

Efficient, Regio- and Stereoselective Formation of Azocan-2-ones via 8-*Endo* Cyclization of α -Carbamoyl Radicals

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Part 2

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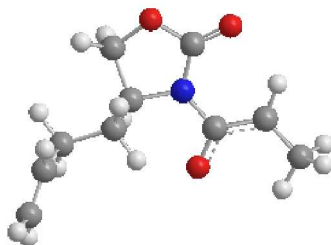
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1. Table S1. The Comparison of UB3LYP/6-31G* and UBHandHLYP/6-31G*

Radicals	Relative energy (kcal/mol)	
	UB3LYP/6-31G*	UBHandHLYP/6-31G*
R-11-Z	8.9	9.4
R-11-E	0	0
TS-11-Z-E	13.0	12.8
TS-11-8E	15.9	17.5
TS-11-7E	25.6	27.1
TS-11-8Z1	22.7	24.7
TS-11-8Z2	23.0	25.0
TS-11-7Z	26.1	27.9
P-12/13	1.9	-1.5
P-11-7E	14.2	10.4
P-14 (bb)	4.0	1.0
P-14 (bc)	3.3	0.3
P-11-7Z	9.5	6.0

2. Calculations (UB3LYP/6-31G*) on the Reactions of Radical R-11

R-11-E



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-11-E HF = -669.8806613

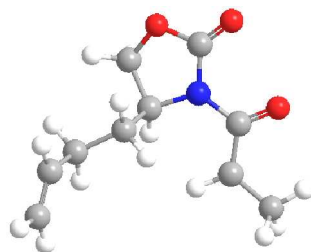
Sum of electronic and thermal Free Energies= -669.693822

O 2

C

C	1	7.60609105			
C	1	1.44482772	2	25.54998357	
O	3	1.23564309	1	123.25638447	2 -80.80799961
N	3	1.41719249	1	118.96485290	4 -179.54432244
C	5	1.47014139	3	119.91310201	1 -178.36631677
C	6	1.53786971	5	112.19204318	3 76.16923698
C	7	1.54077025	6	112.71471384	5 -172.05268444
C	2	1.33304458	1	51.74078827	3 -76.46398894
H	6	1.09309680	5	108.94567706	3 -45.33240935
H	7	1.09912737	6	108.97227953	5 65.21435215
H	7	1.09367900	6	108.36350548	5 -51.33189599
H	8	1.10158381	7	109.57196336	6 -55.64009448
H	8	1.09774933	7	109.39802713	6 60.91765064
H	9	1.09150066	2	119.18972849	1 -124.41489731
H	2	1.08826023	1	86.84966916	3 59.03492764
H	2	1.08663487	1	134.94817887	3 -175.70332789
C	6	1.53905820	5	99.80148569	3 -162.58206163
H	18	1.09562594	6	112.50955266	5 95.00569445
H	18	1.09158562	6	113.46032196	5 -140.26722318
O	18	1.44036594	6	105.07505437	5 -22.73817365
C	21	1.36068343	18	109.99060164	6 20.69106558
O	22	1.20713245	21	122.79974100	18 171.28227613
C	1	1.48521537	3	120.32827222	4 0.68405359
H	24	1.10027008	1	110.64668658	3 -120.14958830
H	24	1.09171752	1	111.30686414	3 1.20706019
H	24	1.09994557	1	110.68731587	3 122.81885075
H	1	1.08279568	3	119.04451284	4 -178.66598649

R-11-Z



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

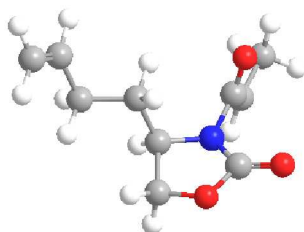
Calculation for R-11-Z HF = -669.8656107

Sum of electronic and thermal Free Energies= -669.679676

0 2

C					
C	1	5.94805300			
C	1	1.45530979	2	105.62920758	
O	3	1.22697105	1	121.59075026	2 146.34022227
N	3	1.41833210	1	116.92906967	4 178.84245808
C	5	1.47086470	3	126.25202502	1 1.36683663
C	6	1.53968442	5	112.53931032	3 78.42479751
C	7	1.54068508	6	113.15160753	5 -171.90998214
C	2	1.33299457	1	61.53499147	3 15.28505786
H	6	1.09475641	5	110.32378410	3 -45.33681548
H	7	1.09835340	6	108.48884921	5 65.35432303
H	7	1.09602238	6	109.25932855	5 -50.15233201
H	8	1.10091941	7	109.36075180	6 -56.03808683
H	8	1.09855803	7	109.71890275	6 60.36400803
H	9	1.09129084	2	119.18875757	1 -135.14683759
H	2	1.08845844	1	73.80139197	3 156.68856465
H	2	1.08649185	1	141.61675688	3 -90.94627450
C	6	1.53900401	5	99.59684358	3 -161.08442456
H	18	1.09647639	6	111.94488508	5 91.15506303
H	18	1.09188632	6	113.40512958	5 -144.62582075
O	18	1.43107713	6	104.66850134	5 -26.90288362
C	21	1.37314426	18	109.99811564	6 23.53192614
O	22	1.19703366	21	122.90799807	18 171.63063320
C	1	1.48550911	3	120.37634430	4 0.17804415
H	24	1.10021753	1	110.95423998	3 -120.34965083
H	24	1.09152231	1	110.50997392	3 0.74109604
H	24	1.09994176	1	110.95326455	3 121.95711208
H	1	1.08483638	3	121.10064081	4 -179.48915282

TS-11-Z-E



#p ub3lyp/6-31g* opt=(ts,modredundant,noeigentest,nrscale,calcf) scfcyc=200
optcyc=500 freq=noraman iop(1/8=5)

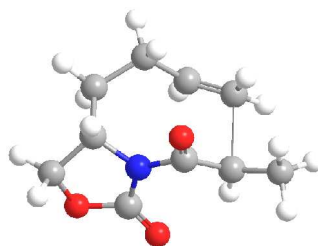
Calculation for TS-11-Z-E HF = -669.8601167

Sum of electronic and thermal Free Energies= -669.673163

0 2

C					
N	1	1.45044199			
C	2	1.39076036	1	119.95334354	
O	1	1.23170813	2	121.05094842	3 -64.05266611
C	1	1.43203535	4	123.72216156	2 179.02632509
C	2	1.47064584	1	122.25537074	4 84.22577803
C	6	1.54407131	2	98.55410955	1 -175.75797251
H	7	1.09200582	6	113.30971779	2 144.64997651
H	7	1.09626556	6	111.81047533	2 -91.19877610
O	3	1.37079882	2	108.14940604	1 165.45850294
O	3	1.20355204	2	127.93699252	1 -16.44477019
C	5	1.48424980	1	122.29869355	4 0.39996278
H	12	1.09953023	5	110.97023227	1 -124.57529104
H	12	1.09185446	5	110.86923406	1 -2.75431913
H	12	1.09999607	5	110.46962539	1 118.04126740
H	5	1.08679855	1	117.94863045	4 179.05255591
H	6	1.09766565	2	109.98960197	1 68.60554881
C	6	1.53849861	2	113.75038040	1 -54.78815359
H	18	1.09616752	6	109.08357834	2 50.52377526
H	18	1.09714806	6	109.15600297	2 -65.08749397
C	18	1.54114587	6	112.67485617	2 172.12655708
H	21	1.09802876	18	110.60474860	6 59.65113001
H	21	1.10181264	18	108.50912397	6 -56.80988666
C	21	1.50512687	18	112.39549201	6 -177.84745396
H	24	1.09139745	21	115.63999857	18 59.07151214
C	24	1.33298912	21	125.18222133	18 -120.22254595
H	26	1.08846267	24	121.77301393	21 -0.45329685
H	26	1.08655075	24	121.76456155	21 179.61654043

TS-11-8E



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-11-8E HF=-669.8611103

Sum of electronic and thermal Free Energies= -669.668486

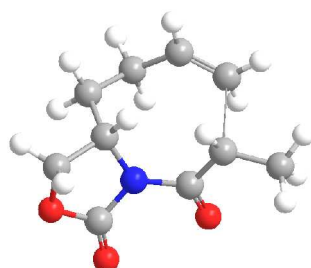
O 2

C

C

	1	2.19163851			
C	1	1.45365587	2	92.78151965	
O	3	1.22967362	1	124.25336894	2 -85.26390298
N	3	1.42351355	1	116.81303520	2 85.63939134
C	5	1.46592359	3	120.91569123	1 -147.19105616
C	6	1.54420939	5	111.78036355	3 86.51675883
C	7	1.54835561	6	115.81011911	5 -48.61700500
C	2	1.37912668	1	111.27205480	3 -45.72805177
H	6	1.09121134	5	109.15171696	3 -36.68531901
H	7	1.09831891	6	107.64288323	5 -171.30292028
H	7	1.09913794	6	108.52899844	5 73.77168710
H	8	1.10141072	7	106.74275761	6 -165.79557846
H	8	1.09613254	7	110.36190092	6 -50.41270603
H	9	1.09045048	2	118.74311614	1 -89.43140180
H	2	1.08760879	1	89.81319968	3 75.70975975
H	2	1.08690676	1	92.48776262	3 -168.58330416
C	6	1.53477485	5	99.52618720	3 -154.80382418
H	18	1.09586165	6	112.41367408	5 90.31243216
H	18	1.09195123	6	113.63632034	5 -144.42318193
O	18	1.44272424	6	104.20721585	5 -27.11387609
C	21	1.36772961	18	109.46814905	6 23.84200130
O	22	1.20693535	21	122.91857928	18 170.13266074
C	1	1.49898249	3	118.87541673	4 22.16107592
H	24	1.10003543	1	110.38540390	3 88.88134387
H	24	1.09610988	1	111.33879741	3 -152.58188669
H	24	1.09320019	1	111.04370838	3 -30.49584495
H	1	1.08349189	3	116.55872907	4 173.55832635

TS-11-8Z1



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

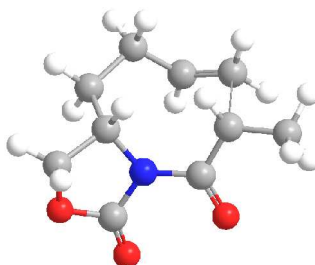
Calculation for TS-11-8Z1 HF=-669.8494126

Sum of electronic and thermal Free Energies= -669.657722

0 2

C					
C	1	2.23604058			
C	1	1.47114310	2	101.97411336	
O	3	1.22183909	1	121.78088857	2 94.89867360
N	3	1.42643320	1	117.32988910	2 -86.16709545
C	5	1.47087725	3	127.62721122	1 18.28126324
C	6	1.54445102	5	113.49600652	3 91.10724557
C	7	1.54408191	6	115.91275549	5 -52.81478497
C	2	1.36975812	1	108.51997264	3 71.87003075
H	6	1.09157964	5	110.76730894	3 -33.60589128
H	7	1.09922827	6	106.91539354	5 -175.55073680
H	7	1.09767621	6	108.59594548	5 69.67144038
H	8	1.09603089	7	109.39819672	6 71.10765949
H	8	1.09978495	7	107.45867008	6 -173.57650604
H	9	1.09089625	2	119.27120928	1 93.41478678
H	2	1.08750687	1	87.85867395	3 -49.11845038
H	2	1.08663110	1	93.95170133	3 -164.53750898
C	5	1.41061248	3	122.55928573	1 -157.62938683
O	18	1.37658127	5	107.55812994	3 165.31927146
C	19	1.43341065	18	109.66697194	5 -9.89148107
H	20	1.09221019	19	108.34880345	18 146.64832073
H	20	1.09700332	19	109.14850639	18 -94.11434039
O	18	1.19734670	5	129.69230922	3 -14.10712343
C	1	1.50185735	3	116.31012311	4 -14.17666212
H	24	1.09485652	1	111.43962155	3 168.12094971
H	24	1.10014305	1	110.44228533	3 -72.45383669
H	24	1.09306261	1	111.07757233	3 45.66055718
H	1	1.08580753	3	118.20674183	4 -159.86011201

TS-11-8Z2



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscalc,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

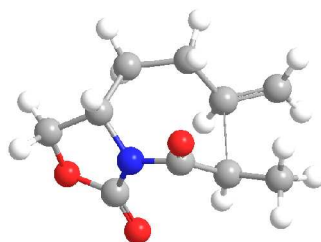
Calculation for TS-11-8Z2 HF =-669.8488665

Sum of electronic and thermal Free Energies= -669.657177

0 2

C					
C	1	2.23703163			
C	1	1.46602887	2	101.96225632	
O	3	1.22231412	1	121.98658403	2 100.30893821
N	3	1.42484030	1	117.28532719	2 -78.60974085
C	5	1.47685373	3	128.50405216	1 -8.94263731
C	6	1.54388726	5	114.18443709	3 99.71754891
C	7	1.54472494	6	117.26182030	5 -70.79985656
C	2	1.36881383	1	106.42588629	3 45.06135021
H	6	1.09285688	5	110.78239992	3 -26.27083350
H	7	1.09888319	6	107.18959754	5 167.55065785
H	7	1.09795883	6	107.83435027	5 53.38269147
H	8	1.10027533	7	106.93367231	6 -178.76357578
H	8	1.09867114	7	109.72083668	6 -63.82853435
H	9	1.08933866	2	119.19183338	1 -96.11739654
H	2	1.08770990	1	86.60035037	3 165.35325118
H	2	1.08638240	1	96.60868019	3 -79.27994111
C	5	1.41519149	3	121.59052286	1 -177.69063897
O	18	1.37441271	5	107.80709170	3 157.55519916
C	19	1.43231311	18	109.53429872	5 -8.74290057
H	20	1.09192222	19	108.19701653	18 146.92824814
H	20	1.09703825	19	109.26783633	18 -93.86292362
O	18	1.19679092	5	129.45776798	3 -23.91945099
C	1	1.49988906	3	117.27233208	4 -11.56517276
H	24	1.09568514	1	111.38157700	3 160.21736920
H	24	1.10053363	1	110.79547072	3 -80.52920551
H	24	1.09257060	1	110.67207859	3 38.03854418
H	1	1.08560949	3	118.26841676	4 -159.18521524

TS-11-7E



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscalc,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

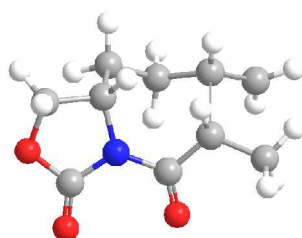
Calculation for TS-11-7E HF =-669.8453206

Sum of electronic and thermal Free Energies= -669.653020

0 2

C					
C	1	2.16135345			
C	1	1.44985363	2	93.33711130	
C	3	2.47881663	1	129.73956107	2 33.14647516
N	3	1.43156487	1	116.86435686	2 68.00595557
O	3	1.22809109	1	124.33635453	2 -100.40367897
H	1	1.08459588	3	116.08033524	6 162.07419894
C	5	1.38652156	3	128.25690151	1 33.57291073
O	8	1.36989438	5	108.00530279	3 -172.48226261
O	8	1.20819132	5	128.85623368	3 7.97980122
C	9	1.44269024	8	109.41752947	5 -5.62705715
H	11	1.09216477	9	108.09028398	8 143.49048910
H	11	1.09562727	9	108.68529977	8 -97.48712027
C	4	1.54580556	3	97.17375438	1 -42.32206989
H	14	1.09930536	4	108.52688711	3 106.42956783
H	14	1.09774791	4	107.77092508	3 -138.78606480
C	2	1.53606949	1	109.98387324	3 18.24577592
H	17	1.09689559	2	106.75526852	1 158.15840763
H	17	1.09643277	2	110.72185187	1 43.19499495
H	2	1.08928422	1	88.43577026	3 -97.47674566
C	2	1.39059260	1	102.49947812	3 146.16301162
H	21	1.08575405	2	121.22335405	1 72.20085082
H	21	1.08706408	2	121.45385489	1 -100.57827027
H	4	1.09159572	3	90.76236683	1 -153.82751926
C	1	1.50175879	3	117.44942538	6 16.48582914
H	25	1.09913063	1	109.72132754	3 77.16439478
H	25	1.09386992	1	111.32066220	3 -163.86190217
H	25	1.09288762	1	111.34292850	3 -41.52353987

TS-11-7Z



#p ub3lvp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

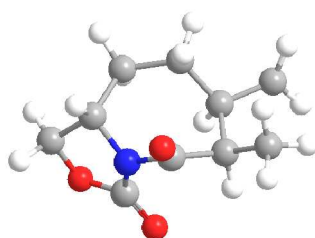
Calculation for TS-11-7Z HF =-669.8431975

Sum of electronic and thermal Free Energies= -669.652166

0 2

C					
C	1	2.22686978			
C	1	1.47479720	2	103.95933965	
N	3	1.42005216	1	115.30003407	2 -73.37627987
C	4	1.46601234	3	123.91787127	1 20.19563947
O	3	1.22049630	1	122.70480375	2 106.89736979
H	1	1.08736650	3	116.31882276	6 -151.46253032
C	4	1.40713289	3	124.50493372	1 -172.13067861
O	8	1.19752042	4	129.53666864	3 1.37404950
O	8	1.37602242	4	107.51628711	3 -178.96797293
C	10	1.43233572	8	109.95173873	4 -9.05126812
H	11	1.09651662	10	109.00665037	8 -96.76759694
H	11	1.09241603	10	108.49717352	8 144.16313292
C	5	1.54266828	4	112.28425732	3 71.82925671
H	14	1.09891327	5	107.96307010	4 -165.36805450
H	14	1.09763798	5	108.39716297	4 79.56508095
C	2	1.52300629	1	103.92905129	3 17.85710613
H	17	1.09656664	2	109.42647142	1 -58.05288377
H	17	1.09822142	2	108.03430424	1 -172.48516637
H	2	1.09021935	1	89.16952471	3 134.31357953
C	2	1.37995528	1	104.30630524	3 -108.34316064
H	21	1.08728692	2	121.21218370	1 95.58209713
H	21	1.08519340	2	121.67963468	1 -77.98259554
H	5	1.09259080	4	110.61373599	3 -52.28673212
C	1	1.50205079	3	115.83464012	6 -11.62517996
H	25	1.09213913	1	111.15362330	3 48.42822048
H	25	1.09417009	1	111.35335043	3 170.65976070
H	25	1.09924614	1	109.98804383	3 -69.96497756

P-11-7E



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

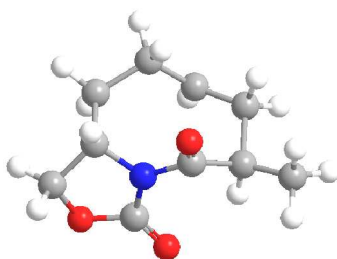
Calculation for P-11-7E HF = -669.8652123

Sum of electronic and thermal Free Energies= -669.671137

0 2

C					
C	1	1.60510000			
C	1	1.51041963	2	105.13095814	
C	3	2.47582614	1	120.98519920	2 17.97653505
N	3	1.43230971	1	116.00559355	2 53.98322351
O	3	1.21233558	1	124.46250595	2 -113.45606867
C	5	1.38846909	3	126.81180940	1 42.46491588
O	7	1.36927154	5	107.86981266	3 -168.77196337
O	7	1.20697322	5	128.46518691	3 12.43424703
C	8	1.44331267	7	109.40415325	5 -4.19379892
C	4	1.54880891	3	95.71518572	1 -31.27958801
C	11	1.54820381	4	116.90052809	3 -11.64253545
C	2	1.49107188	1	111.04226165	3 158.54270138
C	1	1.52979729	3	110.66234972	6 11.02151684
H	1	1.09444962	3	109.06322377	6 132.56210674
H	2	1.09912381	1	104.80649639	3 -85.90205946
H	4	1.09219596	3	92.19750473	1 -143.37357995
H	10	1.09198087	8	108.09086038	7 143.56419153
H	10	1.09547208	8	108.70319741	7 -97.23481031
H	11	1.09892586	4	108.15535877	3 109.82460892
H	11	1.09787955	4	108.07084676	3 -135.41269130
H	12	1.09597046	11	106.40982574	4 -172.68429628
H	12	1.09771834	11	110.75500225	4 -57.92158619
H	13	1.08603177	2	120.30613541	1 69.02924472
H	13	1.08593268	2	121.19261948	1 -99.82821491
H	14	1.09425985	1	110.31733037	3 56.85518757
H	14	1.09362120	1	110.56234724	3 176.85598991
H	14	1.09445162	1	111.57765373	3 -62.32690265

P-12/13



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-12/13 HF = -669.886509

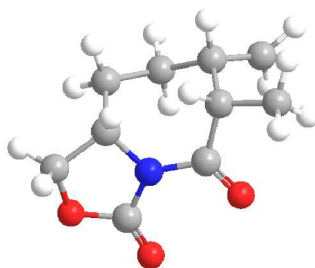
Sum of electronic and thermal Free Energies= -669.690833

0 2

C

C	1	1.58374700			
C	1	1.51266248	2	103.22887750	
O	3	1.21735249	1	123.43906338	2 -80.13570476
N	3	1.41655323	1	116.56969181	2 87.96962923
C	5	1.46765968	3	120.72587874	1 -135.19589498
C	6	1.54560522	5	111.06713502	3 81.36040632
C	7	1.55383439	6	115.99670336	5 -46.77188493
C	2	1.49660277	1	115.34752269	3 -49.72965867
C	6	1.53434228	5	99.36070186	3 -160.14671030
O	10	1.44337496	6	104.17569942	5 -27.48175538
C	11	1.36576602	10	109.72059564	6 23.56270474
O	12	1.20565334	11	123.21378574	10 170.22494349
C	1	1.52886586	3	112.76268781	4 40.21612723
H	1	1.09110707	3	109.62374318	4 164.30319039
H	2	1.09888515	1	106.47839926	3 72.55585422
H	2	1.09727090	1	106.70554241	3 -172.83221355
H	6	1.09131475	5	109.45220210	3 -42.05123459
H	7	1.09850154	6	107.66331805	5 -169.76584341
H	7	1.09867060	6	108.40896930	5 75.27253995
H	8	1.10226580	7	106.04118362	6 -166.46452552
H	8	1.09692510	7	109.88822058	6 -52.18925284
H	9	1.08920490	2	118.32610943	1 -86.91260284
H	10	1.09568949	6	112.47325075	5 89.87293105
H	10	1.09176059	6	113.58856617	5 -144.72867707
H	14	1.09541015	1	111.02178944	3 68.76184786
H	14	1.09550676	1	110.27178842	3 -171.71713210
H	14	1.09407821	1	110.82107400	3 -51.39321088

P-11-7Z



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

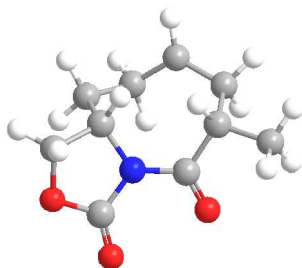
Calculation for P-11-7Z HF = -669.8718233

Sum of electronic and thermal Free Energies= -669.678715

0 2

C					
C	1	1.58638818			
C	1	1.53041491	2	110.36468870	
N	3	1.41234578	1	114.08223548	2 -76.01721139
C	4	1.46900503	3	123.91276002	1 -0.12674872
O	3	1.21176201	1	123.42402819	2 103.00302065
H	1	1.09592111	3	108.45526863	6 -140.86236228
C	4	1.41211025	3	124.23875526	1 168.94090227
O	8	1.19693882	4	129.08808353	3 0.58800495
O	8	1.37067349	4	107.62850207	3 -178.19857945
C	10	1.43222438	8	110.30907068	4 -8.82765649
H	11	1.09616306	10	108.79356225	8 -98.98700175
H	11	1.09217724	10	108.41650218	8 142.31543279
C	5	1.55319146	4	113.25780039	3 67.28887960
H	14	1.09777957	5	108.31769065	4 -146.59664978
H	14	1.09748820	5	108.99583982	4 98.14354875
C	14	1.53787583	5	115.17765485	4 -22.31796912
H	17	1.09764201	14	108.53442851	5 65.05804318
H	17	1.09612611	14	108.08314054	5 179.02098240
H	2	1.09928698	1	104.97289207	3 159.16947159
C	2	1.49580317	1	112.55009647	3 -83.07917381
H	21	1.08639427	2	120.22446860	1 79.30731979
H	21	1.08463403	2	121.42018590	1 -90.85545178
H	5	1.09275627	4	109.56540104	3 -55.80518449
C	1	1.53044167	3	110.65863773	6 -22.68048302
H	25	1.09182579	1	110.94946238	3 56.65592760
H	25	1.09576042	1	110.37206460	3 177.38682910
H	25	1.09484484	1	110.60089966	3 -62.89148453

P-14 (bb)



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-14 (bb) HF = -669.8824216

Sum of electronic and thermal Free Energies= -669.687524

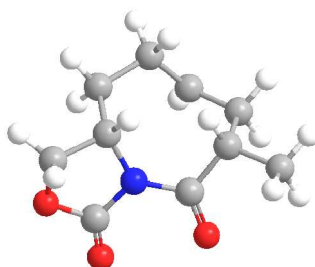
0 2

C

C	1	1.56858633			
C	1	1.53814663	2	111.17977217	
O	3	1.21285116	1	121.26650035	2 90.84721485
N	3	1.41291393	1	117.18560646	2 -90.97025689
C	5	1.47210369	3	127.13003242	1 17.52632984
C	6	1.54087318	5	112.87542529	3 83.19221595
C	7	1.54857385	6	114.72554501	5 -51.55436683
C	2	1.49373810	1	115.66376638	3 70.49149494
H	6	1.09161744	5	110.55747834	3 -40.73596701
H	7	1.09860887	6	107.23827176	5 -173.80471200
H	7	1.09819360	6	108.96770230	5 70.80604077
H	8	1.09726744	7	108.82795769	6 72.43464716
H	8	1.10004460	7	107.10919641	6 -173.17542109
H	9	1.08878811	2	118.87009474	1 100.62592997
H	2	1.10117289	1	106.63320147	3 -52.73872538
H	2	1.09629696	1	106.99212929	3 -166.71736022
C	5	1.41653141	3	123.15123817	1 -166.16620281
O	18	1.37232508	5	107.51447055	3 171.10916719
C	19	1.43439499	18	109.97401299	5 -8.56766131
H	20	1.09206689	19	108.31058975	18 145.32898706
H	20	1.09662170	19	109.00030960	18 -95.51502274
O	18	1.19647534	5	129.42150063	3 -8.32280328
C	1	1.53544115	3	108.74317410	4 -30.68557996
H	24	1.09538634	1	109.97768726	3 -178.91318736
H	24	1.09471952	1	111.22728798	3 -58.87703326
H	24	1.09288891	1	110.67153574	3 60.62721215

H	1	1.09586993	24	108.63812351	3	119.67035850
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P-14 (bc)



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-14 (bc) HF = -669.8831381

Sum of electronic and thermal Free Energies= -669.688617

0 2

C

C

C

O

N

C

C

C

C

H

H

H

H

H

H

H

H

C

O

C

H

H

O

C

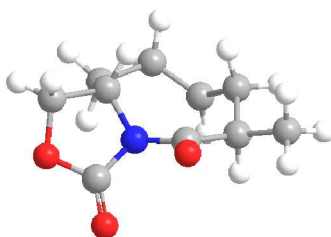
H

1	1.56239345			
1	1.53038986	2	108.45554835	
3	1.21279887	1	121.58609436	2 90.84372885
3	1.41255106	1	116.90551142	2 -87.34047291
5	1.47673373	3	128.12911128	1 -11.08977523
6	1.53920196	5	114.48754501	3 89.42986739
7	1.54949067	6	116.32449948	5 -70.13495016
2	1.49434630	1	114.39077935	3 58.75574841
6	1.09345907	5	110.37996943	3 -35.80265372
7	1.09935214	6	107.08897640	5 168.61815484
7	1.09782077	6	108.39009370	5 53.87054011
8	1.10007621	7	106.61338245	6 -173.95813395
8	1.10009659	7	108.78986825	6 -59.96748655
9	1.08704424	2	119.33123054	1 -119.75590514
2	1.10380401	1	106.22150099	3 -179.01324469
2	1.09577159	1	108.24468915	3 -64.82636903
5	1.41874038	3	122.09722219	1 172.96284974
18	1.36999394	5	107.78423766	3 165.01291089
19	1.43223903	18	109.84643552	5 -8.71498095
20	1.09181830	19	108.20053929	18 145.38129650
20	1.09664332	19	109.07867279	18 -95.53793388
18	1.19624516	5	129.10601567	3 -16.60654430
1	1.53243652	3	110.26982023	4 -31.17279796
24	1.09552071	1	110.19261646	3 176.95455137

H	24	1.09512424	1	111.25301539	3	-63.00753258
H	24	1.09277962	1	110.48987925	3	56.49970006
H	1	1.09518971	3	110.34466182	4	-151.35532424

3. Calculations (UB3LYP/6-31G*) on the Rotational Barriers of P-12/13

TS-12/13-Z-E



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-12/13-Z-E HF = -669.8698697

Sum of electronic and thermal Free Energies= -669.674873

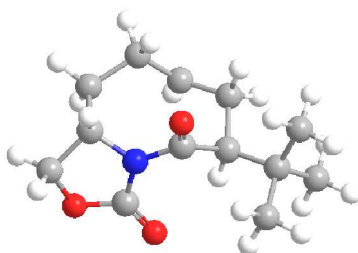
0 2

O

C	1	1.21006687				
N	2	1.44629790	1	119.39413626		
C	3	1.41273542	2	116.27250491	1	-36.77285373
C	2	1.52751748	1	121.95236318	3	-173.54640653
C	5	1.55623217	2	116.21819882	1	-141.54715765
C	3	1.48452071	2	124.52859372	1	105.57374405
C	7	1.53664646	3	113.85655073	2	115.63330295
C	8	1.54719237	7	114.38717336	3	-78.35782941
C	9	1.49095431	8	114.09204206	7	54.48649622
H	7	1.09528779	3	110.17369225	2	-8.95165608
H	8	1.09920251	7	108.12395456	3	160.86760349
H	8	1.09693080	7	108.41347070	3	45.25341811
H	9	1.09811647	8	107.81805778	7	177.70609113
H	9	1.10079462	8	107.93416200	7	-67.55515502
H	10	1.08872109	9	118.83149314	8	83.27390941
H	6	1.09896362	5	109.71291479	2	56.43859499
H	6	1.10212521	5	105.20398917	2	169.49693939
C	7	1.54398109	3	99.78569508	2	-124.98447167
H	19	1.09655968	7	112.07682482	3	90.75431972

H	19	1.09167578	7	113.20588116	3	-144.69919903
O	4	1.36593207	3	108.98570434	2	143.33371915
O	4	1.19996352	3	127.10753646	2	-39.98577039
C	5	1.53364273	2	110.21428980	1	-13.52558511
H	24	1.09166990	5	111.15314658	2	51.72644353
H	24	1.09522393	5	110.03004442	2	172.37443961
H	24	1.09605215	5	111.01905657	2	-67.94888807
H	5	1.10249667	2	103.23074097	1	102.38377107

P-12/13 (R = t-Bu)



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-12/13 (R = t-Bu) HF = -787.8227806

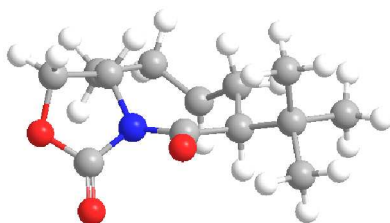
Sum of electronic and thermal Free Energies= -787.546744

0 2

C						
C	1	1.58236396				
C	1	1.51659141	2	102.18543928		
O	3	1.21820662	1	124.43149103	2	-75.23909887
N	3	1.41859441	1	116.16210734	2	92.25401854
C	5	1.46799711	3	120.47068359	1	-134.39949443
C	6	1.54454430	5	111.19849842	3	80.12465676
C	7	1.55480594	6	116.17510610	5	-48.40506637
C	2	1.49877572	1	113.85867812	3	-53.32949127
H	6	1.09140548	5	109.44181341	3	-43.23808796
H	7	1.09862917	6	107.49822529	5	-171.27030531
H	7	1.09882908	6	108.41419229	5	73.84378711
H	8	1.10223076	7	105.93791231	6	-165.95057961
H	8	1.09672354	7	109.85769184	6	-51.70168123
H	9	1.08957483	2	118.02627034	1	-84.29713808
H	2	1.09624080	1	107.77992734	3	68.77533612
H	2	1.09617165	1	107.50640618	3	-175.28463044
C	6	1.53536765	5	99.44075984	3	-161.21987805

H	18	1.09565393	6	112.46585471	5	90.89897572
H	18	1.09178661	6	113.50291087	5	-143.83588103
O	18	1.44304310	6	104.34456127	5	-26.51639800
C	21	1.36516270	18	109.75738771	6	23.12096171
O	22	1.20637945	21	123.17119384	18	169.89242364
C	1	1.56200969	3	115.58192485	4	51.55316942
H	1	1.09171174	3	108.10234490	4	171.67886934
C	24	1.54115844	1	113.56488859	3	-68.44332686
H	26	1.09259634	24	111.44316607	1	56.45385385
H	26	1.09689727	24	109.67616028	1	176.55918003
H	26	1.09625378	24	111.77741521	1	-64.74529358
C	24	1.54295661	1	108.43585388	3	170.07149101
H	30	1.09637434	24	110.09074409	1	-176.68390292
H	30	1.09673177	24	111.41047652	1	-57.23888147
H	30	1.09599884	24	112.13676380	1	64.04426955
C	24	1.54479932	1	107.91105539	3	52.96430261
H	34	1.09639202	24	111.14758950	1	53.00596983
H	34	1.09657529	24	110.45417551	1	172.97356178
H	34	1.09580662	24	111.35822172	1	-67.62650369

TS-12/13-Z-E (R = t-Bu)



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-12/13-Z-E (R = t-Bu) HF = -787.8006054

Sum of electronic and thermal Free Energies= -787.524213

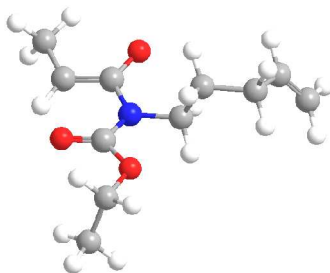
0 2

O						
C	1	1.21181633				
N	2	1.44411990	1	117.91306230		
C	3	1.42005787	2	115.71366877	1	-29.73350908
C	2	1.53946124	1	123.05168147	3	-172.68804933
C	5	1.55711323	2	114.37983299	1	-153.64024468
C	3	1.48683899	2	125.41363258	1	111.01617741

C	7	1.53611219	3	112.91476635	2	121.67395711
C	8	1.54716982	7	113.81138423	3	-75.71709839
C	9	1.49098533	8	113.38430168	7	47.01044974
H	7	1.09399167	3	110.42103027	2	-3.11796707
H	8	1.09890911	7	108.53029969	3	162.75279090
H	8	1.09682666	7	108.03718334	3	47.14110135
H	9	1.09750608	8	108.28548757	7	170.61487711
H	9	1.10085232	8	107.95137847	7	-74.39197499
H	10	1.08812325	9	119.44136624	8	86.82649223
H	6	1.09803897	5	110.50997533	2	60.63764568
H	6	1.09708463	5	106.47107097	2	174.48925962
C	7	1.54041948	3	99.71846983	2	-119.71095520
H	19	1.09661953	7	112.23797716	3	87.57468348
H	19	1.09164555	7	113.37155484	3	-147.45650617
O	4	1.36574992	3	109.01223925	2	139.26759799
O	4	1.19877842	3	127.19068861	2	-44.20884464
C	5	1.57877136	2	113.21819361	1	-20.45723658
H	5	1.10390602	2	101.96488658	1	93.19044127
C	24	1.54262306	5	111.36474628	2	-57.43661406
H	26	1.09289286	24	111.59187011	5	64.29554672
H	26	1.09645234	24	110.07478111	5	-176.06687669
H	26	1.09774176	24	111.52399916	5	-57.27669113
C	24	1.54729125	5	110.22933934	2	-177.81847564
H	30	1.09574829	24	109.22458391	5	-168.26062902
H	30	1.09765886	24	111.81062847	5	-49.64802237
H	30	1.09495297	24	113.09628285	5	72.84685129
C	24	1.54710387	5	110.44718403	2	65.08490312
H	34	1.08892858	24	112.17800648	5	-61.93791950
H	34	1.09797460	24	110.65492532	5	59.17184975
H	34	1.09682494	24	109.65641905	5	177.40050008

4. Calculations (UB3LYP/6-31G*) on the Reactions of R-15

R-15



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

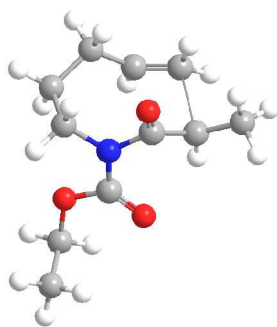
Calculation for R-15 HF = -710.4014116

Sum of electronic and thermal Free Energies= -710.169194

0 2

C					
O	1	1.23556258			
C	1	1.44565951	2	121.57503583	
N	1	1.43199905	2	117.78876603	3 176.75253202
C	4	1.48068221	1	115.53953105	2 -9.13651772
C	5	1.53222515	4	113.08584226	1 89.06220866
C	6	1.54214529	5	112.54922882	4 179.15039305
C	7	1.50591916	6	113.64107162	5 63.49235542
C	8	1.33376930	7	125.35460076	6 -123.87527192
H	5	1.08948316	4	106.56475204	1 -31.86322040
H	5	1.09063138	4	107.75690066	1 -148.25803843
H	6	1.09642598	5	109.27285129	4 57.83895414
H	6	1.09634992	5	108.62204451	4 -59.09903529
H	7	1.10015841	6	107.78335933	5 -175.49507387
H	7	1.09861204	6	109.95751120	5 -59.86826667
H	8	1.09165276	7	115.59086082	6 55.83702771
H	9	1.08865308	8	121.69690605	7 -0.02141637
H	9	1.08676846	8	121.82773629	7 -179.67580399
H	3	1.08024902	1	119.83244370	2 174.29570062
C	4	1.38933001	1	123.56770002	2 162.65627967
O	20	1.21879650	4	126.19747011	1 3.57648844
O	20	1.35552542	4	110.67625494	1 -175.89418641
C	22	1.44784684	20	115.95212361	4 -179.51107088
C	23	1.52072657	22	111.54146661	20 84.42873893
H	24	1.09344584	23	110.59322556	22 -65.12548081
H	24	1.09499590	23	110.88902257	22 55.92534466
H	24	1.09613440	23	109.72832208	22 175.49866330
H	23	1.09276895	22	103.87932652	20 -155.31803040
H	23	1.09217857	22	108.80346780	20 -38.80404566
C	3	1.48629907	1	120.14704017	2 -5.29109011
H	30	1.10020819	3	110.68492247	1 120.74148558
H	30	1.10028954	3	110.58362601	1 -122.23729844
H	30	1.09142184	3	111.33980316	1 -0.66586788

TS-15-8E



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15-8E HF=-710.3844034

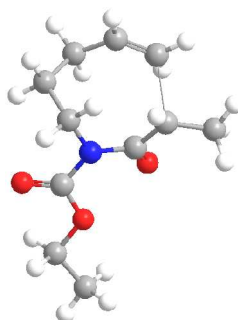
Sum of electronic and thermal Free Energies=-710.146496

0 2

C					
C	1	2.19583499			
C	1	1.45579715	2	95.36348087	
O	3	1.22846660	1	122.78383374	2 -88.03194990
N	3	1.43984708	1	117.84584611	2 81.96488053
C	5	1.47571747	3	116.18807269	1 -141.71101419
C	6	1.53586143	5	112.89104544	3 94.76185596
C	7	1.54841887	6	114.78407512	5 -56.91522039
C	2	1.37786556	1	111.58585888	3 -46.96439333
H	6	1.09082386	5	105.62410830	3 -26.40671850
H	6	1.09076977	5	108.88644413	3 -142.53996550
H	7	1.09856913	6	107.42992849	5 -177.95221136
H	7	1.09699729	6	109.41523113	5 66.72651400
H	8	1.10156354	7	107.15724459	6 -166.35995935
H	8	1.09740525	7	109.79823907	6 -51.12908050
H	9	1.09071701	2	118.77100947	1 -87.47760710
H	2	1.08777200	1	90.68492076	3 74.95393650
H	2	1.08699581	1	91.14023352	3 -169.43659326
H	1	1.08094974	3	117.29926331	4 171.06833435
C	5	1.38300312	3	122.36710899	1 38.24260599
O	20	1.21895073	5	125.93543271	3 4.78685788
O	20	1.35876468	5	110.69737514	3 -176.09129123
C	22	1.44705462	20	115.81735467	5 -176.61365152
C	23	1.52078302	22	111.59129546	20 83.96472661
H	24	1.09505696	23	110.91099343	22 56.31371748
H	24	1.09621298	23	109.78620320	22 175.94145617
H	24	1.09345593	23	110.52125894	22 -64.67761267
H	23	1.09225931	22	108.76987008	20 -39.18928930
H	23	1.09300415	22	103.95227768	20 -155.71425338

C	1	1.49952941	3	118.44883798	4	20.65093433
H	30	1.10018625	1	110.31016495	3	86.22094746
H	30	1.09609471	1	111.26009710	3	-155.22886465
H	30	1.09307388	1	111.16664916	3	-33.02531429

TS-15-8Z1



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15-8Z1 HF =-710.3760249

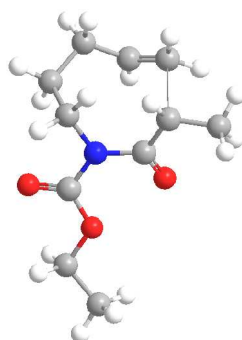
Sum of electronic and thermal Free Energies= -710.138412

0 2

C						
C	1	2.22178552				
C	1	1.47126931	2	100.00179594		
N	3	1.43246437	1	118.02519114	2	-90.64518070
C	4	1.40227859	3	122.74550143	1	-161.38854693
O	5	1.33839549	4	113.44823186	3	21.88828830
C	6	1.44474083	5	115.39533281	4	-179.09466394
C	7	1.51706027	6	107.01147709	5	176.00891029
C	4	1.47703148	3	122.83189443	1	26.54369670
C	9	1.53684945	4	114.91777292	3	90.09833682
C	10	1.54678881	9	114.75695695	4	-57.79136838
C	2	1.37277321	1	110.08824183	3	70.52570956
O	5	1.21957061	4	122.30467820	3	-162.08585962
O	3	1.22503619	1	120.74495019	2	87.75508797
H	9	1.08985882	4	108.11385056	3	-33.03844163
H	9	1.09168375	4	107.25198876	3	-148.68413369
H	7	1.09501149	6	108.96171142	5	-62.49724025
H	7	1.09444018	6	108.89432796	5	54.66347865
H	1	1.08517420	3	118.61049299	14	-164.89258834
C	1	1.50300744	3	116.36433788	14	-19.31995608
H	8	1.09413027	7	110.69600670	6	-59.68685428
H	8	1.09466996	7	110.93291086	6	60.54934060

H	8	1.09561838	7	109.77684832	6	-179.64395025
H	20	1.09514832	1	111.36837904	3	166.99841593
H	20	1.10028856	1	110.43741819	3	-73.73848633
H	20	1.09287852	1	111.11955835	3	44.61924789
H	11	1.09669959	10	109.70169816	9	72.29672308
H	11	1.09975269	10	107.92263551	9	-171.97429833
H	12	1.09107777	2	119.05989617	1	93.79846725
H	2	1.08696621	1	94.28182667	3	-165.53778990
H	2	1.08756968	1	87.23439785	3	-50.18076329
H	10	1.09923052	9	106.77776384	4	-179.16375395
H	10	1.09427652	9	109.05673845	4	65.52808105

TS-15-8Z2



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15-8Z2 HF =-710.3733779

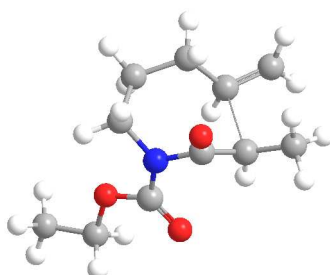
Sum of electronic and thermal Free Energies= -710.137034

0 2

C						
C	1	2.22327450				
C	1	1.47016103	2	101.08692902		
O	3	1.22350637	1	120.79155307	2	91.55996424
N	3	1.43094144	1	117.81812260	2	-86.19534371
C	5	1.48161289	3	124.25515660	1	18.46182325
C	6	1.54101432	5	115.21007925	3	93.12721490
C	7	1.54702668	6	114.98227590	5	-86.79133573
C	2	1.37309847	1	110.50150982	3	31.76495801
H	6	1.09063753	5	108.71511243	3	-31.31507513
H	6	1.09083954	5	106.27280326	3	-146.42047247
H	7	1.09821377	6	107.83335002	5	152.59412167
H	7	1.09420433	6	108.55213942	5	37.93569153
H	8	1.09965792	7	107.94485619	6	-179.64894083

H	8	1.09905576	7	109.10467973	6	-64.10837025
H	9	1.09002435	2	118.57795044	1	-88.82289642
H	2	1.08832108	1	89.70915052	3	153.52317084
H	2	1.08591617	1	91.82738901	3	-90.88850236
H	1	1.08520511	3	118.47859223	4	-163.19861672
C	5	1.40620490	3	122.75504319	1	-166.79487412
O	20	1.21984282	5	121.99009076	3	-163.31995532
O	20	1.33702237	5	113.96230703	3	20.34495900
C	22	1.44514585	20	115.33103336	5	-179.40295389
C	23	1.51703219	22	106.96594551	20	176.69244947
H	24	1.09411083	23	110.71044243	22	-59.69709028
H	24	1.09461561	23	110.91988557	22	60.50819390
H	24	1.09563875	23	109.77373516	22	-179.67180070
H	23	1.09497217	22	108.97506830	20	-61.80333861
H	23	1.09446168	22	108.89086731	20	55.34501609
C	1	1.50147662	3	116.90841736	4	-17.37323532
H	30	1.09596613	1	111.33804533	3	160.68426907
H	30	1.10054319	1	110.62177286	3	-80.20493244
H	30	1.09252323	1	110.77380011	3	38.47277892

TS-15-7E



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15-7E HF=-710.3688758

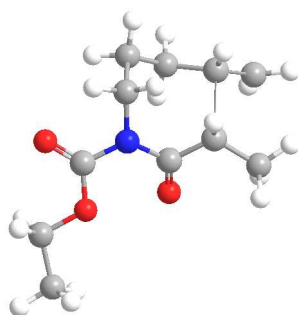
Sum of electronic and thermal Free Energies=-710.132294

0 2

C						
C	1	2.16789378				
C	1	1.45355967	2	94.98536699		
N	3	1.44490307	1	117.20760736	2	65.95447167
C	4	1.47261515	3	113.16627946	1	-122.28914882
O	3	1.22671966	1	123.28449737	2	-101.58945927
H	5	1.08919091	4	108.92935869	3	-163.11185994
C	4	1.37614743	3	121.86978411	1	45.62690908

O	8	1.21988716	4	125.21572643	3	9.77553180
O	8	1.35838330	4	111.37074197	3	-171.41236805
C	10	1.44469283	8	115.08204216	4	-176.31908805
C	11	1.51720446	10	107.30321975	8	178.74894185
H	12	1.09477764	11	110.97893341	10	-60.44308270
H	12	1.09490811	11	111.01821859	10	60.15373956
H	12	1.09541283	11	109.75093643	10	179.85587204
H	11	1.09457694	10	108.92090375	8	-59.78792582
H	11	1.09438800	10	108.90993190	8	57.26272781
C	1	1.50203861	3	117.19975815	6	15.92268547
H	18	1.09282581	1	111.38069425	3	-41.97088315
H	18	1.09917363	1	109.70126893	3	76.66955625
H	18	1.09389916	1	111.26567760	3	-164.28104380
H	1	1.08303431	3	116.48042358	6	160.69302138
C	5	1.53699741	4	111.14569539	3	74.30475737
H	23	1.09856346	5	109.13319023	4	72.16591703
H	23	1.09799310	5	107.63597577	4	-172.77749834
C	2	1.53447917	1	109.79119487	3	19.78391188
H	26	1.09731200	2	106.67367500	1	158.89024001
H	26	1.09720866	2	110.49218985	1	44.17313286
H	2	1.08936588	1	88.38871543	3	-95.79858988
C	2	1.38906036	1	102.40889352	3	147.81690815
H	30	1.08717085	2	121.40315826	1	-100.42384826
H	30	1.08598570	2	121.34493540	1	72.21721308
H	5	1.09197366	4	106.38837084	3	-46.31219364

TS-15-7Z



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15-7Z HF = -710.3688556

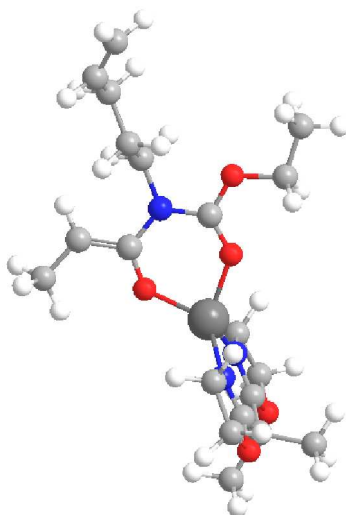
Sum of electronic and thermal Free Energies= -710.132583

0 2
C

C	1	2.21635305			
C	1	1.47446852	2	103.31450666	
N	3	1.42791296	1	116.23121722	2 -75.61038725
C	4	1.47347600	3	119.82806079	1 26.66453531
O	3	1.22351947	1	121.56646744	2 102.60081607
H	5	1.08974256	4	107.00371281	3 -168.04759443
C	4	1.40325340	3	123.32200868	1 -168.47101899
O	8	1.21879468	4	122.70161883	3 -155.69305895
O	8	1.33766061	4	112.82145159	3 27.90267814
C	10	1.44498538	8	115.47314355	4 -178.35740776
C	11	1.51695988	10	107.00796700	8 176.99351663
H	12	1.09414245	11	110.70162871	10 -59.65165146
H	12	1.09464699	11	110.91159822	10 60.59447626
H	12	1.09560525	11	109.78013032	10 -179.61442277
H	11	1.09490764	10	108.93127422	8 -61.49062181
H	11	1.09456656	10	108.87389732	8 55.67539215
C	1	1.50348933	3	115.55945040	6 -15.13004425
H	18	1.09197366	1	111.21145831	3 48.96688385
H	18	1.09412969	1	111.26988256	3 171.13949924
H	18	1.09938300	1	109.97582241	3 -69.55603050
H	1	1.08665249	3	116.57750112	6 -154.47023198
C	5	1.53447832	4	113.22592336	3 70.98078002
H	23	1.09572710	5	108.56088473	4 74.00242448
H	23	1.09912838	5	107.76120852	4 -170.63884641
C	2	1.52366633	1	104.01359695	3 13.74869689
H	26	1.09696488	2	109.38864522	1 -55.61124039
H	26	1.09825913	2	108.23563728	1 -170.17590412
H	2	1.09035615	1	89.28916814	3 130.06551581
C	2	1.38192222	1	104.51672935	3 -112.76469595
H	30	1.08735469	2	121.22067713	1 95.94233713
H	30	1.08545873	2	121.70939984	1 -77.59845286
H	5	1.09238010	4	108.57107578	3 -52.63921223

5. Calculations (UB3LYP/6-31G*) on the Reactions of R-15L

R-15L



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-15L HF=-1521.4958957

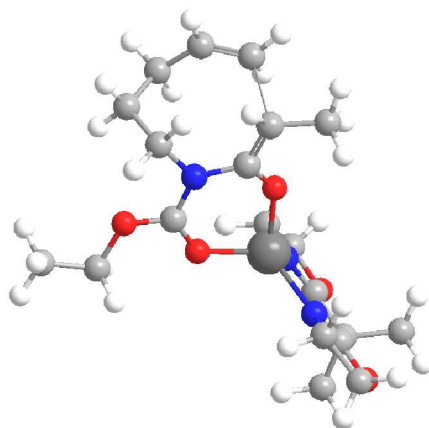
Sum of electronic and thermal Free Energies=-1521.049004

2 2

C					
C	1	6.79533530			
C	1	1.43835336	2	89.88896066	
N	3	1.40468387	1	119.29657255	2 -22.77539887
C	4	1.39541720	3	121.69008873	1 169.68855656
O	5	1.30327842	4	112.85262179	3 -175.16150822
C	6	1.48473873	5	119.14686940	4 -179.52151966
C	7	1.51129878	6	107.08084531	5 -179.33192549
C	4	1.50690007	3	120.56763095	1 -8.09845567
C	9	1.53033854	4	113.59878144	3 89.83698297
C	10	1.54321339	9	111.41210541	4 -179.44176350
C	2	1.33270648	1	16.32651057	3 -174.61331163
O	5	1.24987985	4	125.00720914	3 4.71181039
O	3	1.26526798	1	118.85030593	4 179.38438556
Mg	14	1.96763304	3	134.56017436	1 -172.42765956
N	15	2.05558612	14	121.60134060	3 -123.06208759
N	15	2.05498673	14	120.87491905	3 122.16216883
C	16	1.29822671	15	125.35687697	14 -128.49530573
C	17	1.29808005	15	125.40672540	14 129.43468647
C	19	1.52043898	17	130.67484434	15 0.10807060
C	20	1.56162762	19	107.84888017	17 120.00792787
H	21	1.09128782	20	109.52212864	19 57.24603305
H	21	1.09123392	20	109.46968818	19 176.43432017
H	21	1.09505569	20	111.48161119	19 -63.16457255
C	20	1.56108907	19	107.87689032	17 -121.66855503

H	25	1.09500769	20	111.44950631	19	62.68654588
H	25	1.09117992	20	109.52721365	19	-176.93614261
H	25	1.09110983	20	109.51787746	19	-57.69705813
O	18	1.32484719	16	116.55041603	15	179.31536261
O	19	1.32502859	17	116.54803994	15	-179.97297082
C	29	1.46247524	18	108.76277534	16	-0.22960139
H	31	1.09061510	29	107.27258171	18	121.40134643
H	31	1.09068194	29	107.24501265	18	-120.59693951
C	16	1.48976062	15	126.88249585	14	50.72907685
H	34	1.09395064	16	109.71125695	15	60.45614610
H	34	1.09390477	16	109.77485000	15	-58.57901931
C	17	1.48956458	15	126.82356807	14	-50.50058568
H	37	1.09390358	17	109.73531068	15	-59.57807776
H	37	1.09386443	17	109.73320366	15	59.45633073
C	30	1.46238252	19	108.74762412	17	0.01785720
H	40	1.09064200	30	107.24205379	19	121.00900950
H	40	1.09066386	30	107.26266102	19	-121.00080526
H	9	1.09086577	4	106.83777485	3	-34.73024030
H	9	1.08872022	4	106.40439357	3	-148.08351888
H	7	1.09207583	6	106.99400703	5	-57.86757562
H	7	1.09234888	6	106.97768182	5	59.22274626
H	1	1.08211297	3	119.85171804	14	172.61291274
C	1	1.47788920	3	122.33283041	14	-4.63773352
H	8	1.09357743	7	111.43047819	6	-61.27947455
H	8	1.09351530	7	111.37271030	6	60.94569888
H	8	1.09484034	7	108.56932335	6	179.82308247
H	48	1.10161039	1	109.81664148	3	116.25167759
H	48	1.09981464	1	109.86742443	3	-128.70709952
H	48	1.08991985	1	113.04380922	3	-5.85179955
H	11	1.09726224	10	109.60823015	9	-58.85661466
H	11	1.10089650	10	108.96376879	9	57.51598837
H	12	1.09079880	2	119.47582152	1	134.19027987
H	2	1.08591585	1	132.13679933	3	-119.55000109
H	2	1.08819529	1	110.12034356	3	46.52508626
H	10	1.09570762	9	109.44739053	4	59.49756536
H	10	1.09871915	9	110.17741670	4	-57.41647206

TS-15L-8Z1



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15L-8Z1 HF =-1521.4899306

Sum of electronic and thermal Free Energies= -1521.037666

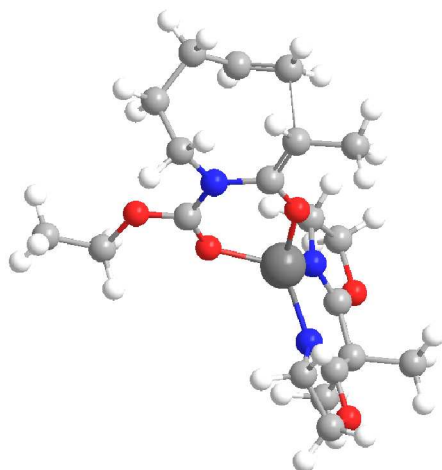
2 2

C

C	1	2.18887360			
C	1	1.43619310	2	102.90143749	
N	3	1.42203405	1	121.23538175	2 -82.96948263
C	4	1.38899767	3	121.70746028	1 -170.99068681
O	5	1.30929223	4	112.79560845	3 -178.96257281
C	6	1.48098926	5	118.89099059	4 -177.70693099
C	7	1.51191083	6	107.15204911	5 -179.59126718
C	4	1.50175949	3	121.49425373	1 8.39539649
C	9	1.53580531	4	114.62919391	3 99.14459121
C	10	1.54879758	9	115.27443523	4 -54.11522116
C	2	1.37952470	1	107.17032000	3 76.35631636
O	5	1.25137349	4	125.76318496	3 2.00658193
O	3	1.26985678	1	118.78836646	2 94.82036087
Mg	14	1.94998221	3	134.77531564	1 161.92379737
N	15	2.06022753	14	121.78930957	3 -107.88235789
N	15	2.05973328	14	122.49470971	3 136.34509782
C	16	1.29701738	15	125.76314400	14 -132.01877976
C	17	1.29767288	15	125.64476911	14 131.13528051
C	18	1.52009573	16	130.59712319	15 0.35291010
C	20	1.56147698	18	107.83005466	16 -119.10189491
H	21	1.09136905	20	109.52982571	18 -176.65381928
H	21	1.09135044	20	109.48901249	18 -57.45959427
H	21	1.09504811	20	111.45785859	18 62.91696694
C	20	1.56070753	18	107.94469156	16 122.53884005
H	25	1.09499973	20	111.43635723	18 -62.77503598

H	25	1.09116450	20	109.52353973	18	57.57551301
H	25	1.09111936	20	109.54928361	18	176.84175054
O	18	1.32591697	16	116.60138014	15	-179.35877483
O	19	1.32577896	17	116.55927149	15	-179.95844741
C	29	1.46216637	18	108.68203296	16	0.15905750
H	31	1.09075608	29	107.26889399	18	120.54787730
H	31	1.09064384	29	107.27840525	18	-121.46362894
C	16	1.48901168	15	126.47770088	14	48.48079273
H	34	1.09389653	16	109.76143461	15	58.59054404
H	34	1.09390812	16	109.67592276	15	-60.40734764
C	17	1.48911196	15	126.60668437	14	-48.64243704
H	37	1.09400602	17	109.73575137	15	-59.62016406
H	37	1.09389681	17	109.71444725	15	59.40147103
C	30	1.46176215	19	108.73389169	17	0.13564144
H	40	1.09071397	30	107.26915768	19	120.92185767
H	40	1.09069901	30	107.28792917	19	-121.08363966
H	9	1.08593965	4	107.25168529	3	-23.93191944
H	9	1.08911025	4	107.24675789	3	-138.28971256
H	7	1.09232061	6	107.23819544	5	-58.09981549
H	7	1.09230852	6	107.16944827	5	58.99591825
H	1	1.08127076	3	118.40367337	14	-160.29299918
C	1	1.50740579	3	117.54461510	14	-14.42925879
H	8	1.09360667	7	111.41856930	6	-60.94963710
H	8	1.09368781	7	111.42124888	6	61.20181104
H	8	1.09480309	7	108.66009005	6	-179.87671694
H	48	1.09254324	1	110.56985933	3	173.53799985
H	48	1.09879054	1	110.06785301	3	-68.19921184
H	48	1.09259930	1	112.29200350	3	51.48347494
H	11	1.09728991	10	110.22408130	9	73.23566087
H	11	1.09817714	10	107.56984805	9	-170.90304926
H	12	1.09005161	2	118.84508395	1	91.33646606
H	2	1.08600071	1	93.51610424	3	-161.22946881
H	2	1.08797594	1	92.34512928	3	-45.63117390
H	10	1.09693588	9	105.93138212	4	-175.55997128
H	10	1.09403519	9	110.23263012	4	69.69429757

TS-15L-8Z2



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15-7Z HF =-1521.4887869

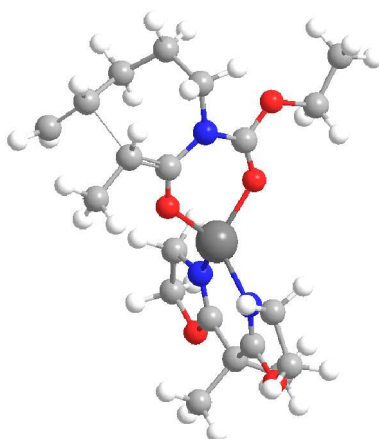
Sum of electronic and thermal Free Energies= -1521.036693

2 2

C					
C	1	2.18832289			
C	1	1.43398623	2	103.17549654	
N	3	1.42151155	1	120.43992090	2 -78.39284749
C	4	1.39140308	3	121.63307270	1 174.67007906
O	5	1.30928675	4	112.86232541	3 -179.82190845
C	6	1.48113301	5	118.92561307	4 -178.88183284
C	7	1.51185816	6	107.14825306	5 179.47956066
C	4	1.50849848	3	122.14048712	1 -8.18238766
C	9	1.53716580	4	115.25311901	3 101.61605026
C	10	1.54849466	9	116.24226110	4 -75.96015519
C	2	1.37940568	1	107.46606267	3 46.17745110
O	5	1.25094539	4	125.90185262	3 0.23251400
O	3	1.26823818	1	119.07728072	2 97.88350250
Mg	14	1.94682674	3	136.27597183	1 -178.39267737
N	15	2.05989919	14	122.04851316	3 -117.23942436
N	15	2.06016113	14	121.95484799	3 127.22845771
C	16	1.29726035	15	125.72014575	14 -129.91462908
C	17	1.29757402	15	125.65741263	14 130.22548578
C	19	1.52008660	17	130.68674476	15 0.28527392
C	20	1.56134083	19	107.81841892	17 119.80046435
H	21	1.09131039	20	109.51845304	19 57.96925536
H	21	1.09132578	20	109.50349282	19 177.16850555
H	21	1.09506988	20	111.45229461	19 -62.44642692
C	20	1.56098093	19	107.93924402	17 -121.87582627

H	25	1.09495485	20	111.45827195	19	63.02423985
H	25	1.09118764	20	109.48873748	19	-176.60303346
H	25	1.09118185	20	109.51640543	19	-57.39313258
O	18	1.32572426	16	116.60918466	15	179.41365730
O	19	1.32597632	17	116.55944951	15	-179.89720350
C	29	1.46225320	18	108.68789598	16	-0.00661111
H	31	1.09070326	29	107.26862567	18	120.88137870
H	31	1.09066947	29	107.27243635	18	-121.12426952
C	16	1.48929257	15	126.53055903	14	49.22840562
H	34	1.09391259	16	109.72921571	15	60.05816083
H	34	1.09390688	16	109.71721881	15	-58.94000411
C	17	1.48877317	15	126.59550976	14	-49.20930296
H	37	1.09386033	17	109.80840113	15	-58.79323102
H	37	1.09405185	17	109.61907716	15	60.24093568
C	30	1.46157370	19	108.71477317	17	-0.67161927
H	40	1.09056060	30	107.30848151	19	122.41303980
H	40	1.09088116	30	107.25339147	19	-119.59387713
H	9	1.08768631	4	107.55996409	3	-23.57354770
H	9	1.08880634	4	106.04700722	3	-137.11330356
H	7	1.09229727	6	107.20153393	5	-59.01094079
H	7	1.09230134	6	107.19359063	5	58.07440225
H	1	1.08090910	3	118.15686368	14	-161.85610279
C	1	1.50430655	3	118.57066098	14	-14.03411314
H	8	1.09362089	7	111.40739851	6	-60.84420464
H	8	1.09364560	7	111.45222339	6	61.30098668
H	8	1.09479729	7	108.64674213	6	-179.77658286
H	48	1.09311351	1	110.63871328	3	166.51980820
H	48	1.09899747	1	110.04545963	3	-75.34927246
H	48	1.09212090	1	112.21707689	3	44.45640396
H	11	1.09865955	10	107.37359037	9	-179.61783053
H	11	1.09671269	10	110.03286348	9	-63.82938789
H	12	1.09067288	2	118.92351955	1	-99.92691181
H	2	1.08745436	1	86.88871684	3	165.84492332
H	2	1.08659784	1	98.36172922	3	-79.06261714
H	10	1.09647217	9	106.53638436	4	163.64203330
H	10	1.09515013	9	109.30622400	4	49.47932711

TS-15L-7Z



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-15L-7Z HF =-1521.482734

Sum of electronic and thermal Free Energies= -1521.030833

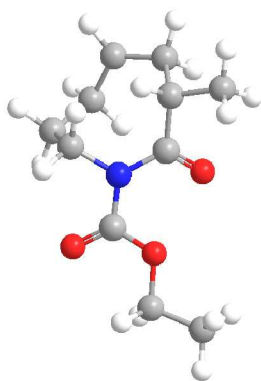
2 2

C					
C	1	2.17323058			
C	2	2.61094893	1	88.72037196	
C	3	1.53787357	2	97.84779356	1 -3.04666931
C	2	1.51888454	1	106.95459086	4 27.73357392
N	4	1.49677816	3	112.91303058	2 61.77737441
C	6	1.41658773	4	118.84135325	3 -79.35534280
O	7	1.26780228	6	120.63972116	4 171.01081970
C	2	1.39030764	1	102.85407776	7 98.08167815
H	5	1.09841192	2	109.34938582	1 69.40030822
H	5	1.09788646	2	106.86815421	1 -177.28943013
H	2	1.08988439	1	89.19273000	7 -145.36290665
H	9	1.08474642	2	121.67674877	1 77.99945540
H	9	1.08734133	2	121.28981073	1 -99.34433140
H	4	1.08822850	3	112.39948761	2 -59.56040940
H	4	1.08674195	3	110.54620178	2 -177.94486938
H	3	1.09508462	2	138.66409858	1 127.69863425
H	3	1.09651370	2	94.59902120	1 -111.31256715
C	6	1.38730685	4	118.54711557	3 95.82703446
O	19	1.25166540	6	125.13639156	4 176.03052480
O	19	1.30812716	6	113.15397536	4 -3.17798790
C	21	1.48136876	19	118.98201845	6 177.18509490
C	22	1.51182610	21	107.09088488	19 -178.46532338
H	23	1.09363874	22	111.40634165	21 -60.90775196
H	23	1.09361387	22	111.38706520	21 61.21668329
H	23	1.09478435	22	108.66336408	21 -179.85797066

H	22	1.09230080	21	107.21357288	19	-56.99357297
H	22	1.09233437	21	107.15320311	19	60.13265889
Mg	8	1.95378391	7	133.71347612	6	17.89073039
N	29	2.06039272	8	121.97435763	7	105.87406631
N	29	2.05979792	8	121.63754286	7	-138.95860259
C	30	1.29705675	29	125.72010037	8	128.91427964
C	30	1.48919102	29	126.54057053	8	-51.13573672
C	31	1.29761283	29	125.62047014	8	-128.96970908
C	31	1.48902278	29	126.62873809	8	49.90938892
C	32	1.52002660	30	130.61790469	29	0.13281975
O	32	1.32587031	30	116.61503418	29	-179.79946714
C	37	1.46213416	32	108.67977076	30	0.35945837
H	33	1.09384472	30	109.76888161	29	58.82718938
H	33	1.09400354	30	109.66836893	29	-60.16282732
O	34	1.32594840	31	116.55305389	29	179.36470134
H	35	1.09403398	31	109.62654681	29	-59.60195832
H	35	1.09385052	31	109.82149337	29	59.39957965
C	41	1.46156557	34	108.72843999	31	0.62237053
C	36	1.56124329	32	107.85294348	30	-120.35426232
C	36	1.56101928	32	107.88692142	30	121.27853203
H	38	1.09078109	37	107.25414564	32	120.19752858
H	38	1.09061618	37	107.29937661	32	-121.80825190
H	44	1.09084645	41	107.25308140	34	119.72233024
H	44	1.09056665	41	107.30725895	34	-122.27888487
H	45	1.09124967	36	109.54133100	32	-176.74789209
H	45	1.09124077	36	109.49390396	32	-57.51330861
H	45	1.09502470	36	111.43974312	32	62.84142709
H	46	1.09505860	36	111.43166549	32	-62.94535325
H	46	1.09126177	36	109.53139609	32	57.40673287
H	46	1.09121866	36	109.54310375	32	176.65350150
C	1	1.50707315	7	117.67154207	6	-168.24208070
H	57	1.09142233	1	112.39157540	7	-48.49766291
H	57	1.09827788	1	109.79130774	7	71.51465805
H	57	1.09295888	1	110.55442427	7	-170.59824797
H	1	1.08146489	7	116.64687277	6	-26.83033852

6. Calculations (UB3LYP/6-31G*) on the Relative Energies of P-15 & P-20

P-15-1



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-15-1 HF = -710.40784

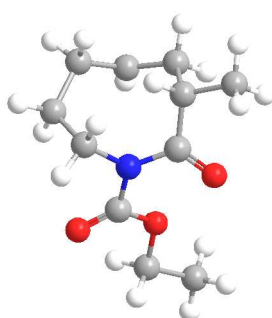
Sum of electronic and thermal Free Energies= -710.167296

0 2

C				
C	1	1.56838661		
C	1	1.53651989	2	110.18785761
N	3	1.41839759	1	117.93770725
C	4	1.41023327	3	122.51698769
O	5	1.33605308	4	112.94649210
C	6	1.44628385	5	115.45535431
C	7	1.51671594	6	107.04759373
C	4	1.47931836	3	121.86656081
C	9	1.53419666	4	114.17177610
C	10	1.55124628	9	114.15283400
C	2	1.49520022	1	115.83604456
O	5	1.21731463	4	122.42683977
O	3	1.21606295	1	120.00629068
H	9	1.09082391	4	108.13959626
H	9	1.09051836	4	106.96036372
H	7	1.09487994	6	108.83795804
H	7	1.09432396	6	108.79057552
H	1	1.09402001	3	110.78447767
C	1	1.53670050	3	108.68940203
H	8	1.09409245	7	110.70112103
H	8	1.09466215	7	110.96568059
H	8	1.09554038	7	109.72483103
H	20	1.09561123	1	109.99561995
H	20	1.09528506	1	111.18143294
H	20	1.09282528	1	110.64595457
H	11	1.09787181	10	109.10019186
H	11	1.10012115	10	107.38830582

H	12	1.08885339	2	118.74894252	1	102.93213657
H	2	1.09643507	1	107.22351890	3	-168.91916960
H	2	1.10148106	1	106.11429746	3	-54.98982470
H	10	1.09863551	9	107.07381504	4	-176.87940059
H	10	1.09538470	9	109.25766265	4	67.43591776

P-15-2



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-15-2 HF = -710.4074526

Sum of electronic and thermal Free Energies= -710.167408

0 2

C

C

C

N

C

O

C

C

C

C

C

C

O

O

H

H

H

H

H

C

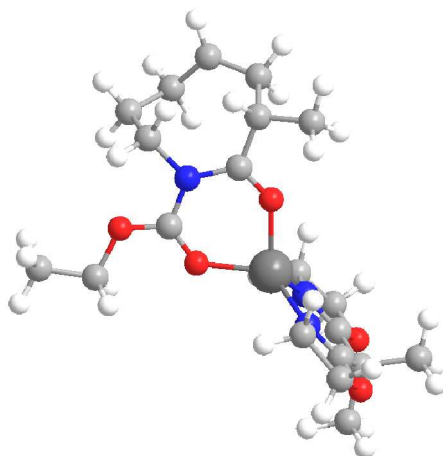
H

H

1	1.56601757				
1	1.53157009	2	109.10911123		
3	1.42077295	1	116.80740591	2	-75.69597696
4	1.40915081	3	123.11244286	1	156.82243384
5	1.33659362	4	113.34404728	3	-18.77175508
6	1.44631101	5	115.33766993	4	179.53347236
7	1.51670448	6	107.03005649	5	-176.44655861
4	1.48187894	3	122.93260141	1	-29.12905364
9	1.53308989	4	114.35662850	3	103.01277117
10	1.55045486	9	115.30704268	4	-68.88445564
2	1.49495564	1	115.45987793	3	60.86293665
5	1.21793439	4	122.33823067	3	164.78877389
3	1.21458706	1	121.03200180	2	101.19820805
9	1.09152900	4	108.47918252	3	-21.73874187
9	1.09095243	4	106.10504335	3	-136.72140947
7	1.09419114	6	108.80895285	5	-55.08521794
7	1.09499856	6	108.86843490	5	62.01755484
1	1.09399416	3	110.44525470	14	-141.20046488
1	1.53155734	3	110.42790731	14	-21.23388977
8	1.09462340	7	110.96411064	6	-60.42922366
8	1.09412486	7	110.73656552	6	59.87199884

H	8	1.09555183	7	109.71928797	6	179.78191734
H	20	1.09563964	1	110.12587555	3	179.69369644
H	20	1.09468466	1	111.19982253	3	-60.23841382
H	20	1.09314624	1	110.83960473	3	59.21476946
H	11	1.10023044	10	107.25007188	9	-177.98451928
H	11	1.10016681	10	108.82628517	9	-63.55400313
H	12	1.08739088	2	118.98154924	1	-120.67428134
H	2	1.10396621	1	105.61266607	20	-55.03427922
H	2	1.09650086	1	108.31008316	20	58.51681966
H	10	1.09892192	9	107.70538793	4	169.32634006
H	10	1.09646901	9	108.33361419	4	54.61100962

P-15L-1



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-15L-1 HF =-1521.5077669

Sum of electronic and thermal Free Energies= -1521.052459

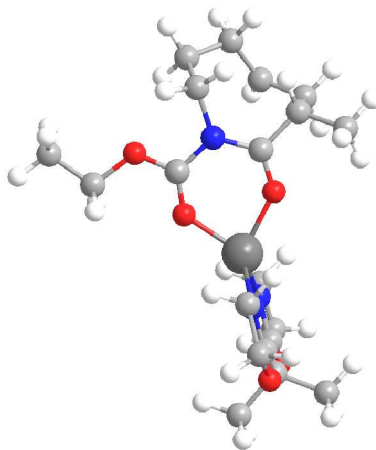
2 2

C						
C	1	1.59531737				
C	1	1.51189975	2	110.45949128		
N	3	1.39595401	1	121.26565025	2	-84.60505973
C	4	1.40444991	3	121.67051204	1	-176.94803938
O	5	1.30161121	4	112.64942812	3	-178.73775572
C	6	1.48646342	5	119.21330265	4	-178.38042121
C	7	1.51107655	6	107.09675547	5	179.85829977
C	4	1.50832517	3	121.57806390	1	6.44136003
C	9	1.53186448	4	113.27453199	3	94.29980172
C	10	1.55063455	9	114.06189354	4	-54.69124934
C	2	1.48760482	1	116.59432223	3	73.56524670
O	5	1.24806458	4	125.21513295	3	2.03356768

O	3	1.25242184	1	117.80237193	2	94.20903528
Mg	14	1.96888509	3	136.49291526	1	172.31925649
N	15	2.05418659	14	121.54676082	3	-115.50155434
N	15	2.05398943	14	120.93229646	3	129.49773691
C	16	1.29833601	15	125.28449166	14	-127.67979159
C	17	1.29858474	15	125.24575203	14	127.91750565
C	18	1.52042959	16	130.69375561	15	-0.49944834
C	20	1.56126443	18	107.88631717	16	-121.41153380
H	21	1.09118846	20	109.52090426	18	-176.63633107
H	21	1.09122821	20	109.51391739	18	-57.42929488
H	21	1.09503911	20	111.46063634	18	62.95484068
C	20	1.56164048	18	107.80041550	16	120.27759829
H	25	1.09502593	20	111.47186276	18	-62.76885315
H	25	1.09123744	20	109.48084701	18	57.62130084
H	25	1.09123193	20	109.51528360	18	176.81531306
O	18	1.32459399	16	116.55230666	15	179.35508541
O	19	1.32462326	17	116.52469210	15	-178.91038026
C	29	1.46251684	18	108.77134298	16	-0.40882592
H	31	1.09055569	29	107.27779081	18	121.81127290
H	31	1.09071509	29	107.23419508	18	-120.18392309
C	16	1.48992093	15	126.96672811	14	51.75370520
H	34	1.09397460	16	109.69429732	15	60.64274325
H	34	1.09383191	16	109.78549102	15	-58.41068472
C	17	1.48988531	15	126.99148680	14	-50.52285321
H	37	1.09387730	17	109.80275651	15	-60.28169985
H	37	1.09396797	17	109.69549202	15	58.78476519
C	30	1.46224702	19	108.79763757	17	-0.27614468
H	40	1.09055770	30	107.27006766	19	121.64160044
H	40	1.09071197	30	107.23656892	19	-120.34792148
H	9	1.08632957	4	106.97256400	3	-27.71750166
H	9	1.08825445	4	107.02474653	3	-142.53461631
H	7	1.09219169	6	106.91680469	5	-58.63210681
H	7	1.09215226	6	106.90028678	5	58.40393829
H	1	1.09163672	3	110.21643651	14	-146.88649259
C	1	1.53788983	3	110.36652689	14	-27.22065671
H	8	1.09349960	7	111.43243231	6	-61.05429261
H	8	1.09354592	7	111.45804744	6	61.22087313
H	8	1.09488175	7	108.52251289	6	-179.90933197
H	48	1.09325886	1	108.74840121	3	-174.10619711
H	48	1.09452141	1	111.74956030	3	-55.20894601
H	48	1.09293842	1	111.62441528	3	66.50696166
H	11	1.10038914	10	109.34940173	9	74.56395438
H	11	1.09756524	10	107.32896732	9	-170.89499634
H	12	1.08713988	2	118.57717911	1	100.48081670
H	2	1.09418185	1	104.78776700	3	-164.29429323

H	2	1.10062055	1	106.62409577	3	-51.32551099
H	10	1.09662496	9	105.95068325	4	-175.42354654
H	10	1.09541765	9	110.44727512	4	69.56436283

P-15L-2



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-15L-2 HF =-1521.5082631

Sum of electronic and thermal Free Energies= -1521.054243

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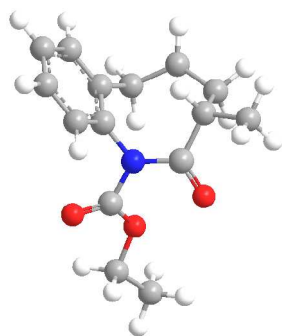
C

C

C	1	1.57769824				
C	1	1.50918652	2	107.16253414		
N	3	1.39368832	1	120.35830330	2	-87.29884415
C	4	1.40549683	3	121.35679656	1	168.11965643
O	5	1.30128036	4	112.80365957	3	-175.26033760
C	6	1.48679712	5	119.21904032	4	-179.44235743
C	7	1.51100957	6	107.11167097	5	179.45230024
C	4	1.51397606	3	122.07703372	1	-10.51210204
C	9	1.53197756	4	114.85656853	3	92.48736083
C	10	1.55036922	9	115.88309924	4	-73.34644187
C	2	1.49329425	1	115.10994273	3	58.66602881
O	5	1.24782986	4	125.07806912	3	4.45657009
O	3	1.25098190	1	118.04052483	2	88.57097316
Mg	14	1.96974297	3	136.25925087	1	-171.96359060
N	15	2.05402599	14	121.92001351	3	-120.30886642
N	15	2.05355572	14	120.59182536	3	124.64077684
C	16	1.29848212	15	125.25990733	14	-128.29137873
C	17	1.29848284	15	125.27693800	14	129.24985000
C	19	1.52038944	17	130.70591803	15	0.62562042
C	20	1.56139779	19	107.82309756	17	120.26961755

H	21	1.09127580	20	109.49069513	19	58.01417604
H	21	1.09132447	20	109.53784579	19	177.20002080
H	21	1.09506199	20	111.46889516	19	-62.39289995
C	20	1.56158859	19	107.86298647	17	-121.42949383
H	25	1.09498440	20	111.48006395	19	62.92871012
H	25	1.09117447	20	109.50180053	19	-176.67208535
H	25	1.09120334	20	109.49649499	19	-57.47467529
O	18	1.32453983	16	116.54241183	15	179.47449234
O	19	1.32464276	17	116.52651021	15	-179.45393978
C	29	1.46254183	18	108.77914512	16	0.01706973
H	31	1.09065537	29	107.24568928	18	120.79598449
H	31	1.09062148	29	107.25696868	18	-121.20296828
C	16	1.48988797	15	126.98019945	14	50.87060048
H	34	1.09387533	16	109.76807666	15	59.99317064
H	34	1.09392463	16	109.73118704	15	-59.08532220
C	17	1.48960700	15	126.95328949	14	-49.56794554
H	37	1.09379209	17	109.84457119	15	-59.20533571
H	37	1.09401639	17	109.63229414	15	59.85978149
C	30	1.46237334	19	108.77359531	17	-0.68736806
H	40	1.09048315	30	107.28054624	19	122.50304596
H	40	1.09083580	30	107.22166060	19	-119.50474295
H	9	1.08877437	4	107.08022775	3	-32.53132942
H	9	1.08791509	4	105.59046931	3	-145.84012053
H	7	1.09208440	6	106.86882038	5	-59.04077628
H	7	1.09221189	6	106.90246688	5	57.97943015
H	1	1.08961201	3	110.65270260	14	-154.88136186
C	1	1.53532557	3	111.78403124	14	-33.59297444
H	8	1.09354112	7	111.44755600	6	-61.08628749
H	8	1.09347168	7	111.45310803	6	61.20586261
H	8	1.09488297	7	108.50220713	6	-179.93570053
H	48	1.09349061	1	108.95360449	3	-179.29487217
H	48	1.09460132	1	111.63040305	3	-60.41012709
H	48	1.09282839	1	111.62592863	3	61.26068466
H	11	1.09693111	10	106.95749918	9	-175.29838577
H	11	1.09964368	10	108.55830491	9	-61.19705446
H	12	1.08663504	2	118.78925572	1	-134.22074736
H	2	1.10267048	1	104.36299310	3	-179.74646215
H	2	1.09570963	1	108.49921232	3	-66.67550834
H	10	1.09719562	9	106.14960861	4	166.06410971
H	10	1.09583278	9	109.31361546	4	51.84369113

P-20-boat-boat



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-20a-boat-boat HF=-862.8302162

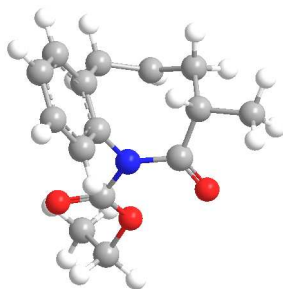
Sum of electronic and thermal Free Energies=-862.571443

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C					
C	1	1.57753063			
C	1	1.53052479	2	109.22383074	
O	3	1.21642939	1	121.44357171	2 95.36720106
N	3	1.41378857	1	117.22038033	2 -83.23058922
C	2	2.63192463	1	99.34020013	3 61.31384563
C	2	1.49436361	1	115.92969359	3 86.00138579
H	6	1.09669140	2	87.82922344	1 -87.87618203
H	6	1.09659018	2	135.80416672	1 158.92093837
H	7	1.08827503	2	117.87432812	1 102.20124853
H	2	1.10157393	1	107.19988769	3 -38.65249939
H	2	1.09588331	1	107.06882901	3 -152.29646952
H	1	1.09423242	3	110.05236553	4 -145.88862925
C	5	1.42629122	3	120.73738824	1 171.89235135
O	14	1.21084561	5	123.47566784	3 138.95311147
O	14	1.33571665	5	111.28317339	3 -44.70166142
C	16	1.44798330	14	115.59660976	5 175.09112372
C	17	1.51634106	16	107.13622075	14 -176.24984142
H	18	1.09475556	17	110.97074418	16 -60.71634622
H	18	1.09411702	17	110.69414049	16 59.72612100
H	18	1.09547101	17	109.71399853	16 179.58783834
H	17	1.09432405	16	108.57646076	14 -54.94825874
H	17	1.09461355	16	108.67527689	14 62.12573968
C	1	1.53314579	3	109.41639980	4 -25.82609610
H	24	1.09550791	1	109.97124618	3 -177.88780505
H	24	1.09480740	1	111.23216320	3 -57.90625901
H	24	1.09349398	1	110.89302764	3 61.64287759
C	5	1.44544784	3	123.40219049	1 -16.07622762
C	28	1.40520782	5	119.40860135	3 82.14359358
C	28	1.39720305	5	119.53955509	3 -100.04136057

C	29	1.40104547	28	117.98126969	5	178.60642197
C	30	1.39356963	28	120.04792672	5	-178.34236425
H	30	1.08431930	28	119.01336218	5	0.63465208
C	31	1.39387300	29	121.27771352	28	-0.72922528
H	31	1.08762127	29	118.91578854	28	179.70935053
H	32	1.08617498	30	119.87034953	28	179.85524098
H	34	1.08672387	31	119.83510648	29	-179.41332446

P-20-boat-chair



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-20a-boat-chair HF=-862.8282233

Sum of electronic and thermal Free Energies=-862.570918

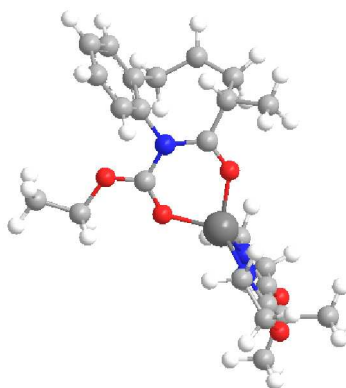
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C

C	1	1.57436013				
C	1	1.52998933	2	109.38364835		
O	3	1.21148135	1	122.54369199	2	101.38175295
N	3	1.42884189	1	114.68737503	2	-76.71580650
C	2	2.65915497	1	103.87720572	3	61.30570476
C	2	1.49766868	1	116.98364639	3	35.37137393
H	6	1.10032867	2	133.68363819	1	-95.37246659
H	6	1.10526456	2	106.03019142	1	134.67186575
H	7	1.08621376	2	117.95145819	1	-117.79490868
H	2	1.10295883	1	106.37451327	3	159.99752634
H	2	1.09603204	1	107.21508622	3	-86.43786808
H	1	1.09233786	3	108.88133696	4	-140.85814956
C	5	1.41178137	3	125.09452985	1	162.79627894
O	14	1.21548561	5	121.94650319	3	168.91528992
O	14	1.33696572	5	112.86667530	3	-13.36674994
C	16	1.44803830	14	115.87068114	5	-179.93191713
C	17	1.52081993	16	111.47222423	14	84.96059623
H	18	1.09353928	17	110.58552365	16	-65.40063576
H	18	1.09499589	17	110.79265670	16	55.68449692
H	18	1.09623333	17	109.74480352	16	175.19361454

H	17	1.09241020	16	103.74458543	14	-154.83494012
H	17	1.09240272	16	108.92561414	14	-38.25807131
C	1	1.53024217	3	110.84275247	4	-21.08261322
H	24	1.09580071	1	110.08385968	3	176.43006535
H	24	1.09500885	1	111.24860872	3	-63.68308057
H	24	1.09352511	1	110.78415638	3	56.02045247
C	5	1.44925388	3	120.07527860	1	-21.01734864
C	28	1.40428446	5	120.58775814	3	85.83609368
C	28	1.39585881	5	118.37337024	3	-93.12625626
C	29	1.40067434	28	117.67406311	5	-178.16940653
C	30	1.39339362	28	120.34992665	5	178.68908755
H	30	1.08576347	28	118.83811057	5	-1.57387565
C	31	1.39448284	29	121.60887143	28	-0.75867355
H	31	1.08751713	29	118.77271074	28	179.42571145
H	32	1.08618007	30	119.99990380	28	179.87180520
H	34	1.08659825	31	119.83722863	29	-179.88468641

P-20L-boat-boat



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-20aL-boat-boat HF =-1673.9362399

Sum of electronic and thermal Free Energies= -1673.463997

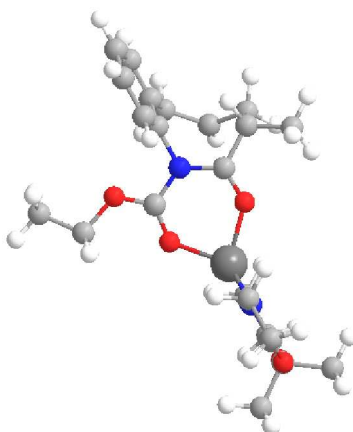
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C						
C	1	1.59199291				
C	1	1.50475784	2	108.44933141		
N	3	1.39367076	1	119.55449566	2	-92.75693897
C	4	1.40837893	3	122.28628564	1	175.27096630
O	5	1.29700305	4	112.64032009	3	-174.69543866
C	6	1.48432861	5	119.25877481	4	-179.29960186
C	7	1.51123859	6	106.95962934	5	178.66882868
C	4	1.46935914	3	120.45766570	1	-1.93607704

C	9	1.40152376	4	119.64963252	3	75.15982578
C	10	1.52488950	9	122.37670698	4	-7.13453598
C	2	1.48989082	1	116.48598450	3	80.54186474
O	5	1.24879724	4	124.59972803	3	5.22511726
O	3	1.25252477	1	118.86052258	2	84.22573043
Mg	14	1.96832742	3	135.51357211	1	179.26110413
N	15	2.05504963	14	122.04703109	3	-117.79436035
N	15	2.05453751	14	120.20859605	3	127.61843142
C	16	1.29824747	15	125.36108859	14	-128.00399238
C	17	1.29813559	15	125.37158537	14	128.11095560
C	19	1.52052071	17	130.69787957	15	1.86089292
C	20	1.56099770	19	107.81466654	17	120.33734833
H	21	1.09132204	20	109.51250326	19	57.56658470
H	21	1.09120857	20	109.51998597	19	176.75184859
H	21	1.09500849	20	111.46306339	19	-62.84104635
C	20	1.56152172	19	107.90944311	17	-121.34268730
H	25	1.09498667	20	111.46628656	19	62.90418993
H	25	1.09125557	20	109.47223284	19	-176.69606505
H	25	1.09125020	20	109.51246865	19	-57.50199607
O	18	1.32480895	16	116.54924691	15	-179.42824278
O	19	1.32497895	17	116.52846333	15	-178.27001261
C	29	1.46247296	18	108.76289940	16	0.39426135
H	31	1.09076630	29	107.23183825	18	120.00506988
H	31	1.09054509	29	107.28963016	18	-121.98872938
C	16	1.48964138	15	126.88649187	14	52.20249994
H	34	1.09384676	16	109.82835053	15	58.35017395
H	34	1.09400253	16	109.63208999	15	-60.71919297
C	17	1.48944925	15	126.84322503	14	-50.10036351
H	37	1.09404664	17	109.64903290	15	-62.09267978
H	37	1.09377850	17	109.80541938	15	56.97650602
C	30	1.46219911	19	108.76702607	17	0.71081675
H	40	1.09079740	30	107.22709373	19	119.66562679
H	40	1.09052578	30	107.29739223	19	-122.32440451
H	7	1.09246641	6	106.99201550	5	-59.90352809
H	7	1.09242947	6	107.04927199	5	57.15619639
H	1	1.09085892	3	109.81970881	14	-157.56510375
C	1	1.53849614	3	110.49442066	14	-36.38829402
H	8	1.09330262	7	111.30717861	6	-61.17725003
H	8	1.09332692	7	111.30164869	6	60.71144831
H	8	1.09482421	7	108.61828603	6	179.76193647
H	46	1.09330700	1	108.90655070	3	-175.44323655
H	46	1.09490447	1	111.65654749	3	-56.62138187
H	46	1.09325075	1	111.55912043	3	64.99640365
H	11	1.09985494	10	110.61323100	9	37.43406712
H	11	1.09428353	10	108.92967534	9	154.28234800

H	12	1.08558737	2	118.19893070	1	117.46931657
H	2	1.09391697	1	105.77706094	3	-157.63174481
H	2	1.10336066	1	106.79551022	3	-45.05850008
C	10	1.40234376	9	116.95795546	4	178.36272066
C	9	1.39616944	4	117.92907377	3	-106.00765072
C	59	1.39209840	9	119.36485392	4	-178.48980812
H	60	1.08513514	59	119.95290841	9	-179.79474769
C	58	1.39350763	10	121.44946011	9	-0.09925073
H	62	1.08558325	58	119.69871430	10	-179.64814070
H	58	1.08649482	10	118.85835133	9	179.72688514
H	59	1.08642073	9	120.09899785	4	1.29595947

P-20L-boat-chair



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for P-20aL-boat-chair HF =-1673.9366733

Sum of electronic and thermal Free Energies=-1673.462312

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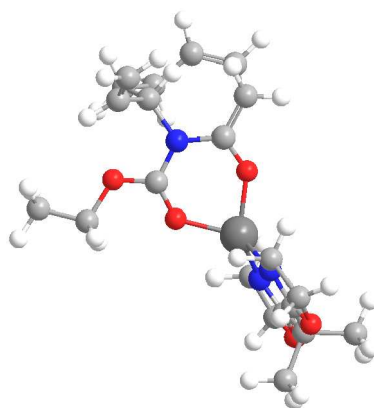
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C	1	1.50760674	2	106.90075377		
N	3	1.39506717	1	117.73369480	2	-85.17275042
C	4	1.40281906	3	122.57856933	1	170.02675987
O	5	1.29795157	4	112.59000332	3	-172.66401443
C	6	1.48431556	5	119.22614273	4	-178.91942116
C	7	1.51128217	6	106.97382483	5	179.48950546
C	4	1.47076812	3	119.58760199	1	-7.94511600
C	9	1.40208328	4	120.16633250	3	78.81828135
C	10	1.51755385	9	123.05271260	4	2.36912234
C	2	1.50087224	1	116.77887119	3	32.68013263
O	5	1.24915939	4	124.46734082	3	7.14341669

O	3	1.24875163	1	120.23802280	2	91.80756783
Mg	14	1.97302503	3	134.51170212	1	-175.29183680
N	15	2.05528317	14	119.82875816	3	-120.64330297
N	15	2.05500200	14	121.68155843	3	125.46370490
C	16	1.29797617	15	125.37410300	14	-127.87283154
C	17	1.29819837	15	125.34214979	14	126.85785278
C	18	1.52023955	16	130.68199363	15	-1.05190920
C	20	1.56144281	18	107.84126783	16	-120.51955910
H	21	1.09118007	20	109.52113204	18	-176.71027943
H	21	1.09123053	20	109.50250745	18	-57.49619376
H	21	1.09503680	20	111.47880800	18	62.88586860
C	20	1.56153605	18	107.87632221	16	121.17792259
H	25	1.09500860	20	111.47779092	18	-62.88577270
H	25	1.09118629	20	109.50701162	18	57.49818192
H	25	1.09119978	20	109.51031497	18	176.71329579
O	18	1.32507305	16	116.55854604	15	178.99007798
O	19	1.32502801	17	116.54419186	15	-179.71077170
C	29	1.46223241	18	108.74546961	16	-0.16284909
H	31	1.09064755	29	107.26034837	18	121.19725109
H	31	1.09067520	29	107.25407410	18	-120.80052380
C	16	1.48954803	15	126.85981374	14	50.85627042
H	34	1.09393884	16	109.73431358	15	60.70067944
H	34	1.09388112	16	109.74055615	15	-58.37510914
C	17	1.48956976	15	126.89396488	14	-52.65183594
H	37	1.09388338	17	109.75419355	15	-59.75847141
H	37	1.09387312	17	109.70942004	15	59.27092505
C	30	1.46222784	19	108.75438720	17	0.01430339
H	40	1.09065454	30	107.25742208	19	121.09890745
H	40	1.09068736	30	107.25458915	19	-120.90997331
H	7	1.09235973	6	107.06855027	5	-59.00324153
H	7	1.09247681	6	107.00261935	5	58.06953899
H	1	1.09009619	3	108.55169000	14	-151.59799584
C	1	1.53269252	3	112.39287377	14	-30.44392431
H	8	1.09331673	7	111.28936423	6	-60.61815465
H	8	1.09336008	7	111.33270955	6	61.28421849
H	8	1.09483675	7	108.63286434	6	-179.66993839
H	46	1.09382581	1	109.02885670	3	177.52663901
H	46	1.09479735	1	111.60059760	3	-63.67776281
H	46	1.09336929	1	111.61031139	3	58.07102462
H	11	1.10165940	10	109.26334783	9	74.43724776
H	11	1.10332121	10	107.64222967	9	-173.17126502
H	12	1.08741466	2	116.87625067	1	-134.24009093
H	2	1.10183026	1	105.76780798	3	157.17493873
H	2	1.09471914	1	107.15850760	3	-89.43163666
C	10	1.40158703	9	116.61351891	4	-178.70093607

C	9	1.39509899	4	117.26131357	3	-99.92759649
C	59	1.39320661	9	119.46218760	4	179.04256423
H	60	1.08516156	59	119.98076962	9	-179.93414680
C	58	1.39493282	10	121.74498149	9	-0.34318754
H	62	1.08552339	58	119.68463822	10	-179.98306141
H	58	1.08636236	10	118.78058122	9	179.67744698
H	59	1.08659657	9	119.99893013	4	-0.71510974

7. Calculations (UB3LYP/6-31G*) on the Reactions of R-26L

R-26L (R=H)



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-26L (R=H) HF=-1559.5581131

Sum of electronic and thermal Free Energies= -1559.105359

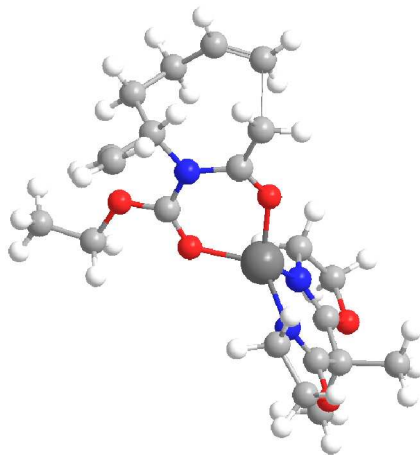
2 2

C					
C	1	2.67983418			
C	1	1.42264889	2	99.98705659	
N	3	1.41304752	1	121.79065728	2 -83.50744070
C	4	1.39030206	3	120.67326587	1 -174.86669632
O	5	1.30665242	4	113.25939234	3 -169.19385598
C	6	1.48179908	5	118.71567842	4 -176.60617082
C	7	1.51199806	6	107.38396900	5 179.34288814
C	4	1.53783997	3	120.19545668	1 7.13852529
C	9	1.54095743	4	112.12511395	3 103.33184069
C	10	1.54593000	9	115.10196169	4 -52.02095151
C	2	1.35179369	1	93.71944981	3 75.51535297
O	5	1.25111575	4	125.47067175	3 11.57850559
O	3	1.27085093	1	117.30505810	4 178.26993296
Mg	14	1.95271302	3	133.94935137	1 158.17161612

N	15	2.05811153	14	122.49131477	3	-103.40331458
N	15	2.05862286	14	121.01202833	3	141.34681753
C	16	1.29722884	15	125.66161091	14	-128.93713658
C	17	1.29778740	15	125.53282158	14	129.12511369
C	18	1.52017764	16	130.62557386	15	0.42264751
C	20	1.56108391	18	107.93949335	16	-121.14413497
H	21	1.09127761	20	109.52564187	18	-176.67003736
H	21	1.09126811	20	109.53375485	18	-57.43852915
H	21	1.09506346	20	111.45965155	18	62.92273638
C	20	1.56128282	18	107.81305278	16	120.48698989
H	25	1.09500016	20	111.44444244	18	-62.86484548
H	25	1.09117634	20	109.48662388	18	57.49664648
H	25	1.09116732	20	109.53399213	18	176.74919435
O	18	1.32576232	16	116.58936769	15	-179.74978023
O	19	1.32564234	17	116.56042659	15	-178.56431646
C	29	1.46224128	18	108.68466663	16	0.36004775
H	31	1.09077846	29	107.24563889	18	120.09189629
H	31	1.09057384	29	107.27342247	18	-121.90665419
C	16	1.48924539	15	126.57185289	14	50.92008914
H	34	1.09380969	16	109.80656065	15	58.68879969
H	34	1.09399484	16	109.63898458	15	-60.31614322
C	17	1.48927642	15	126.70092209	14	-49.01501349
H	37	1.09395832	17	109.74772494	15	-60.93447127
H	37	1.09390261	17	109.70844378	15	58.07484419
C	30	1.46188216	19	108.73440567	17	0.01358463
H	40	1.09068102	30	107.27684627	19	121.12362668
H	40	1.09072517	30	107.26566054	19	-120.88438920
H	9	1.08383469	4	103.50655727	3	-11.94492111
H	7	1.09219285	6	107.16092011	5	-59.24190594
H	7	1.09225830	6	107.14615608	5	57.79247442
H	1	1.07781614	3	125.65926184	14	-163.94523892
H	8	1.09373686	7	111.56709249	6	-61.72287214
H	8	1.09372586	7	111.51151681	6	60.64778250
H	8	1.09485882	7	108.57325811	6	179.49752530
H	11	1.09748782	10	110.84283934	9	69.35489599
H	11	1.09908850	10	107.21915281	9	-175.12760588
H	12	1.09106509	2	118.68483540	1	95.21530248
H	2	1.08617336	1	95.37677682	3	-162.33708696
H	2	1.08776445	1	87.71777592	3	-45.83281868
H	10	1.09676637	9	105.55805278	4	-172.73111564
H	10	1.09251956	9	110.61631793	4	72.56034830
C	9	1.51081836	4	112.78546791	3	-126.59990188
H	57	1.08505821	9	117.33891886	4	-82.31158586
C	57	1.33405090	9	122.52060016	4	101.63992809
H	59	1.08847327	57	122.56927542	9	-2.29247805

H	59	1.08597571	57	121.38096577	9	176.77434993
H	1	1.08273234	3	115.11500881	14	1.40507905

TS-26L (R=H)-8-endo



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

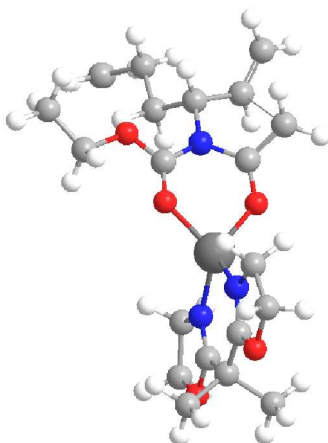
Calculation for TS-26L (R=H)-8-endo HF =-1559.5577222
Sum of electronic and thermal Free Energies= -1559.103061

2 2

C					
C	1	2.35055004			
C	1	1.42449515	2	103.08849828	
N	3	1.41645093	1	121.71634706	2 -81.88006394
C	4	1.38918883	3	120.78468218	1 -179.05261887
O	5	1.30798383	4	113.24105533	3 -167.03617731
C	6	1.48115408	5	118.65167590	4 -176.41268377
C	7	1.51206529	6	107.39830996	5 179.03206479
C	4	1.53545398	3	120.18505765	1 2.52431100
C	9	1.54191834	4	112.64253916	3 102.60012357
C	10	1.54885986	9	115.22423530	4 -50.96695522
C	2	1.36664981	1	100.92260603	3 77.23492915
O	5	1.25122219	4	125.58678326	3 13.60859235
O	3	1.27167737	1	117.64902801	2 94.34623217
Mg	14	1.94854087	3	133.94025544	1 160.00639843
N	15	2.05938645	14	122.82182957	3 -101.66597287
N	15	2.05962938	14	120.76833075	3 143.16958725
C	16	1.29704046	15	125.72112036	14 -128.37591896
C	17	1.29753572	15	125.61213617	14 129.24902956
C	18	1.52007993	16	130.61710173	15 0.06307801
C	20	1.56097210	18	107.93360635	16 -121.15611303

H	21	1.09125489	20	109.53069095	18	-176.78332811
H	21	1.09128597	20	109.53132347	18	-57.55329693
H	21	1.09504676	20	111.44599818	18	62.80423379
C	20	1.56121547	18	107.80728391	16	120.47391207
H	25	1.09501778	20	111.42787511	18	-62.79139391
H	25	1.09119027	20	109.49516700	18	57.56926257
H	25	1.09123163	20	109.55924302	18	176.82386152
O	18	1.32598577	16	116.60095002	15	179.90169239
O	19	1.32591616	17	116.56733600	15	-178.67436364
C	29	1.46216128	18	108.67150022	16	0.10352337
H	31	1.09072751	29	107.26119250	18	120.63749062
H	31	1.09064409	29	107.26748170	18	-121.36268601
C	16	1.48910630	15	126.51211385	14	51.24989648
H	34	1.09387351	16	109.76184907	15	59.36363091
H	34	1.09395424	16	109.67392728	15	-59.62882283
C	17	1.48909362	15	126.61584452	14	-48.89403600
H	37	1.09390687	17	109.77009831	15	-60.53260358
H	37	1.09395233	17	109.66938167	15	58.46537485
C	30	1.46178846	19	108.71332932	17	-0.21337650
H	40	1.09064464	30	107.28725144	19	121.57702776
H	40	1.09077926	30	107.26129180	19	-120.43098825
H	9	1.08424377	4	103.49878829	3	-13.18664035
H	7	1.09219225	6	107.17549058	5	-59.58807448
H	7	1.09228781	6	107.20513366	5	57.44476093
H	1	1.07843046	3	124.42415070	14	-158.59067419
H	8	1.09375812	7	111.57864598	6	-61.79709974
H	8	1.09378178	7	111.50088068	6	60.56328701
H	8	1.09485132	7	108.59602493	6	179.40502417
H	11	1.09703285	10	110.63601508	9	70.65497858
H	11	1.09881722	10	107.24014154	9	-173.60576612
H	12	1.09057199	2	118.66075317	1	93.00330901
H	2	1.08623797	1	93.99961824	3	-160.34588707
H	2	1.08726024	1	90.03280594	3	-44.14141020
H	10	1.09657802	9	105.59867680	4	-171.84659094
H	10	1.09259255	9	110.63424097	4	73.30048667
C	9	1.51131814	4	112.71164769	3	-127.49044994
H	57	1.08509218	9	117.31317438	4	-82.43321758
C	57	1.33403596	9	122.54183130	4	101.49905763
H	59	1.08846303	57	122.55307366	9	-2.23012447
H	59	1.08598777	57	121.36540616	9	176.83231830
H	1	1.08338521	3	114.00663448	14	-4.90081312

TS-26L (R=H)-5-exo



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-26L (R=H)-5-exo HF =-1559.54 85287

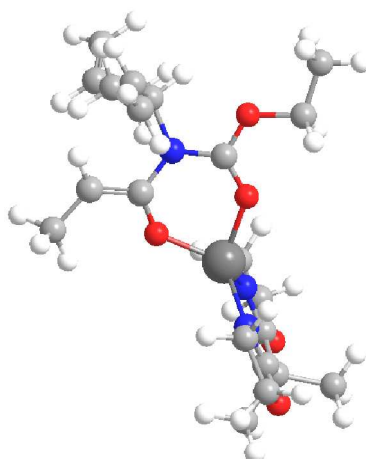
Sum of electronic and thermal Free Energies= -1559.097977

2 2

C					
C	1	2.33322470			
C	1	1.42394477	2	85.89824808	
N	3	1.41204540	1	115.43671794	2 -40.99935785
C	4	1.38391782	3	119.96198906	1 -141.95062156
O	5	1.30334920	4	113.65205375	3 156.37852567
C	6	1.48527949	5	119.01503181	4 178.93900432
C	7	1.51127147	6	107.17252188	5 179.89140554
C	4	1.52012838	3	116.83568769	1 31.57290343
O	5	1.25308482	4	123.49102492	3 -21.82480762
O	3	1.26181340	1	122.65458844	2 137.57994494
Mg	11	1.97570520	3	128.51323887	1 154.69201470
N	12	2.05529241	11	118.94372405	3 -120.05477610
N	12	2.05755666	11	121.98470771	3 126.81373935
C	13	1.29737087	12	125.54637357	11 -126.84740489
C	14	1.29808112	12	125.35034162	11 124.89458125
C	15	1.52026421	13	130.62717816	12 -1.19503638
C	17	1.56083212	15	107.93127106	13 -121.45251874
H	18	1.09120632	17	109.52379176	15 -176.66261548
H	18	1.09124040	17	109.52068515	15 -57.43215556
H	18	1.09502867	17	111.45772793	15 62.94113980
C	17	1.56158623	15	107.79965707	13 120.19172183
H	22	1.09501737	17	111.45521650	15 -62.73412700
H	22	1.09124829	17	109.46574293	15 57.62695038
H	22	1.09128516	17	109.53510113	15 176.83262415
O	15	1.32538517	13	116.58045696	12 178.62236288

O	16	1.32540039	14	116.52974845	12	-179.28861334
C	26	1.46259041	15	108.69495342	13	-0.73723163
H	28	1.09051940	26	107.28435184	15	122.34461540
H	28	1.09079862	26	107.22829311	15	-119.65178765
C	13	1.48942050	12	126.66843007	11	51.75631758
H	31	1.09400666	13	109.64298345	12	61.71281898
H	31	1.09375260	13	109.78676207	12	-57.32168832
C	14	1.48920938	12	126.88346471	11	-54.09755845
H	34	1.09397447	14	109.75901348	12	-60.29638134
H	34	1.09396104	14	109.71920654	12	58.77283599
C	27	1.46176473	16	108.76426876	14	0.10291176
H	37	1.09068327	27	107.27730591	16	120.96716510
H	37	1.09070884	27	107.27129601	16	-121.02630838
H	7	1.09254253	6	107.07977225	5	-58.50306998
H	7	1.09184223	6	106.96071261	5	58.54415077
H	1	1.08185192	3	119.49451625	11	-138.39652890
H	8	1.09352001	7	111.36209343	6	-60.45234181
H	8	1.09368280	7	111.54097362	6	61.74705392
H	8	1.09484794	7	108.58701889	6	-179.31891956
H	2	1.08988521	1	93.88308064	3	-72.58811439
C	2	1.35967279	1	102.43048649	3	167.38256273
H	47	1.08745982	2	122.01625865	1	-85.61727454
H	47	1.08565050	2	121.08186720	1	92.84778064
H	9	1.09481602	4	108.21607176	3	-107.24434980
C	9	1.54657684	4	110.92932953	3	131.60282912
H	51	1.09768553	9	108.90121563	4	-63.21690933
H	51	1.09217510	9	109.46527401	4	53.85062123
C	51	1.54453919	9	113.05237542	4	174.71476449
H	54	1.09540209	51	110.50939009	9	62.70501270
H	54	1.10056459	51	108.67033737	9	-54.25710884
C	54	1.50732195	51	111.41884176	9	-175.25735499
H	57	1.09096786	54	116.00356454	51	62.76445704
C	57	1.33265199	54	124.54982105	51	-117.67063984
H	59	1.08815707	57	121.94681915	54	-0.36223425
H	59	1.08593628	57	121.64167599	54	-179.20436177
H	1	1.08448712	3	118.52046676	11	19.11293668

R-26L (R=Me)



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-26L (R=Me) HF =-1598.8816436

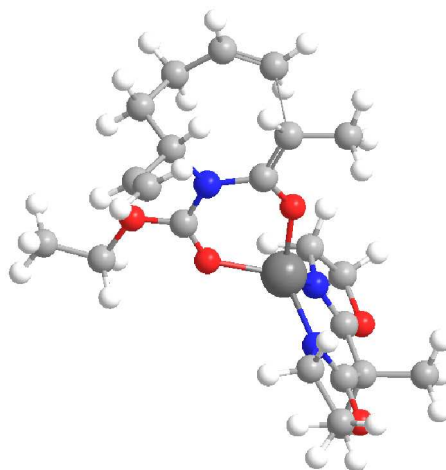
Sum of electronic and thermal Free Energies= -1598.405498

2 2

C				
C	1	6.13563495		
C	1	1.43364093	2	75.64898284
N	3	1.41107024	1	119.17379835
C	4	1.39343670	3	120.63435991
O	5	1.30398558	4	113.53747088
C	6	1.48316647	5	119.22655596
C	7	1.51147206	6	107.05043553
C	4	1.52147292	3	121.04860918
C	9	1.54548061	4	112.49707156
C	10	1.54079625	9	114.26514675
C	2	1.33263757	1	9.82171804
O	5	1.25187107	4	124.76222633
O	3	1.26619173	1	119.19945872
Mg	14	1.96682614	3	133.45891388
N	15	2.05689973	14	120.25263160
N	15	2.05584683	14	121.81833989
C	16	1.29803582	15	125.42933887
C	17	1.29783354	15	125.49657516
C	19	1.52039754	17	130.67109404
C	20	1.56107409	19	107.94174441
H	21	1.09121816	20	109.54012366
H	21	1.09122686	20	109.51492367
H	21	1.09504125	20	111.46200298
C	20	1.56147517	19	107.79407517
H	25	1.09503134	20	111.44923606

H	25	1.09123447	20	109.52535183	19	-176.61604329
H	25	1.09124116	20	109.47056075	19	-57.40899062
O	18	1.32516790	16	116.54968072	15	178.74504127
O	19	1.32515264	17	116.56186352	15	179.82247053
C	29	1.46221157	18	108.75182417	16	-0.07072515
H	31	1.09066594	29	107.25545156	18	120.98654770
H	31	1.09066739	29	107.26370397	18	-121.01914024
C	16	1.48959489	15	126.79672320	14	50.62419305
H	34	1.09393155	16	109.75421355	15	60.81691531
H	34	1.09388960	16	109.73333283	15	-58.20792095
C	17	1.48960591	15	126.73637756	14	-53.10383998
H	37	1.09390896	17	109.70609633	15	-59.58944965
H	37	1.09385870	17	109.75828544	15	59.44320526
C	30	1.46242894	19	108.73678345	17	0.20436776
H	40	1.09071172	30	107.25288018	19	120.56997604
H	40	1.09063472	30	107.26816661	19	-121.44398533
H	9	1.09090722	4	103.42524108	3	-163.32808227
H	7	1.09212182	6	106.93886823	5	-59.71102791
H	7	1.09242037	6	107.18429257	5	57.39600282
H	1	1.08243291	3	118.54182202	14	168.93104315
C	1	1.47805773	3	122.56439026	14	-7.14420936
H	8	1.09362961	7	111.44201776	6	-61.75164325
H	8	1.09343365	7	111.32458496	6	60.37963049
H	8	1.09484183	7	108.60706377	6	179.31243432
H	47	1.10118736	1	109.79024506	3	117.19734220
H	47	1.10004980	1	109.84100354	3	-127.92042447
H	47	1.09015793	1	113.17204579	3	-5.16450307
H	11	1.09824954	10	109.42921943	9	-54.25743596
H	11	1.10276274	10	109.44231944	9	62.36365925
H	12	1.09082729	2	119.43018655	1	139.37381159
H	2	1.08583315	1	128.83902875	3	145.55283654
H	2	1.08821056	1	114.31644519	3	-42.44551940
H	10	1.09622596	9	105.62938667	4	-176.11862103
H	10	1.09609040	9	112.19742997	4	69.51460382
C	9	1.51320732	4	113.34772532	3	81.61395891
H	61	1.08895355	9	112.95139410	4	-173.39411973
C	61	1.33271548	9	127.56540046	4	10.05100746
H	63	1.08805562	61	122.94013731	9	-2.57986967
H	63	1.08527206	61	120.94789751	9	177.11358634

TS-26L (R=Me)-8-endo-1



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

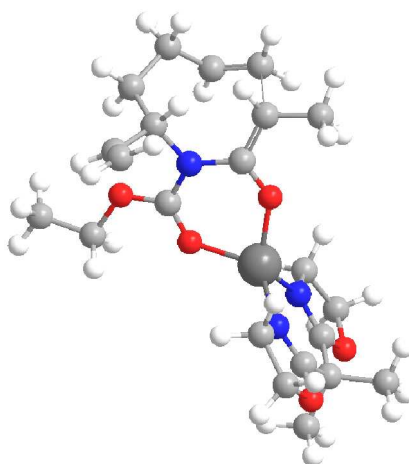
Calculation for TS-26L (R=Me)-8-endo-1 HF=-1598.8770188
Sum of electronic and thermal Free Energies=-1598.394537

2 2

C					
C	1	2.19356372			
C	1	1.43885318	2	101.24146503	
N	3	1.42058708	1	121.93218659	2 -77.59107200
C	4	1.38880392	3	120.94590394	1 176.51056365
O	5	1.30910558	4	113.15809595	3 -168.26260325
C	6	1.47993450	5	118.67740371	4 -176.62655446
C	7	1.51238597	6	107.37762983	5 179.76265559
C	4	1.53648868	3	120.70052745	1 -3.96942409
C	9	1.54260911	4	113.12351176	3 106.20636765
C	10	1.54924210	9	114.85591151	4 -48.16032946
C	2	1.38000131	1	107.17149101	3 79.85866132
O	5	1.25168402	4	126.00579338	3 12.18447922
O	3	1.27052249	1	117.80907511	2 98.10478487
Mg	14	1.94569986	3	135.37132994	1 166.98270244
N	15	2.06046170	14	123.44389728	3 -104.92921589
N	15	2.06058797	14	120.80785613	3 139.41593497
C	16	1.29701300	15	125.76576957	14 -129.11962108
C	17	1.29735353	15	125.68799200	14 129.85839616
C	18	1.51998825	16	130.61989075	15 1.10899945
C	20	1.56092900	18	108.02381964	16 -122.17323595
H	21	1.09125684	20	109.52573010	18 -176.73323093
H	21	1.09115050	20	109.53109889	18 -57.48905410
H	21	1.09502425	20	111.45949846	18 62.88135196
C	20	1.56145534	18	107.74816219	16 119.49393661

H	25	1.09503473	20	111.45503036	18	-62.72484869
H	25	1.09129635	20	109.49699638	18	57.63731737
H	25	1.09118951	20	109.53824585	18	176.87235458
O	18	1.32612726	16	116.60562160	15	-179.26507226
O	19	1.32609794	17	116.58405147	15	-178.49812489
C	29	1.46199544	18	108.66866907	16	0.15435477
H	31	1.09075516	29	107.26411983	18	120.62816038
H	31	1.09066742	29	107.27881344	18	-121.38790719
C	16	1.48902490	15	126.47655540	14	51.57571694
H	34	1.09387079	16	109.76362619	15	58.50176877
H	34	1.09392317	16	109.68317461	15	-60.47539528
C	17	1.48896143	15	126.54989665	14	-48.46923759
H	37	1.09400432	17	109.69471798	15	-61.35194558
H	37	1.09383193	17	109.75074420	15	57.63950183
C	30	1.46175772	19	108.69507512	17	0.28977291
H	40	1.09077899	30	107.26667493	19	120.46601250
H	40	1.09065747	30	107.29225476	19	-121.54607729
H	9	1.08369645	4	103.49518967	3	-9.65935584
H	7	1.09213534	6	107.27743478	5	-58.82926455
H	7	1.09241819	6	107.23900726	5	58.23426623
H	1	1.08017032	3	119.17027461	14	-158.68560165
C	1	1.50636635	3	117.69366013	14	-12.01417888
H	8	1.09377627	7	111.57579736	6	-61.35553016
H	8	1.09378476	7	111.48761995	6	60.94673375
H	8	1.09483360	7	108.63343146	6	179.80072136
H	47	1.09271443	1	110.42924336	3	173.35681403
H	47	1.09885157	1	110.17204616	3	-68.34721077
H	47	1.09267902	1	112.40330716	3	51.35444265
H	11	1.09700688	10	110.29801158	9	70.90943183
H	11	1.09830432	10	107.36384833	9	-173.19131862
H	12	1.09024143	2	118.58028948	1	89.95271705
H	2	1.08604852	1	92.91053863	3	-158.02022169
H	2	1.08800552	1	93.15136705	3	-42.54686998
H	10	1.09646293	9	105.54057371	4	-168.86748519
H	10	1.09209169	9	110.87186995	4	76.13688564
C	9	1.51152519	4	112.36132681	3	-123.77467249
H	61	1.08530996	9	117.33992179	4	-81.12311021
C	61	1.33409598	9	122.55261814	4	102.73596440
H	63	1.08844369	61	122.53010675	9	-2.12092834
H	63	1.08601834	61	121.37649859	9	176.83349736

TS-26L (R=Me)-8-endo-2



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

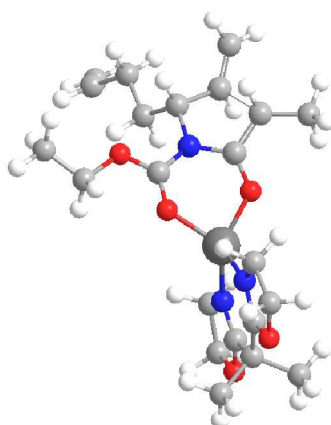
Calculation for TS-26L (R=Me)-8-endo-2 HF =-1598.8747965
Sum of electronic and thermal Free Energies= -1598.395083

2 2

C					
C					
C	1	2.19793616	2	103.29088044	
N	3	1.42137063	1	120.81374340	2 -73.57060810
C	4	1.38934026	3	120.70163825	1 165.22860248
O	5	1.30912442	4	113.30373089	3 -167.23942464
C	6	1.47995456	5	118.73083695	4 -176.77587730
C	7	1.51230611	6	107.35206165	5 -179.05995891
C	4	1.54360166	3	121.03482531	1 -18.20930655
C	9	1.54355887	4	113.58674862	3 106.28645044
C	10	1.54980001	9	115.85632501	4 -71.94459096
C	2	1.37888037	1	106.35733565	3 47.86424564
O	5	1.25158411	4	125.95495534	3 12.60765628
O	3	1.26968352	1	118.41800695	2 101.50516287
Mg	14	1.94485290	3	135.63335396	1 179.62710740
N	15	2.06031575	14	120.93418398	3 -110.94327205
N	15	2.06038644	14	123.13826463	3 133.64711129
C	16	1.29704743	15	125.80559682	14 -129.53610119
C	17	1.29732538	15	125.75346516	14 128.94205213
C	18	1.52024546	16	130.61964915	15 -1.80926224
C	20	1.56103222	18	107.79624442	16 -119.97525716
H	21	1.09117958	20	109.53471905	18 -177.00541045
H	21	1.09131268	20	109.49819055	18 -57.77676018
H	21	1.09501569	20	111.43742781	18 62.59919133
C	20	1.56084282	18	107.98858959	16 121.65069044

H	25	1.09501213	20	111.43911356	18	-63.09292567
H	25	1.09127874	20	109.53241155	18	57.30563782
H	25	1.09132031	20	109.52262540	18	176.52552701
O	18	1.32611129	16	116.58813384	15	178.42202380
O	19	1.32600631	17	116.57738284	15	179.66770424
C	29	1.46192433	18	108.68037678	16	-0.64009724
H	31	1.09058615	29	107.30890487	18	122.23413912
H	31	1.09083656	29	107.24545164	18	-119.76719440
C	16	1.48880712	15	126.41950044	14	48.87410679
H	34	1.09406052	16	109.63088477	15	61.82294331
H	34	1.09378330	16	109.78293148	15	-57.17046463
C	17	1.48884657	15	126.49463834	14	-51.24956955
H	37	1.09390706	17	109.75055225	15	-58.97047428
H	37	1.09396829	17	109.66878770	15	60.02296629
C	30	1.46184797	19	108.70659568	17	-0.10857608
H	40	1.09067916	30	107.29219259	19	121.34482352
H	40	1.09076120	30	107.27310914	19	-120.66503195
H	9	1.08621045	4	103.65628521	3	-11.59103462
H	7	1.09195012	6	107.32359317	5	-57.63116429
H	7	1.09252559	6	107.19901126	5	59.44067092
H	1	1.08018858	3	118.65125795	14	-159.98557885
C	1	1.50385433	3	118.59991845	14	-11.52845759
H	8	1.09373447	7	111.58415561	6	-61.23663571
H	8	1.09378532	7	111.46680804	6	61.02148945
H	8	1.09481308	7	108.63619948	6	179.87715526
H	47	1.09303106	1	110.55974818	3	168.09562605
H	47	1.09912865	1	110.20596419	3	-73.64921098
H	47	1.09225257	1	112.22182958	3	46.11930629
H	11	1.09899582	10	107.10921545	9	179.65410950
H	11	1.09694107	10	110.05849019	9	-64.90820628
H	12	1.09031977	2	118.99472380	1	-101.12073622
H	2	1.08739224	1	86.50953621	3	167.40665238
H	2	1.08673590	1	99.39192978	3	-77.55261435
H	10	1.09603774	9	106.34065085	4	168.52091568
H	10	1.09271630	9	109.91061682	4	53.88982648
C	9	1.51430961	4	111.35061091	3	-124.90057089
H	61	1.08542186	9	117.26092291	4	-86.87696957
C	61	1.33412397	9	122.56421460	4	97.04012919
H	63	1.08845831	61	122.45115051	9	-2.00430933
H	63	1.08605113	61	121.35846869	9	176.78940239

TS-26L (R=Me)-5-exo



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

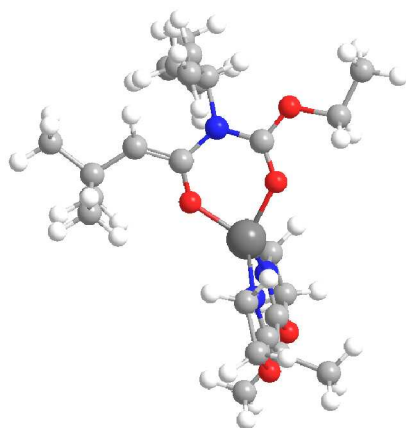
Calculation for TS-26L (R=Me)-5-exo HF =-1598.8733165
Sum of electronic and thermal Free Energies= -1598.395779

2 2

C					
C	1	2.19774911			
C	1	1.43176720	2	88.04851027	
N	3	1.41300185	1	114.39690034	2 -40.34366779
C	4	1.38042265	3	120.57648928	1 -144.08367927
O	5	1.30409681	4	113.76975890	3 156.73377728
C	6	1.48415980	5	119.02736728	4 178.46252910
C	7	1.51149616	6	107.16236047	5 178.99687996
C	4	1.51590414	3	115.46914902	1 28.70782357
O	5	1.25404595	4	123.41125538	3 -21.68674787
O	3	1.26299033	1	123.54545740	2 136.60180334
Mg	11	1.97420235	3	128.01550141	1 157.76351587
N	12	2.05723920	11	120.14394135	3 -120.60452810
N	12	2.05869584	11	121.03174886	3 126.23768406
C	13	1.29723331	12	125.61720176	11 -127.55173314
C	14	1.29769673	12	125.49757531	11 126.31568183
C	15	1.52026885	13	130.65238870	12 0.24936404
C	17	1.56093806	15	107.95232987	13 -121.50922700
H	18	1.09123372	17	109.55191369	15 -176.93360311
H	18	1.09123507	17	109.50575801	15 -57.69833411
H	18	1.09503718	17	111.44301779	15 62.65723358
C	17	1.56141914	15	107.77188153	13 120.12257640
H	22	1.09502380	17	111.43963410	15 -62.69919764
H	22	1.09119321	17	109.47303807	15 57.65670462
H	22	1.09119690	17	109.53793233	15 176.90533292
O	15	1.32571145	13	116.58605364	12 179.99807436

O	16	1.32576779	14	116.54298754	12	-178.93696148
C	26	1.46236157	15	108.68602042	13	0.48213523
H	28	1.09078761	26	107.23836676	15	119.98329257
H	28	1.09055770	26	107.27717657	15	-122.00819538
C	13	1.48918719	12	126.60961248	11	52.10762031
H	31	1.09380357	13	109.78013246	12	58.87984553
H	31	1.09396218	13	109.63185475	12	-60.12384186
C	14	1.48905217	12	126.72881624	11	-52.19175235
H	34	1.09398295	14	109.75703797	12	-60.52107030
H	34	1.09397961	14	109.68930621	12	58.51445673
C	27	1.46171050	16	108.74181080	14	0.02481496
H	37	1.09067959	27	107.28164116	16	121.14236443
H	37	1.09072745	27	107.27920916	16	-120.85692843
H	7	1.09265878	6	107.10898473	5	-59.45615705
H	7	1.09179361	6	107.05412990	5	57.62809397
H	1	1.08585040	3	114.98285170	11	-136.54189961
C	1	1.49511655	3	121.43324134	11	15.45269443
H	8	1.09351572	7	111.33690293	6	-60.50381434
H	8	1.09368406	7	111.52821765	6	61.64055940
H	8	1.09483583	7	108.62516254	6	-179.40380690
H	43	1.09399349	1	110.53559225	3	157.36329382
H	43	1.09916038	1	110.20151187	3	-84.79170755
H	43	1.09299286	1	112.13697992	3	35.32714123
H	2	1.09054333	1	95.29873992	3	-72.17098482
C	2	1.37155098	1	105.26896987	3	167.67049443
H	51	1.08713506	2	121.90005968	1	-84.92268762
H	51	1.08539594	2	121.07259032	1	92.10755658
H	9	1.09529188	4	108.39234092	3	-106.22985968
C	9	1.54540414	4	111.42789410	3	132.26615427
H	55	1.09772021	9	108.92065757	4	-63.05328601
H	55	1.09238139	9	109.42740561	4	53.94712043
C	55	1.54397729	9	113.08430504	4	174.84584642
H	58	1.09551959	55	110.44189843	9	62.25131979
H	58	1.10054475	55	108.68276721	9	-54.67134273
C	58	1.50741551	55	111.48881881	9	-175.69939458
H	61	1.09097246	58	116.00351778	55	62.85891134
C	61	1.33263926	58	124.54768627	55	-117.50612855
H	63	1.08819709	61	121.92883258	58	-0.42555511
H	63	1.08594044	61	121.65685292	58	-179.28938480

R-26L (R=*t*-Bu)



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-26L (R=*t*-Bu) HF =-1716.821142

Sum of electronic and thermal Free Energies= -1716.265028

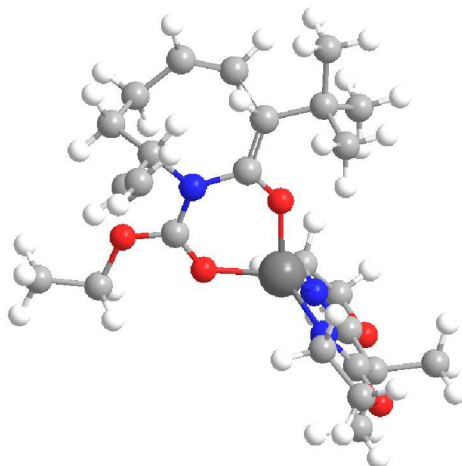
2 2

C				
C	1	6.07556860		
C	1	1.43367065	2	76.77089007
N	3	1.41728439	1	118.35638064
C	4	1.39108333	3	120.83365303
O	5	1.30500671	4	113.55513277
C	6	1.48187959	5	119.20114486
C	7	1.51160383	6	107.03817627
C	4	1.52081782	3	121.10639086
C	9	1.54506830	4	112.51555073
C	10	1.54068683	9	114.21929886
C	2	1.33263236	1	9.39202343
O	5	1.25269939	4	124.88975651
O	3	1.26631788	1	120.60864154
Mg	14	1.96448616	3	133.57381672
N	15	2.05809998	14	119.58520379
N	15	2.05754707	14	122.79404667
C	16	1.29775142	15	125.54268900
C	17	1.29774245	15	125.56046287
C	18	1.52029848	16	130.67413456
C	20	1.56107718	18	107.85234789
H	21	1.09116789	20	109.51993901
H	21	1.09119397	20	109.53014914
H	21	1.09500146	20	111.44972149
C	20	1.56128923	18	107.90120133
H	25	1.09508042	20	111.44829004
H	25	1.09123017	20	109.52850141

H	25	1.09130931	20	109.50597646	18	176.85142155
O	18	1.32551802	16	116.56207686	15	178.15964886
O	19	1.32536594	17	116.57647197	15	179.37409956
C	29	1.46213849	18	108.72572463	16	-0.64843005
H	31	1.09054432	29	107.29390981	18	122.21432568
H	31	1.09080029	29	107.24104731	18	-119.78547373
C	16	1.48942172	15	126.68187772	14	49.92449799
H	34	1.09402718	16	109.66173830	15	62.13510282
H	34	1.09375746	16	109.79919853	15	-56.88144352
C	17	1.48954489	15	126.68351934	14	-53.69944798
H	37	1.09385281	17	109.73654330	15	-58.73703002
H	37	1.09388559	17	109.71376521	15	60.26067512
C	30	1.46235058	19	108.72333718	17	-0.12016078
H	40	1.09066948	30	107.27133794	19	121.21598469
H	40	1.09072071	30	107.25855569	19	-120.80365554
H	9	1.09126687	4	103.51210207	3	-160.92149013
H	7	1.09212461	6	107.04116333	5	-58.65528806
H	7	1.09253211	6	107.22536236	5	58.46539538
H	1	1.08427765	3	116.06913045	14	162.49565665
C	1	1.50183232	3	126.31674940	14	-10.98504093
H	8	1.09367586	7	111.43082243	6	-61.58978104
H	8	1.09342620	7	111.29933453	6	60.46255596
H	8	1.09482423	7	108.65306054	6	179.44005745
H	11	1.09819629	10	109.39474452	9	-54.66313430
H	11	1.10263065	10	109.45279074	9	61.93143868
H	12	1.09104360	2	119.39205905	1	137.65133073
H	2	1.08585146	1	128.36011256	3	145.19693236
H	2	1.08819710	1	114.80199997	3	-42.69555700
H	10	1.09625964	9	105.71994201	4	-176.75067339
H	10	1.09642724	9	112.05312260	4	68.86815140
C	9	1.51314586	4	113.42527189	3	83.96175343
H	58	1.08895962	9	112.93806330	4	-174.15922794
C	58	1.33246949	9	127.59048031	4	9.23218984
H	60	1.08802240	58	122.86341873	9	-2.74968526
H	60	1.08526155	58	120.97888119	9	177.06915171
C	47	1.54727706	1	113.19155154	3	-45.88809285
H	63	1.09556462	47	111.13636455	1	-58.27161023
H	63	1.09206355	47	112.21341862	1	63.76815660
H	63	1.09450388	47	108.90700627	1	-176.50442590
C	47	1.56249642	1	107.69749827	3	75.46802724
H	67	1.09479225	47	111.62709607	1	57.65117717
H	67	1.09537274	47	108.36927829	1	176.30618979
H	67	1.09393110	47	111.30456187	1	-64.47882555
C	47	1.54572306	1	108.06702518	3	-167.19284667
H	71	1.09409457	47	109.99426230	1	-176.70234809

H	71	1.09574034	47	111.63081321	1	-57.13632674
H	71	1.09576087	47	111.39418544	1	64.04396728

TS-26L (R= *t*-Bu)-8-endo



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-26L (R= *t*-Bu)-8-endo HF =-1716.8119771
Sum of electronic and thermal Free Energies= -1716.249825

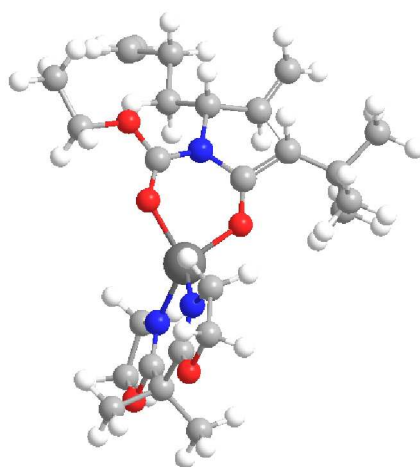
2 2

C					
C	1	2.18001179			
C	1	1.44122715	2	98.36105265	
N	3	1.42914352	1	121.21160343	2 -76.11577299
C	4	1.38797509	3	121.03370523	1 171.24114341
O	5	1.31044350	4	113.10369517	3 -167.45607378
C	6	1.47877374	5	118.71996533	4 -176.70256368
C	7	1.51260297	6	107.32389616	5 -179.57343324
C	4	1.53724376	3	121.22524595	1 -9.88216614
C	9	1.54346031	4	113.62879167	3 108.22332596
C	10	1.54875630	9	114.94833348	4 -43.00436249
C	2	1.38341635	1	106.65387242	3 85.09358516
O	5	1.25220768	4	126.38869399	3 12.73887755
O	3	1.26920726	1	119.35400223	2 99.19603355
Mg	14	1.94300842	3	136.50388553	1 172.80790744
N	15	2.06162060	14	123.19964629	3 -107.30325063
N	15	2.06191070	14	121.43537254	3 136.83371366
C	16	1.29696880	15	125.84200621	14 -129.76997383
C	17	1.29714924	15	125.78951828	14 130.72407460
C	18	1.52000627	16	130.62446146	15 0.22601547

C	20	1.56089923	18	107.92763016	16	-121.07051888
H	21	1.09127873	20	109.53219383	18	-176.81994284
H	21	1.09126298	20	109.53426535	18	-57.58006457
H	21	1.09505078	20	111.43390413	18	62.79725454
C	20	1.56109314	18	107.84289451	16	120.55905927
H	25	1.09505426	20	111.42408781	18	-62.80028280
H	25	1.09124164	20	109.51467007	18	57.57576547
H	25	1.09123467	20	109.52854028	18	176.81351718
O	18	1.32627085	16	116.60625364	15	-179.87190491
O	19	1.32626441	17	116.59568157	15	-179.43087242
C	29	1.46199324	18	108.66279497	16	-0.07661110
H	31	1.09072861	29	107.28037551	18	121.08303634
H	31	1.09072060	29	107.26982906	18	-120.93769849
C	16	1.48895909	15	126.40166620	14	50.32501265
H	34	1.09395147	16	109.73275066	15	59.40219688
H	34	1.09393701	16	109.70283546	15	-59.54241713
C	17	1.48892099	15	126.46155981	14	-48.37782608
H	37	1.09390973	17	109.75280148	15	-59.91686651
H	37	1.09390170	17	109.67106358	15	59.06693650
C	30	1.46175730	19	108.68233707	17	-0.06460533
H	40	1.09068619	30	107.28435310	19	121.28901879
H	40	1.09077538	30	107.28221194	19	-120.72734024
H	9	1.08281555	4	103.43031846	3	-7.95512403
H	7	1.09203908	6	107.35272451	5	-58.17762013
H	7	1.09252825	6	107.28519539	5	58.92552402
H	1	1.08011611	3	116.82663802	14	-161.57987238
C	1	1.53998723	3	122.12157991	14	-19.24308672
H	8	1.09379262	7	111.56513425	6	-61.32121806
H	8	1.09376948	7	111.41936868	6	60.90119697
H	8	1.09479610	7	108.68131371	6	179.77031751
H	11	1.09696015	10	110.01091167	9	70.25165960
H	11	1.09820371	10	107.30221842	9	-173.98125407
H	12	1.09018144	2	118.43821552	1	87.09922802
H	2	1.08432553	1	93.06188861	3	-153.46818853
H	2	1.08762096	1	95.65995625	3	-37.93343754
H	10	1.09634014	9	105.62002694	4	-163.99961222
H	10	1.09184550	9	110.79962995	4	81.01402450
C	9	1.51144372	4	112.03527813	3	-121.78848691
H	58	1.08563493	9	117.35922234	4	-79.14892927
C	58	1.33418260	9	122.58431411	4	104.78932981
H	60	1.08836459	58	122.49147162	9	-2.10312860
H	60	1.08603665	58	121.37860823	9	176.76887292
C	47	1.54539370	1	108.27889104	3	-175.97290432
H	63	1.09417990	47	109.82451534	1	174.84271098
H	63	1.09507090	47	112.58436118	1	-65.96190900

H	63	1.09631617	47	111.61080453	1	55.76409994
C	47	1.55434608	1	107.20226514	3	-60.23829178
H	67	1.09588570	47	111.55254253	1	-56.15296618
H	67	1.09437733	47	111.61601307	1	65.65171977
H	67	1.09534609	47	109.36091946	1	-174.94448865
C	47	1.54271746	1	115.19578108	3	61.75124055
H	71	1.09181443	47	112.19801640	1	-61.50518534
H	71	1.09485709	47	111.96002052	1	60.61214317
H	71	1.09486873	47	109.06569355	1	178.85878431

TS-26L (R= *t*-Bu)-5-exo



#p ub3lvp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-26L (R= *t*-Bu)-5-exo HF=-1716.8127544
Sum of electronic and thermal Free Energies=-1716.255365

2 2

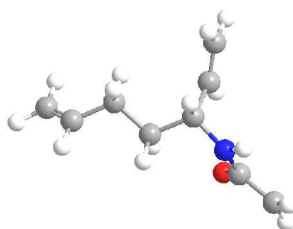
C						
C	1	2.16775400				
C	1	1.43641765	2	88.56680115		
N	3	1.41737733	1	113.66611907	2	-40.44425948
C	4	1.37880933	3	120.77337321	1	-142.82432752
O	5	1.30525723	4	113.76868222	3	156.10327179
C	6	1.48303040	5	118.98991015	4	178.46050355
C	7	1.51167039	6	107.15244958	5	179.82807359
C	4	1.51106149	3	115.27691490	1	28.26531207
O	5	1.25457843	4	123.60405248	3	-22.40302500
O	3	1.26315068	1	125.27805689	2	137.08347331
Mg	11	1.97094757	3	128.48932975	1	156.97817329
N	12	2.05842333	11	120.46982284	3	-120.32731218

N	12	2.05988605	11	121.12321031	3	126.33288069
C	13	1.29700799	12	125.72476751	11	-127.67316665
C	14	1.29759505	12	125.57371084	11	126.56742292
C	15	1.52023929	13	130.63065658	12	0.37192643
C	17	1.56076968	15	107.96722710	13	-121.76091919
H	18	1.09123832	17	109.51011739	15	-176.81308110
H	18	1.09120207	17	109.49618212	15	-57.59710524
H	18	1.09501866	17	111.45878053	15	62.76897217
C	17	1.56129367	15	107.80840121	13	119.88302359
H	22	1.09503965	17	111.44692396	15	-62.90973834
H	22	1.09125919	17	109.47218241	15	57.46003724
H	22	1.09123591	17	109.52894226	15	176.68561504
O	15	1.32591113	13	116.59371625	12	-179.87156249
O	16	1.32589295	14	116.55382448	12	-178.96156496
C	26	1.46221756	15	108.68274711	13	-0.26662100
H	28	1.09064323	26	107.27744647	15	121.49263237
H	28	1.09073968	26	107.25645817	15	-120.51111348
C	13	1.48922299	12	126.50523280	11	52.56805026
H	31	1.09397053	13	109.70164325	12	59.65226124
H	31	1.09382752	13	109.74063782	12	-59.32550389
C	14	1.48919024	12	126.66371734	11	-52.03762697
H	34	1.09397731	14	109.76823589	12	-60.42377828
H	34	1.09395270	14	109.70641352	12	58.60685601
C	27	1.46172299	16	108.73522544	14	-0.10531141
H	37	1.09067553	27	107.28607268	16	121.28864448
H	37	1.09073188	27	107.27167451	16	-120.70279216
H	7	1.09263821	6	107.19209738	5	-58.60045035
H	7	1.09189027	6	107.07659308	5	58.49206219
H	1	1.08839347	3	112.84759403	11	-135.61233983
C	1	1.52129470	3	123.95653497	11	11.40654290
H	8	1.09351530	7	111.32878350	6	-60.54125400
H	8	1.09369337	7	111.49197665	6	61.56418127
H	8	1.09480157	7	108.65294886	6	-179.46778445
H	2	1.08992777	1	96.17844661	3	-71.59922665
C	2	1.37718935	1	107.81472993	3	167.56523329
H	48	1.08693232	2	121.80964918	1	-83.15287303
H	48	1.08467334	2	121.22552498	1	94.29844809
H	9	1.09558587	4	108.47150282	3	-105.94879942
C	9	1.54517000	4	111.40125612	3	132.51030342
H	52	1.09767055	9	108.89619286	4	-63.81471506
H	52	1.09258433	9	109.33418310	4	53.03306260
C	52	1.54364006	9	113.31304973	4	173.92376858
H	55	1.09568543	52	110.47992372	9	62.51686246
H	55	1.10060520	52	108.69929320	9	-54.42319648
C	55	1.50740612	52	111.53212010	9	-175.41386198

H	58	1.09101338	55	115.98365655	52	62.65956505
C	58	1.33262191	55	124.58392973	52	-117.72801903
H	60	1.08817473	58	121.92522850	55	-0.40313884
H	60	1.08594884	58	121.66238487	55	-179.27146154
C	43	1.54291565	1	109.34765376	3	175.31624343
H	63	1.09409078	43	111.76194440	1	-65.90093268
H	63	1.09619134	43	111.67438495	1	55.60399014
H	63	1.09431642	43	109.82119212	1	174.88604885
C	43	1.55729478	1	107.54197293	3	-67.85523746
H	67	1.09583007	43	111.42429265	1	-57.36021374
H	67	1.09337430	43	111.50960224	1	64.60927125
H	67	1.09523131	43	109.00376990	1	-175.97526361
C	43	1.54181200	1	112.47201197	3	53.21171012
H	71	1.09406575	43	112.15164927	1	-59.58484475
H	71	1.09600538	43	111.38876311	1	62.34087563
H	71	1.09452299	43	109.62612944	1	-179.19155008

8. Calculations (UB3LYP/6-31G*) on the Reactions of R-29

R-29-Z



#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-29-Z HF=-481.2678415

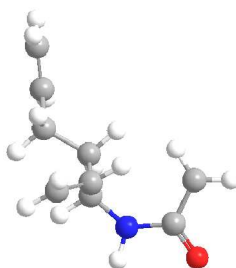
Sum of electronic and thermal Free Energies=-481.096294

0 2

C						
C	1	4.37136425				
C	1	1.45793791	2	23.66629792		
N	3	1.37994712	1	115.38207622	2	-57.26115137
C	4	1.47614870	3	123.77060504	1	173.21173773
O	3	1.23648271	1	121.64618363	4	-178.81255991
H	1	1.08613173	3	123.18684261	6	-179.02251560
H	2	1.08799346	1	73.97587818	3	-70.36355963
C	2	1.33319272	1	138.72865566	3	171.03751352
H	9	1.08903318	2	121.91807535	1	-79.03817095

H	9	1.08696331	2	121.75673058	1	101.26158845
H	5	1.09754261	4	105.02099125	3	-178.57103267
C	5	1.54470246	4	111.05988758	3	65.20185065
H	13	1.09307324	5	109.25960320	4	-68.29562979
H	13	1.09816804	5	107.61368002	4	47.41314468
C	13	1.54008167	5	112.90756803	4	168.59695512
H	16	1.09626735	13	110.05896584	5	60.81442256
H	16	1.10228181	13	108.77932622	5	-55.46878048
C	16	1.50488782	13	112.31915501	5	-176.48137400
H	19	1.09188553	16	115.78855985	13	59.48165025
C	19	1.33333301	16	125.19563964	13	-119.85795234
H	21	1.08838312	19	121.61095146	16	-0.37158673
H	21	1.08685215	19	121.86262333	16	179.64123876
H	4	1.01070760	3	116.88504460	1	14.53809492
H	1	1.08269870	3	117.68766810	6	0.57191046

R-29-E



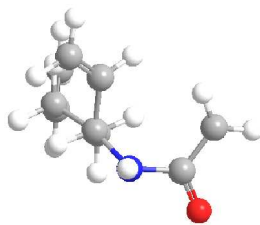
#p ub3lyp/6-31g* opt scfcyc=200 optcyc=500 freq=noraman

Calculation for R-29-E HF = -481.2606768

Sum of electronic and thermal Free Energies= -481.089380

0 2

C						
C	1	3.37781000				
C	1	1.45445092	2	71.01320315		
N	3	1.38405680	1	120.32923722	2	30.54929345
C	4	1.47479613	3	131.40017985	1	-13.09133139
O	3	1.23787788	1	120.07731439	4	178.91761346
H	1	1.08237080	3	124.59592384	6	179.52810950
H	2	1.08989635	1	51.58967705	3	145.76536540
C	2	1.33297463	1	162.35928553	3	80.92151259
H	9	1.08848728	2	121.79181334	1	-125.12890364
H	9	1.08667856	2	121.79135587	1	54.68480998

TS-29-Z-E

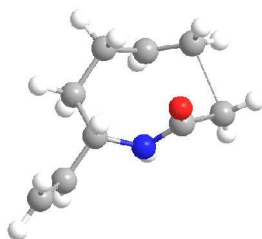
Calculation for TS-29-Z-E HF = -481.2377786

0 2

S69

H	4	1.09880849	3	104.24294156	2	166.05172535
C	4	1.53885762	3	109.47570707	2	51.05719612
H	13	1.09886991	4	109.87168648	3	-71.38579728
H	13	1.09679631	4	107.73854586	3	44.32836804
C	13	1.53994143	4	113.32402063	3	166.35266567
H	16	1.09678829	13	110.20115570	4	59.30942746
H	16	1.10128761	13	108.37512616	4	-56.80174572
C	16	1.50479210	13	112.42071592	4	-177.81028518
H	19	1.09163935	16	115.76418859	13	58.90632015
C	19	1.33338157	16	125.15256393	13	-120.44900933
H	21	1.08852651	19	121.63152270	16	-0.53754465
H	21	1.08677556	19	121.86723262	16	179.73087954
H	3	1.01799200	2	110.29353976	1	-73.10161130
H	1	1.08516382	2	118.29990020	6	5.59848043

TS-29-8-endo(E)



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-29-8-endo(E) HF=-481.2556752

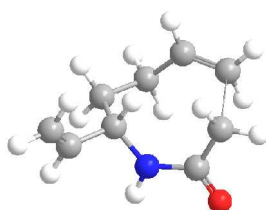
Sum of electronic and thermal Free Energies=-481.078941

0 2

C						
O	1	1.23327465				
C	1	1.46263657	2	122.42823997		
N	1	1.38835363	2	122.26234687	3	-173.87136720
C	4	1.46748562	1	119.37114002	2	27.19168936
C	5	1.54959831	4	110.96728106	1	90.75943296
C	6	1.55064040	5	115.05518494	4	-52.02576041
C	7	1.50513100	6	115.29039168	5	76.49983082
C	8	1.37125047	7	125.19866077	6	-122.89093598
H	4	1.01334756	1	115.11512888	2	169.84963510
H	5	1.09313765	4	105.03696011	1	-27.14787922
H	6	1.09724796	5	107.87428827	4	-174.10166302
H	6	1.10133049	5	109.22627857	4	71.16236325
H	7	1.10150811	6	106.91601766	5	-163.46922269

H	7	1.09625348	6	109.76810023	5	-48.25469699
H	8	1.09188507	7	116.06753028	6	53.96778116
H	9	1.08670143	8	119.82970321	7	-13.16828084
H	9	1.08658474	8	120.15638549	7	-169.90098538
H	3	1.08679456	1	120.66861827	2	167.66553958
H	3	1.08429530	1	116.76516435	2	14.98917604
C	5	1.50934909	4	110.99971836	1	-145.28622935
H	21	1.09223477	5	115.81856647	4	-57.36015147
C	21	1.33214854	5	124.68321096	4	123.92401912
H	23	1.08679782	21	121.82467850	5	178.83192939
H	23	1.08802970	21	121.62821356	5	-1.52875259

TS-29-8-endo(Z)



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-29-8-endo(Z) HF =-481.2550818

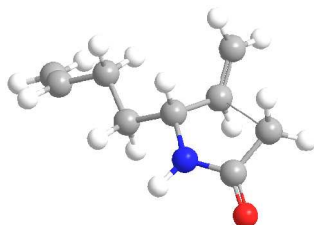
Sum of electronic and thermal Free Energies= -481.078967

0 2

C						
C	1	2.28456234				
C	2	1.46672678	1	101.01865547		
O	3	1.23481160	2	121.32174757	1	95.84590984
N	3	1.38389698	2	118.87428356	1	-82.95200591
C	5	1.46337184	3	129.10289932	2	12.56001675
C	6	1.55032478	5	112.65058605	3	96.56393402
C	7	1.54695515	6	114.44960491	5	-51.31224241
C	1	1.36607312	2	107.31928148	3	70.90124993
H	5	1.01416410	3	111.90630730	2	176.24810186
H	6	1.09231110	5	107.24505803	3	-22.05878972
H	7	1.09803086	6	107.49024740	5	-173.89445753
H	7	1.09914228	6	109.46865351	5	71.03854126
H	8	1.09592566	7	109.54581914	6	70.93280510
H	8	1.10023236	7	107.53546490	6	-173.49915958
H	9	1.09119414	1	119.05160046	2	93.81967116
H	1	1.08667309	9	120.43857066	8	176.30307377
H	1	1.08686403	9	120.37160121	8	17.97069014

H	2	1.08420376	1	96.93760301	9	-172.67144324
H	2	1.08454360	1	99.44356510	9	-54.24663178

TS-29-5-exo



#p ub3lyp/6-31g* opt=(ts,z-matrix,noeigentest,nrscale,calcfc) scfcyc=200 optcyc=500
freq=noraman iop(1/8=5)

Calculation for TS-29-5-exo HF =-481.2525081

Sum of electronic and thermal Free Energies= -481.079417

0 2

C						
C	1	2.26556204				
C	1	1.48321952	2	90.75242599		
N	3	1.37147252	1	112.34228122	2	-29.71327246
C	4	1.46067547	3	121.18954991	1	14.21348418
O	3	1.22727803	1	124.06231828	2	150.07237245
H	1	1.08647781	3	117.97138525	6	-112.76923806
H	2	1.09033744	1	90.76564111	3	-76.39678058
C	2	1.36312842	1	109.37884218	3	162.90112937
H	9	1.08740824	2	121.56000679	1	-84.98665812
H	9	1.08559992	2	121.40302986	1	89.50799024
H	5	1.10274321	4	110.37994256	3	-95.74035370
C	5	1.54459035	4	109.13096858	3	145.71837623
H	13	1.09769744	5	109.12584586	4	-65.46651512
H	13	1.10004930	5	107.87711449	4	49.90159814
C	13	1.53855455	5	114.29748107	4	171.06288334
H	16	1.09569756	13	109.95979095	5	60.92660473
H	16	1.10126839	13	108.54680366	5	-55.35684327
C	16	1.50534991	13	112.28072729	5	-176.39317356
H	19	1.09182205	16	115.88778797	13	60.33729197
C	19	1.33328569	16	125.06796248	13	-119.13080967
H	21	1.08837969	19	121.65773212	16	-0.46781239
H	21	1.08669496	19	121.83925863	16	179.78660285
H	4	1.01203242	3	117.00941490	1	-179.56347502
H	1	1.08568503	3	117.04777144	6	33.14354134