	0.44919900
C	-2.33866300	1.01302700	-0.23559800
H	-0.47516100	2.07706400	0.25362600
H	-1.21326900	1.23632500	1.61460600
C	-2.59869700	-0.51536500	-0.30026000
H	-1.65183200	-1.22670000	1.51832500
H	-1.15124000	-2.15043100	0.09333100
H	-3.15554600	1.55730800	0.24544800
H	-2.23539400	1.42647600	-1.24424100
H	-3.55865500	-0.79381800	0.14267800
H	-2.61467900	-0.85884900	-1.33948900
C	1.34671100	-1.32691000	-0.94529500
H	1.85665500	-1.82929100	-1.75968200
C	1.67565700	-1.44422500	0.41851200
H	2.47898300	-2.05090300	0.82108300

5-Cp-Adduct

C	-0.81598800	-0.00143500	1.12211800
C	-0.83399200	0.17320100	-1.11173000
C	-1.69345700	-1.21547100	0.69052100
C	-1.67111800	-1.11658800	-0.86142900
H	-1.26764900	-2.16175400	1.03688200
H	-1.17624100	-1.98751600	-1.30361400
H	-0.46383800	0.28468500	-2.13492200
H	-0.43139200	-0.05329600	2.14441000
H	-2.67018500	-1.04364500	-1.29794000
H	-2.70281100	-1.13939500	1.10233900
C	0.24803500	0.04415000	-0.00834700
C	1.15680700	-1.20601100	-0.13055700
C	1.23344400	1.24288900	0.08850800
C	2.55278200	-0.74211800	0.29863400
H	1.19322500	-1.52630200	-1.18094500
H	0.79768500	-2.05970400	0.45148600
C	2.61424800	0.67763900	-0.26499400

H	1.24833400	1.62206800	1.11800100
H	0.93695900	2.07737500	-0.55133500
H	2.61635900	-0.70603000	1.39376100
H	3.35200400	-1.39705300	-0.06014700
H	3.43737800	1.27627600	0.13551100
H	2.73620400	0.63110400	-1.35472100
C	-1.66696900	1.31693100	-0.56247400
H	-2.25118400	2.00576200	-1.16335100
C	-1.64711300	1.22103800	0.77033300
H	-2.21492900	1.81207300	1.48108400

6-Cp

C	1.63522400	-0.00003100	-1.11395500
C	2.73699800	-0.00000400	-0.34797000
C	0.98950100	0.00000300	1.13858600
C	2.33035300	0.00002500	1.06634300
H	0.39835400	0.00000800	2.04736300
H	3.01882900	0.00004700	1.90416000
H	3.76447400	0.00000300	-0.69400200
H	1.59199700	-0.00005400	-2.19837400
C	0.39710300	-0.00002900	-0.25314700
C	-0.45720600	1.26248000	-0.51586100
C	-0.45724400	-1.26250700	-0.51582200
C	-1.75847100	1.26174700	0.29013300
H	-0.70218400	1.29433900	-1.58699100
H	0.14173800	2.15243300	-0.29419500
C	-1.75850800	-1.26171400	0.29017600
H	-0.70223200	-1.29439500	-1.58694900
H	0.14166500	-2.15247900	-0.29413100
C	-2.57899400	0.00002200	0.01320700
H	-2.34261700	2.15640600	0.04757300
H	-1.52739000	1.31898200	1.36209100
H	-2.34267200	-2.15636800	0.04763600
H	-1.52742900	-1.31892500	1.36213500
H	-3.49464300	0.00004800	0.61449100
H	-2.89042200	0.00001000	-1.04095400

6-Cp-TS

C	0.60446000	-0.33558800	1.07808600
C	1.59280500	-1.30631400	0.97107100

C	1.21446900	-0.53087000	-1.12932600
C	1.96676200	-1.42617200	-0.38003100
C	1.96842300	1.45107000	0.81945900
C	2.34665200	1.32897300	-0.49884100
H	1.19316200	2.14982900	1.11964800
H	1.88397900	1.92964300	-1.27557600
H	1.21000800	-0.48574700	-2.21539500
H	2.79261000	-2.02044500	-0.75457400
H	2.08642300	-1.79165700	1.80561100
H	0.07032500	-0.11191700	1.99667800
H	3.31920100	0.92430100	-0.75206300
H	2.64267400	1.14865100	1.61163100
C	0.00021100	-0.15154500	-0.30443500
C	-0.70554600	1.17193400	-0.63398700
C	-1.06548800	-1.28102700	-0.52462300
C	-1.94762700	1.40225400	0.23225700
H	-1.01210900	1.13261200	-1.68971500
H	-0.03278600	2.02402300	-0.53873300
C	-2.32152600	-1.08169300	0.32600000
H	-1.35202700	-1.27257100	-1.58566100
H	-0.60847000	-2.25111900	-0.31653600
C	-2.96740200	0.27729100	0.05768800
H	-2.39834100	2.36804000	-0.02152900
H	-1.64714400	1.46598500	1.28767400
H	-3.03351300	-1.88888200	0.11932600
H	-2.05619700	-1.15968100	1.38869000
H	-3.83005800	0.43197200	0.71498000
H	-3.34488900	0.29707700	-0.97435700

6-Cp-Adduct

C	-0.74097500	0.07482000	1.06535400
C	-1.68167500	1.25274400	0.88342200
C	-1.36864500	0.10700500	-1.08786000
C	-2.05592100	1.27203900	-0.39886000
C	-1.66100200	-1.18156500	0.95521900
C	-2.10263800	-1.15582800	-0.53537100
H	-1.11264400	-2.09619300	1.20060400
H	-1.79454800	-2.06088900	-1.06650400
H	-1.30115400	0.15434000	-2.17810400
H	-2.79782300	1.91539600	-0.85975300

H	-2.05407400	1.87733200	1.68841300
H	-0.11420000	0.09339800	1.95984600
H	-3.18506000	-1.06151700	-0.64949300
H	-2.50558300	-1.11110900	1.64465400
C	-0.01595800	0.05301500	-0.31829500
C	0.81556500	-1.21146400	-0.59427800
C	0.89411500	1.26514000	-0.58065100
C	2.07924900	-1.27345700	0.27047500
H	1.10984500	-1.19485100	-1.65436200
H	0.23463700	-2.12546700	-0.45230100
C	2.16280800	1.23957500	0.27778100
H	1.18518800	1.24670100	-1.64152700
H	0.35001300	2.19766800	-0.41719500
C	2.96128500	-0.04422500	0.05145200
H	2.63757400	-2.18944000	0.04726200
H	1.79074500	-1.33224100	1.32945300
H	2.78012200	2.11692200	0.05430700
H	1.88592600	1.31420500	1.33836900
H	3.83797600	-0.07631200	0.70790000
H	3.33580500	-0.05474500	-0.98189400

7-Cp

C	-1.64536800	-0.63026600	-0.98680700
C	-2.91472900	-0.39467300	-0.62202200
C	-2.91472400	0.39467500	0.62203200
C	-1.64536100	0.63026900	0.98680500
C	-0.68878100	-0.00000200	-0.00000200
C	0.16495800	1.06937600	-0.72615000
C	1.41046500	1.55200600	0.03177500
C	2.65684400	0.71301200	-0.27843200
C	2.65684300	-0.71301200	0.27844300
C	1.41046700	-1.55200400	-0.03178200
C	0.16495600	-1.06938200	0.72614200
H	0.49182300	0.66503600	-1.69304000
H	-0.49766600	1.91017900	-0.95820100
H	1.61830700	2.58799500	-0.25820000
H	1.22232400	1.57153100	1.11410500
H	2.76991500	0.67106100	-1.37073700
H	3.54616400	1.23055800	0.10074600
H	3.54616700	-1.23055600	-0.10072800

H	2.76990100	-0.67106300	1.37074900
H	1.22233300	-1.57151400	-1.11411500
H	1.61830700	-2.58799700	0.25817900
H	-0.49766600	-1.91018900	0.95818600
H	0.49181700	-0.66504700	1.69303600
H	-3.80734300	-0.72483100	-1.14148400
H	-1.31024600	-1.17665000	-1.86276100
H	-1.31023000	1.17665500	1.86275600
H	-3.80733500	0.72483500	1.14149900

7-Cp-TS

C	-1.18688900	-0.67590400	1.01923000
C	-2.14363500	-1.47885200	0.41388900
C	-2.19923100	-1.15616200	-0.95480200
C	-1.28688900	-0.13922700	-1.21126700
C	-2.54786600	1.50410000	-0.29421700
C	-2.43261400	1.22127200	1.04863800
H	-0.85791700	-0.77543300	2.05057100
H	-2.82266700	-2.14752200	0.93077800
H	-2.92764400	-1.53700300	-1.66200300
H	-1.04053600	0.22566600	-2.20543900
C	-0.27851100	-0.13397000	-0.07262500
C	0.76085600	-1.25508400	-0.42627900
C	1.96192400	-1.37030500	0.52729700
C	3.18314700	-0.58136800	0.04531800
C	3.02236800	0.93848200	0.08588100
C	1.73798100	1.48351700	-0.55113300
C	0.46542700	1.17417400	0.25832300
H	0.21909900	-2.20109100	-0.47414300
H	1.14553700	-1.07091900	-1.43711500
H	1.68290900	-1.05861700	1.54294900
H	2.24511400	-2.42615400	0.60296600
H	4.06111200	-0.85816700	0.64112100
H	3.40034100	-0.89308000	-0.98573100
H	3.04431800	1.27380400	1.13226800
H	3.89203100	1.39638300	-0.40044700
H	1.83811200	2.57248900	-0.61978500
H	1.63944800	1.12690400	-1.58521200
H	0.74074900	1.14570900	1.32227900
H	-0.21933200	2.01477900	0.15631400

H	-3.45172200	1.24078600	-0.83077100
H	-1.95302900	2.28230500	-0.76160000
H	-1.72177600	1.75391200	1.67276300
H	-3.25055900	0.75120400	1.58072700

7-Cp-Adduct

C	-1.70811900	-0.00810000	-1.01739500
C	-2.22020200	1.27224300	-0.37980300
C	-1.65521000	1.36998000	0.82690200
C	-0.76103600	0.15630600	1.00773700
C	-1.73931700	-1.04619600	1.17841900
C	-2.41825100	-1.14319800	-0.21692000
H	-1.80497600	-0.08304200	-2.10401400
H	-2.99044000	1.91012300	-0.80043400
H	-1.86807000	2.10339500	1.59753300
H	-0.00536900	0.23061400	1.79248300
C	-0.25207600	-0.05536100	-0.45118100
C	0.62335600	1.08916000	-1.00574700
C	1.65015900	1.69249200	-0.04127500
C	2.58372500	0.70613700	0.68680800
C	2.85948700	-0.61306900	-0.04335600
C	1.73451200	-1.64553200	0.10169000
C	0.45854600	-1.39514700	-0.70946100
H	1.14330800	0.71382500	-1.89605400
H	-0.01203900	1.90845600	-1.35307300
H	2.25992700	2.39719300	-0.61959500
H	1.11833500	2.29713600	0.70469700
H	3.53405800	1.21517600	0.88381100
H	2.17447600	0.45830700	1.67441100
H	3.06842400	-0.42877000	-1.10626200
H	3.77302300	-1.05220400	0.37433700
H	2.12023600	-2.63048800	-0.18812300
H	1.47456000	-1.72463200	1.16757800
H	0.70428200	-1.43663200	-1.77998100
H	-0.21280000	-2.23853700	-0.52685800
H	-2.45524300	-0.86189800	1.98298700
H	-1.19337000	-1.96227000	1.42573000
H	-2.26556500	-2.12271500	-0.67842900
H	-3.49621100	-0.97132400	-0.16925400

8-Cp

C	-1.89262600	-0.80885100	0.85449700
C	-3.14172800	-0.49874100	0.47505400
C	-3.07749800	0.47523900	-0.62691800
C	-1.79047400	0.74567500	-0.89561000
H	-1.60423700	-1.49259700	1.64646100
H	-4.06029100	-0.89198000	0.89612000
H	-3.94237400	0.89285800	-1.13033700
H	-1.41519000	1.41129500	-1.66600000
C	2.11366300	1.29889500	-0.41792500
C	2.83260700	0.13972300	0.29901600
C	2.49276800	-1.26749200	-0.21050500
C	1.06207500	-1.78370100	-0.01052100
C	-0.02303400	-1.03085100	-0.80434500
C	-0.88603100	-0.04321800	0.02195400
C	-0.08044100	0.88205100	0.96072300
C	0.89756700	1.87363000	0.32571700
H	3.91395500	0.26777100	0.17521300
H	2.65120200	0.19826800	1.38088300
H	2.72277000	-1.30615200	-1.28489800
H	3.17832600	-1.97582100	0.27098200
H	1.05351100	-2.83523600	-0.31851900
H	0.81755900	-1.79051100	1.05985000
H	0.44006700	-0.50149200	-1.64353000
H	-0.72083600	-1.74591900	-1.25407900
H	-0.81228800	1.45621900	1.54163000
H	0.45584100	0.25934800	1.68764000
H	0.35063300	2.54965700	-0.34302100
H	1.27484000	2.50217000	1.14304400
H	2.82006100	2.12484200	-0.55893300
H	1.83536200	0.98313400	-1.42932800

8-Cp-TS

C	1.48090800	-0.92721100	-0.85783400
C	2.40002000	-1.53971800	-0.01597500
C	2.34973400	-0.90982500	1.24081200
C	1.40545700	0.10924700	1.19137400
C	2.65934100	1.56345200	0.00592300
C	2.75533800	0.92805700	-1.21246700
H	1.23467200	-1.27398900	-1.85808700

H	3.12332200	-2.28967300	-0.31608600
H	3.02752800	-1.09650000	2.06620800
H	1.08089100	0.67967200	2.05785600
H	3.48554800	1.53010700	0.70567400
H	1.96280700	2.38292500	0.15789700
H	2.15382200	1.23600800	-2.06157300
H	3.64958500	0.37174900	-1.46683300
C	-2.50712800	1.25800900	0.71564800
C	-3.25754100	0.40269700	-0.32166500
C	-3.04053800	-1.11322900	-0.21390400
C	-1.63396900	-1.66476200	-0.47841800
C	-0.56055800	-1.22726800	0.53910100
C	0.48576700	-0.17703000	0.01637400
C	-0.25431800	0.99082600	-0.64610400
C	-1.16762100	1.84988000	0.23822700
H	-4.33310600	0.57598300	-0.20132800
H	-3.01563800	0.74667400	-1.33654000
H	-3.34366900	-1.42671700	0.79540200
H	-3.73644400	-1.60525900	-0.90472400
H	-1.70720900	-2.75800700	-0.45277600
H	-1.32303400	-1.42004400	-1.50179000
H	-1.05137600	-0.81800400	1.42704900
H	0.00250000	-2.09638000	0.88303100
H	0.46515700	1.66882600	-1.10255400
H	-0.83957900	0.59456300	-1.48425100
H	-0.60105200	2.21413000	1.10565200
H	-1.40496000	2.74285800	-0.35388300
H	-3.14140100	2.10539200	1.00021600
H	-2.37771500	0.67693300	1.63489500

8-Cp-Adduct

C	-1.50709800	0.44728000	1.01476300
C	-2.37777500	-0.77466400	1.25182400
C	-2.46228500	-1.43505800	0.09399600
C	-1.64945400	-0.66133000	-0.92888500
C	2.51557200	1.19356700	0.70990200
C	3.26787200	0.25594300	-0.25194700
C	2.95178600	-1.23869500	-0.10343000
C	1.52871900	-1.71994900	-0.41537900
C	0.43102600	-1.19260100	0.53275300

C	-0.49165100	-0.09519100	-0.03851600
C	0.32864200	0.99477300	-0.74621700
C	1.25731100	1.85408300	0.12156600
H	3.10133200	0.57460600	-1.29013700
H	4.34439700	0.36879400	-0.07900700
H	3.64871300	-1.79653300	-0.74141800
H	3.18729100	-1.53134000	0.93001000
H	1.27705000	-1.49722200	-1.46036900
H	1.54571500	-2.81393900	-0.35149100
H	-0.19215400	-2.02915900	0.85103400
H	0.89723800	-0.81757500	1.45099900
H	0.91773100	0.52583500	-1.54308700
H	-0.33640400	1.68681300	-1.26598000
H	1.59454000	2.68239900	-0.51497500
H	0.67806800	2.31813100	0.93099400
H	2.28057700	0.65292000	1.63292300
H	3.18709500	2.00480500	1.01418200
C	-2.51667500	0.61177400	-1.19450300
C	-2.39682200	1.39096100	0.14684300
H	-1.08067000	0.91582800	1.90576800
H	-2.91330000	-0.98449100	2.17154800
H	-3.08172400	-2.29700700	-0.13021300
H	-1.35294500	-1.20563100	-1.82981600
H	-3.54844500	0.33489000	-1.42357500
H	-2.14214800	1.19291000	-2.04149900
H	-1.92023400	2.36632700	0.00815100
H	-3.36672100	1.56328500	0.61935300

3N

C	-0.53190300	-1.12032700	0.00016200
C	-0.53226900	1.12041100	0.00016500
H	-0.28203000	2.17686100	0.00067700
H	-0.28131300	-2.17670300	-0.00004800
N	-1.75139700	-0.71464600	-0.00002800
N	-1.75162600	0.71433700	-0.00018500
C	0.41474600	0.00018200	-0.00000300
C	1.74845600	-0.00003900	0.73819400
C	1.74838200	0.00008800	-0.73832500
H	1.99992900	-0.91560800	1.26166400
H	2.00019400	0.91542800	1.26171500

H	2.00008600	0.91566700	-1.26167300
H	1.99982200	-0.91536900	-1.26200500

TS-3N

C	0.11069700	-0.45516400	1.10480100
C	0.11067400	-0.45541300	-1.10471500
C	1.46123000	1.20707500	0.69119200
C	1.46168000	1.20666000	-0.69133000
H	0.83504700	1.91018600	1.23303100
H	0.83603000	1.90954000	-1.23408400
H	-0.11230500	-0.37644400	-2.16419600
H	-0.11225200	-0.37604800	2.16427700
H	2.30418700	0.80248600	-1.23964600
H	2.30349300	0.80353700	1.24034900
N	0.93258700	-1.41657600	-0.66676200
N	0.93258800	-1.41643200	0.66704000
C	-0.77619200	-0.03459300	0.00000100
C	-2.26696700	-0.33069100	0.00000200
C	-1.76763800	1.07975100	-0.00016800
H	-2.69023800	-0.73033100	0.91487800
H	-2.69020800	-0.73059100	-0.91477400
H	-1.86540800	1.65637800	-0.91522600
H	-1.86547600	1.65659700	0.91474700

4N

C	-1.00801400	-1.11039800	-0.00001900
C	-0.68874500	1.10365400	-0.00003500
H	-0.29688100	2.11763700	-0.00005200
H	-0.91633700	-2.19313800	-0.00001400
C	0.12730200	-0.14681300	-0.00004100
C	1.25837300	-0.20927000	1.07288600
C	1.25844800	-0.20928300	-1.07287200
C	2.25587900	0.27287500	0.00003900
H	1.44585700	-1.24871700	1.35607700
H	1.11714700	0.39103600	1.97391100
H	1.44595400	-1.24873300	-1.35603800
H	1.11729200	0.39101000	-1.97391600
H	3.25531200	-0.16622300	0.00007800
H	2.34701000	1.36255500	0.00003500
N	-2.15543900	-0.54319600	0.00001900

N	-1.94953400	0.88462200	0.00000500
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TS-4N

C	0.28882100	-0.41122200	1.07965900
C	0.53970600	-0.53593300	-1.10763600
C	1.65853900	1.28407300	0.72770200
C	1.75350100	1.25082100	-0.64555000
H	0.98637800	1.98208400	1.21811600
H	1.13238500	1.90461700	-1.25262900
H	0.44537900	-0.51895900	-2.18985800
H	-0.04435000	-0.27651200	2.10518400
H	2.63834300	0.85343100	-1.12774600
H	2.45748700	0.88865900	1.34337100
C	-0.51360600	-0.09589200	-0.14653900
C	-1.86684700	-0.89874900	-0.17332900
C	-1.35143200	1.18953500	-0.23806000
C	-2.58034700	0.39673700	0.25992900
H	-1.93316900	-1.78082100	0.46576400
H	-2.12150700	-1.17377700	-1.20022800
H	-1.01962000	2.05077600	0.34748900
H	-1.47130700	1.49300300	-1.28326400
H	-2.67826000	0.45543800	1.34737900
H	-3.54646600	0.61846900	-0.19699000
N	1.33237900	-1.43627800	-0.53186500
N	1.17972000	-1.35981300	0.80134400

5N

C	1.39806400	1.04266500	0.15912200
C	0.81466700	-1.09074300	-0.16669600
H	0.30882300	-2.04214900	-0.31180400
H	1.43780500	2.11646400	0.32297800
N	2.09268800	-1.02507200	-0.15698300
N	2.46913600	0.35088000	0.05337600
C	0.14681600	0.23603700	0.03623100
C	-0.80488800	0.26842700	1.25265500
C	-0.80429500	0.63053100	-1.11521100
C	-2.10320200	-0.37345200	0.72820400
H	-0.97628500	1.31647700	1.52398100
H	-0.38679500	-0.23881600	2.12602800
C	-2.10755000	-0.13063000	-0.80438500

H	-0.38805200	0.40191600	-2.09978200
H	-0.96935500	1.71294800	-1.06544500
H	-2.10543000	-1.44597000	0.94482100
H	-2.98230800	0.05070000	1.21964100
H	-2.12525600	-1.08338200	-1.34191200
H	-2.98359100	0.43414000	-1.13277900

TS-5N

C	0.91362700	-0.58746900	1.07861900
C	0.41164700	-0.35221500	-1.05525400
C	2.11172900	1.20814900	0.55875000
C	1.83560200	1.32253100	-0.78469000
H	1.59840600	1.83173300	1.28555100
H	1.11794100	2.05250200	-1.14800700
H	-0.03301800	-0.17095000	-2.03026800
H	0.94859600	-0.62827300	2.16398600
H	2.53889600	0.95211600	-1.52068500
H	3.04148600	0.76261800	0.89089100
N	1.64436000	-1.44323700	0.36812800
N	1.33763800	-1.30107600	-0.93219700
C	-0.26164800	-0.12350800	0.27342500
C	-0.98839600	1.19129800	0.55393900
C	-1.44128700	-1.13894800	0.41327700
C	-2.32099400	1.06945200	-0.21185400
H	-0.42197400	2.08068200	0.27295000
H	-1.17647400	1.25155700	1.63329100
C	-2.60712300	-0.45231800	-0.31646200
H	-1.67041800	-1.24427100	1.47979700
H	-1.18924300	-2.12708800	0.02275000
H	-3.12413100	1.61228600	0.29248000
H	-2.22060500	1.50853400	-1.20947000
H	-3.57035000	-0.72629300	0.12097600
H	-2.63203400	-0.76678500	-1.36425300

6N

C	1.68169500	0.00013700	-1.03687100
C	1.04967700	0.00002000	1.10584700
H	0.53118000	-0.00008800	2.06035700
H	1.74545900	0.00018400	-2.12207800
C	0.40538000	0.00003500	-0.25136800

C	-0.43733800	1.26935300	-0.51352300
C	-0.43729000	-1.26928600	-0.51365500
C	-1.74231400	1.26152200	0.28642700
H	-0.67145000	1.30447200	-1.58608400
H	0.16015500	2.15775400	-0.28316700
C	-1.74226200	-1.26158800	0.28630200
H	-0.67140900	-1.30430800	-1.58621800
H	0.16023100	-2.15769100	-0.28339300
C	-2.55969400	-0.00003600	0.00127800
H	-2.32370100	2.15688100	0.04261400
H	-1.51708500	1.31660800	1.35976800
H	-2.32361500	-2.15694600	0.04240400
H	-1.51702700	-1.31676900	1.35963600
H	-3.47842700	-0.00008400	0.59677800
H	-2.86428800	0.00001100	-1.05455200
N	2.32905200	-0.00013700	1.06711000
N	2.73707000	-0.00000100	-0.31463700

TS-6N

C	0.63154400	-0.35183900	1.04291900
C	1.21077000	-0.58372000	-1.07015600
C	2.03741100	1.35411000	0.81384300
C	2.40902500	1.20646700	-0.50256000
H	1.29040900	2.08702000	1.10662900
H	1.96701200	1.81980600	-1.28245500
H	1.28422400	-0.62803600	-2.15365100
H	0.16252700	-0.17322000	2.00604600
H	3.35162700	0.73556700	-0.75356200
H	2.68709400	1.00464800	1.60691200
C	-0.01138800	-0.14677500	-0.30731000
C	-0.68302400	1.18427700	-0.65017200
C	-1.07913800	-1.28033700	-0.49562600
C	-1.92268700	1.44059400	0.21260400
H	-0.98625700	1.14617500	-1.70623400
H	0.01314600	2.01899300	-0.55503500
C	-2.32995300	-1.03911800	0.35177700
H	-1.36146900	-1.29805400	-1.55679700
H	-0.62773500	-2.24743100	-0.25923200
C	-2.95404000	0.32359900	0.05146700
H	-2.36163700	2.40741600	-0.05561800

H	-1.62206600	1.51463800	1.26735800
H	-3.05331000	-1.83987000	0.16350700
H	-2.06707000	-1.09747500	1.41616900
H	-3.81750000	0.50176700	0.70094900
H	-3.32603000	0.32871200	-0.98254400
N	1.58175500	-1.28090100	0.95528000
N	1.93480300	-1.42255700	-0.33287400

DiMeN

C	-0.47123100	-0.01508900	1.11728400
C	-0.47124300	0.01428300	-1.11729100
H	-0.22748800	0.02877500	-2.17651200
H	-0.22747800	-0.02909000	2.17651200
C	0.53184600	-0.00001600	-0.00001200
N	-1.68690300	0.00973200	-0.72158200
N	-1.68689400	-0.00975400	0.72158800
C	1.39982600	1.26842900	0.01660400
H	2.04220500	1.27443900	0.90238800
H	2.04185100	1.29780300	-0.86897100
H	0.78070400	2.16935200	0.02860600
C	1.40063500	-1.26788200	-0.01660000
H	2.04306300	-1.27345500	-0.90235100
H	2.04262400	-1.29682100	0.86901300
H	0.78210000	-2.16920800	-0.02864300

TS-DiMeN

C	-0.05256300	-0.39928900	1.10202100
C	-0.05241600	-0.39946300	-1.10196900
C	1.85423000	0.67377700	0.68774000
C	1.85430900	0.67348200	-0.68784200
H	1.54819200	1.55230000	1.24843200
H	1.54839900	1.55176900	-1.24899200
H	-0.22092600	-0.25051500	-2.16525300
H	-0.22114900	-0.25011300	2.16526200
H	2.45168700	-0.04685900	-1.23320700
H	2.45154300	-0.04631700	1.23350000
C	-0.81054100	0.29700700	-0.00007100
N	0.39786900	-1.57484000	-0.67224400
N	0.39780200	-1.57471700	0.67255800
C	-2.25212000	-0.29373900	-0.00011100

H	-2.79417100	0.05243500	0.88499200
H	-2.79425900	0.05278900	-0.88502100
H	-2.23443000	-1.38502600	-0.00032500
C	-0.93227700	1.81503900	-0.00003700
H	-1.49260100	2.14322200	-0.88170700
H	-1.49205000	2.14314300	0.88202000
H	0.02833600	2.32918700	-0.00028800
N			
C	1.12301300	0.20364600	0.00004200
C	-1.12298400	0.20378300	0.00001600
H	-2.18172600	0.43969900	0.00016000
H	2.18178600	0.43942600	-0.00001300
C	0.00007200	1.19083300	-0.00003200
H	0.00013200	1.83893800	0.88448100
H	0.00011100	1.83890200	-0.88457000
N	-0.71853100	-1.01042500	-0.00003400
N	0.71840100	-1.01050900	0.00000300
TS-N			
C	0.52589600	1.10631600	0.25688100
C	0.52598900	-1.10630900	0.25680300
C	-1.59756300	0.68898500	-0.16021300
C	-1.59761400	-0.68901600	-0.16017800
H	-1.92464100	1.23867900	0.71776700
H	-1.92467900	-1.23865000	0.71784300
H	0.54806200	-2.16831600	0.47552500
H	0.54788600	2.16831500	0.47564800
H	-1.61345400	-1.23858400	-1.09360600
H	-1.61333800	1.23850700	-1.09366900
C	0.57677700	-0.00002100	1.26629900
H	-0.18053000	-0.00007900	2.04757700
H	1.57687100	0.00000300	1.72879000
N	0.99879300	-0.66994600	-0.90953800
N	0.99876600	0.67000200	-0.90952400

S3. Distortion/Interaction Analysis

The distortion/interaction analysis was performed on transition state structures with forming bond lengths of 2.26 Å.

Electronic Activation Energies

8-Cp	-546.508460
7-Cp	-507.210538
6-Cp	-467.918326
5-Cp	-428.606738
4-Cp	-389.277096
3-Cp	-349.973903

Diene Distortion Energies

8-Cp	-467.946547
7-Cp	-428.648586
6-Cp	-389.355908
5-Cp	-350.044497
4-Cp	-310.713587
3-Cp	-271.416721

Dienophile Distortion Energies

3-Cp	-78.554505
4-Cp	-78.553905
5-Cp	-78.553521
6-Cp	-78.553183
7-Cp	-78.552812
8-Cp	-78.552745

TS-3-Cp-Ethylene 2.26 Å Geometry

C	0.10299700	-0.44308200	1.15634900
C	0.10572300	-0.45386800	-1.14968900
C	1.31784000	1.40284100	0.68271500
C	1.35407200	1.37314000	-0.69005400
H	0.59090200	2.02413600	1.19680700
H	0.67100900	1.98249500	-1.27393700
H	-0.19152800	-0.30327400	-2.18288900
H	-0.19312300	-0.28589000	2.18885500
H	2.24243300	1.03718200	-1.21203500
H	2.18020800	1.10932900	1.26953900
C	-0.75947200	-0.08979900	0.00046100

C	-2.23706800	-0.45119200	-0.00373900
C	-1.80104000	0.98146000	-0.00930200
H	-2.65168900	-0.86053300	0.91091400
H	-2.64492700	-0.87146000	-0.91648200
H	-1.92276100	1.54951200	-0.92714100
H	-1.93169100	1.55740300	0.90235200
C	1.00009800	-1.41279100	-0.69657400
H	1.68230600	-1.97856600	-1.32049700
C	0.99848800	-1.40574900	0.71327800
H	1.67904200	-1.96609300	1.34385500

TS-4-Cp-Ethylene 2.26 Å Geometry

C	-0.53579700	-0.48629600	-1.16503200
C	-0.26923700	-0.39600400	1.11996200
C	-1.66152400	1.40011000	-0.63417200
C	-1.57646200	1.40770600	0.73865800
H	-0.99473800	2.01946600	-1.22785100
H	-0.86876000	2.05397400	1.24803300
H	0.13625400	-0.20918500	2.11052900
H	-0.36390300	-0.38086200	-2.23258300
H	-2.40879200	1.06822300	1.34392100
H	-2.56930700	1.08150300	-1.13203200
C	-1.20219500	-1.37648400	0.81763000
H	-1.80033200	-1.91931500	1.54092000
C	-1.36482900	-1.43297700	-0.58221900
H	-2.10451200	-2.03030300	-1.10334100
C	0.50003100	-0.11355700	-0.14603400
C	1.83198600	-0.95145100	-0.19237600
C	1.38579700	1.14668700	-0.22505400
C	2.58692400	0.31050000	0.26577300
H	2.08290900	-1.20934500	-1.22508000
H	1.87396100	-1.85002100	0.42604500
H	1.51790600	1.45202600	-1.26879500
H	1.08688400	2.01689600	0.36479000
H	3.56290700	0.50902800	-0.18211700
H	2.68135800	0.34851600	1.35474900

TS-5-Cp-Ethylene 2.26 Å Geometry

C	-0.91767200	-0.53092400	-1.13915600
C	-0.38022800	-0.34001600	1.08973200
C	-2.03920700	1.34039400	-0.54930100

C	-1.76040600	1.42537800	0.79631900
H	-1.49685000	1.94645300	-1.26883800
H	-1.01112600	2.11470800	1.17296300
H	0.13426800	-0.11414200	2.01991800
H	-0.87860200	-0.47818800	-2.22397500
H	-2.49182500	1.10245800	1.52772600
H	-2.99827200	0.96809300	-0.88865000
C	0.25067000	-0.13056000	-0.27419300
C	1.01452500	1.17332100	-0.53558600
C	1.41957200	-1.15350800	-0.44968900
C	2.33822400	1.01363800	0.23641000
H	0.47384900	2.07675700	-0.25178400
H	1.21243600	1.23754200	-1.61358000
C	2.59978200	-0.51459800	0.29871900
H	1.65124100	-1.22666300	-1.51902200
H	1.15247200	-2.15002800	-0.09320500
H	3.15460100	1.55959700	-0.24358700
H	2.23433700	1.42531900	1.24571900
H	3.55931400	-0.79155200	-0.14607900
H	2.61781000	-0.85936400	1.33748500
C	-1.34635100	-1.32711700	0.94585600
H	-1.85650200	-1.82938300	1.76018800
C	-1.67530400	-1.44445200	-0.41820100
H	-2.47877900	-2.05094900	-0.82074100

TS-6-Cp-Ethylene 2.26 Å Geometry

C	0.60395500	-0.33417300	1.07813000
C	1.59230600	-1.30614800	0.97146900
C	1.21670200	-0.52778500	-1.12830400
C	1.96745500	-1.42539600	-0.37844400
C	1.96530200	1.45119400	0.81967700
C	2.34526600	1.32638600	-0.49902100
H	1.19111300	2.15235600	1.11700400
H	1.88609300	1.92939400	-1.27605700
H	1.21256200	-0.48365600	-2.21445000
H	2.79349500	-2.01966600	-0.75257900
H	2.08457700	-1.79220700	1.80639300
H	0.06838600	-0.11226400	1.99631900
H	3.31926000	0.92337700	-0.74939900
H	2.63954700	1.15189100	1.61304300

C	0.00039200	-0.15101300	-0.30496400
C	-0.70635200	1.17171000	-0.63503800
C	-1.06412600	-1.28109700	-0.52616600
C	-1.94713200	1.40172100	0.23301700
H	-1.01504700	1.13049000	-1.69008400
H	-0.03383000	2.02435400	-0.54273100
C	-2.32063900	-1.08309000	0.32420600
H	-1.35020800	-1.27260100	-1.58732200
H	-0.60666900	-2.25099500	-0.31811200
C	-2.96680200	0.27648700	0.05900900
H	-2.39853300	2.36745400	-0.01974500
H	-1.64530000	1.46504400	1.28805500
H	-3.03270100	-1.88959900	0.11510600
H	-2.05602300	-1.16389600	1.38685600
H	-3.82805600	0.43004100	0.71841500
H	-3.34663500	0.29771400	-0.97213700

TS-7-Cp-Ethylene 2.26 Å Geometry

C	1.19117100	-0.67274800	-1.01904000
C	2.14594800	-1.47782800	-0.41006600
C	2.19868000	-1.15432200	0.95711500
C	1.28607100	-0.13509300	1.21083900
C	2.54367800	1.50404500	0.29473300
C	2.43039300	1.21696700	-1.04913100
H	0.86286800	-0.77587500	-2.05029400
H	2.82560200	-2.14724300	-0.92517500
H	2.92526800	-1.53475800	1.66642000
H	1.03703700	0.22893000	2.20468500
C	0.27866200	-0.13344700	0.07112100
C	-0.75924300	-1.25600100	0.42373900
C	-1.96152100	-1.37076000	-0.52835500
C	-3.18241700	-0.58252100	-0.04414000
C	-3.02298000	0.93758200	-0.08339600
C	-1.73732900	1.48287500	0.55082700
C	-0.46700200	1.17291900	-0.26184100
H	-0.21683900	-2.20173500	0.46952400
H	-1.14302400	-1.07391000	1.43530900
H	-1.68396800	-1.05872900	-1.54429700
H	-2.24474200	-2.42660400	-0.60403700
H	-4.06101800	-0.85930700	-0.63901300

H	-3.39805800	-0.89537300	0.98688700
H	-3.04790200	1.27410000	-1.12931900
H	-3.89180400	1.39414700	0.40567700
H	-1.83736300	2.57180500	0.62006200
H	-1.63633500	1.12585100	1.58453300
H	-0.74569300	1.14040500	-1.32480600
H	0.21742100	2.01443700	-0.16525800
H	3.44843700	1.24509300	0.83191100
H	1.95002900	2.28613800	0.75717100
H	1.72345300	1.75213800	-1.67558000
H	3.25197700	0.75048900	-1.57882400

TS-8-Cp-Ethylene 2.26 Å Geometry

C	1.48820200	-0.92089500	-0.85702700
C	2.40257300	-1.53623100	-0.00917500
C	2.34585900	-0.90723700	1.24616600
C	1.39941800	0.11118500	1.19307200
C	2.65653500	1.56439700	0.00335200
C	2.75081600	0.91956600	-1.21214500
H	1.24489300	-1.27128200	-1.85685700
H	3.12827100	-2.28495700	-0.30653300
H	3.01977900	-1.09331400	2.07488600
H	1.06999100	0.68044200	2.05846300
H	3.48335200	1.53478900	0.70253700
H	1.96197300	2.38658200	0.14931400
H	2.15398000	1.23018400	-2.06364100
H	3.64810300	0.36752200	-1.46517600
C	-2.50024700	1.25598600	0.72105500
C	-3.25684000	0.40495800	-0.31544100
C	-3.04084100	-1.11159800	-0.21413600
C	-1.63585900	-1.66518800	-0.48382000
C	-0.55889700	-1.23299300	0.53207800
C	0.48489500	-0.17732000	0.01468200
C	-0.25551100	0.98933000	-0.64933300
C	-1.16625500	1.85139700	0.23421300
H	-4.33170500	0.57874100	-0.18974600
H	-3.01915800	0.75227600	-1.33019100
H	-3.34169800	-1.42846800	0.79480000
H	-3.73924900	-1.60027800	-0.90482100
H	-1.71211500	-2.75828600	-0.45951500

H	-1.32663500	-1.42004900	-1.50762000
H	-1.04736000	-0.83226900	1.42516800
H	0.00672600	-2.10388000	0.86711800
H	0.46340500	1.66491500	-1.11034100
H	-0.84354100	0.59128600	-1.48467300
H	-0.59667100	2.22312300	1.09643700
H	-1.41052400	2.73959300	-0.36237600
H	-3.13332900	2.10087100	1.01554400
H	-2.36157500	0.67031900	1.63597900